



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:15 PM UTC

PDB ID : 5MPB / pdb_00005mpb
EMDB ID : EMD-3536
Title : 26S proteasome in presence of AMP-PNP (s3)
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 : 7.80 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

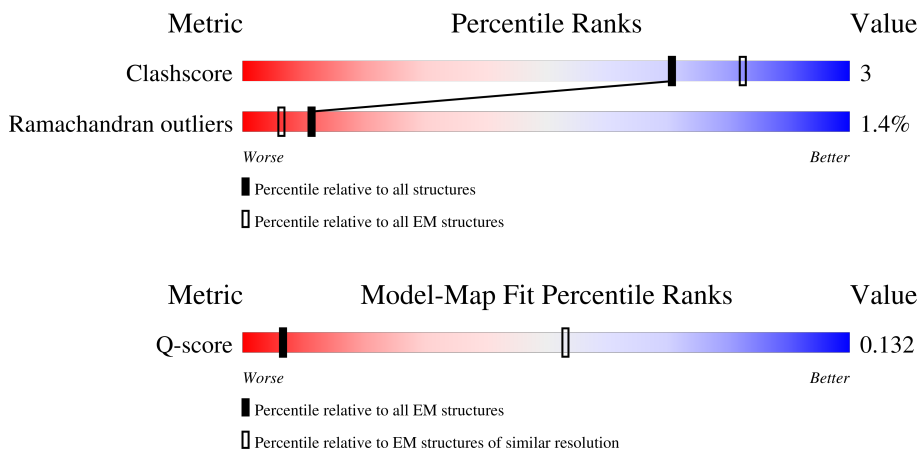
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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	-
Q-score	-	25397	370 (7.30 - 8.30)

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	21% 53% 38% • •
1	a	252	20% 45% 46% 5% •
2	B	250	26% 56% 40% •
2	b	250	26% 51% 44% •
3	C	258	18% 60% 33% • 5%

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Mol	Chain	Length	Quality of chain
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	1	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	
16	I	437	

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Mol	Chain	Length	Quality of chain
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	ADP	M	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 108771 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	386	Total	C	N	O	S	0	0
			3033	1906	543	567	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		

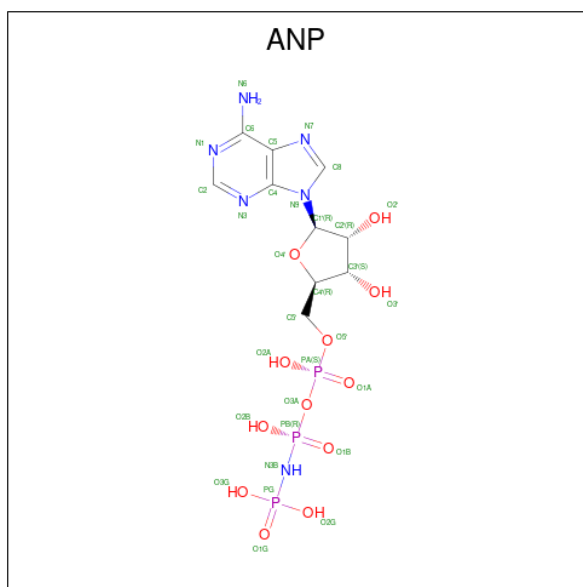
- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN8.

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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			31	10	6	12	3	

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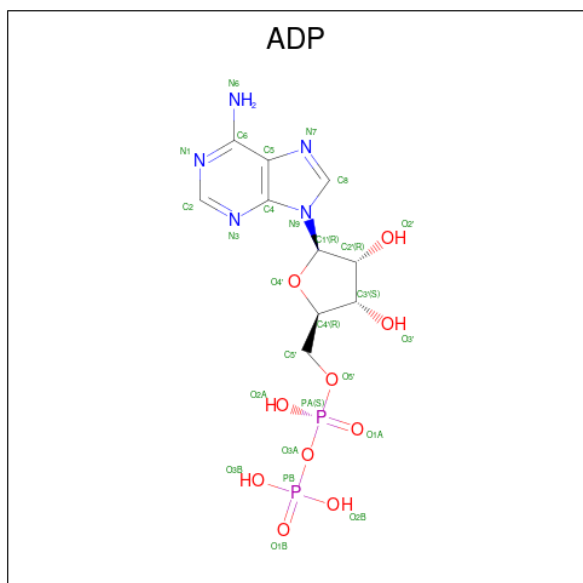
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Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	L	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

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

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

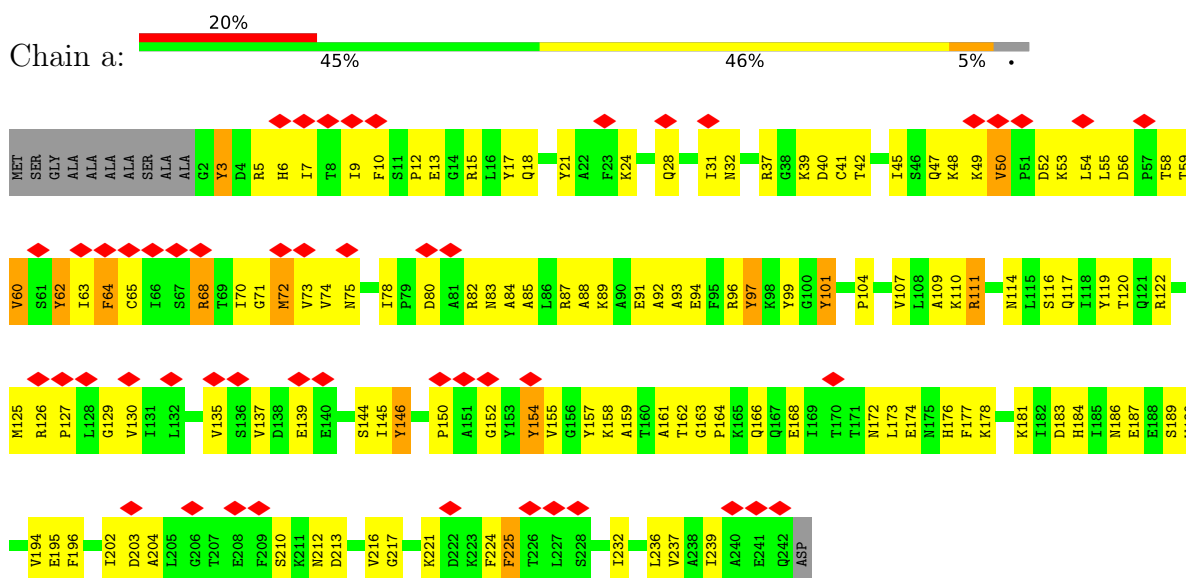


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	M	1	27	10	5	10	2	0

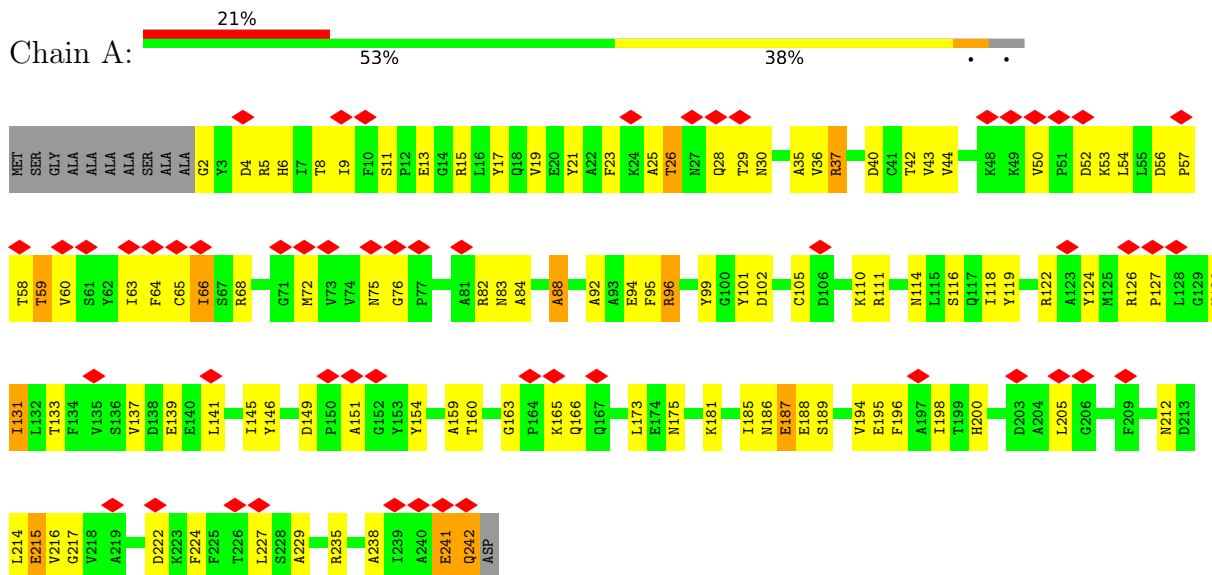
3 Residue-property plots

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

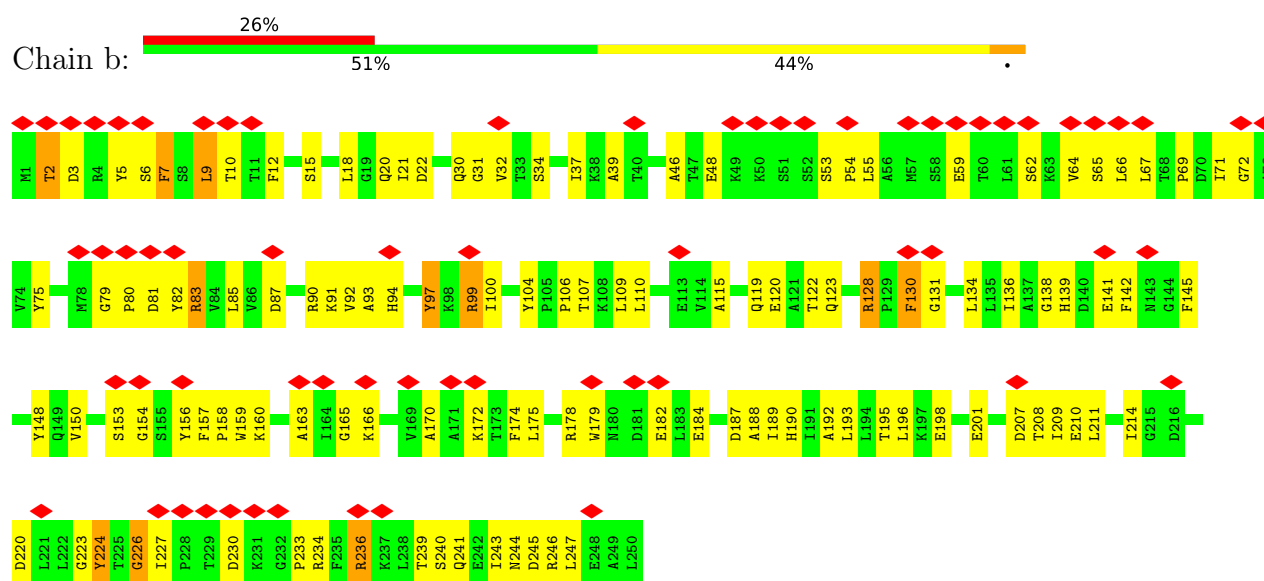
- Molecule 1: Proteasome subunit alpha type-1



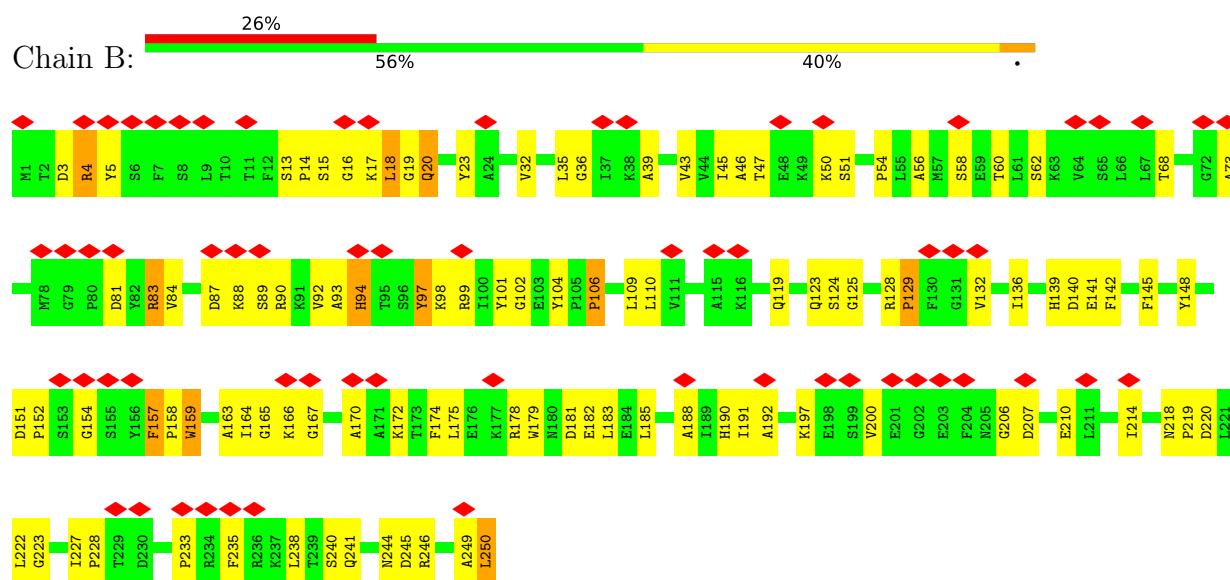
- Molecule 1: Proteasome subunit alpha type-1



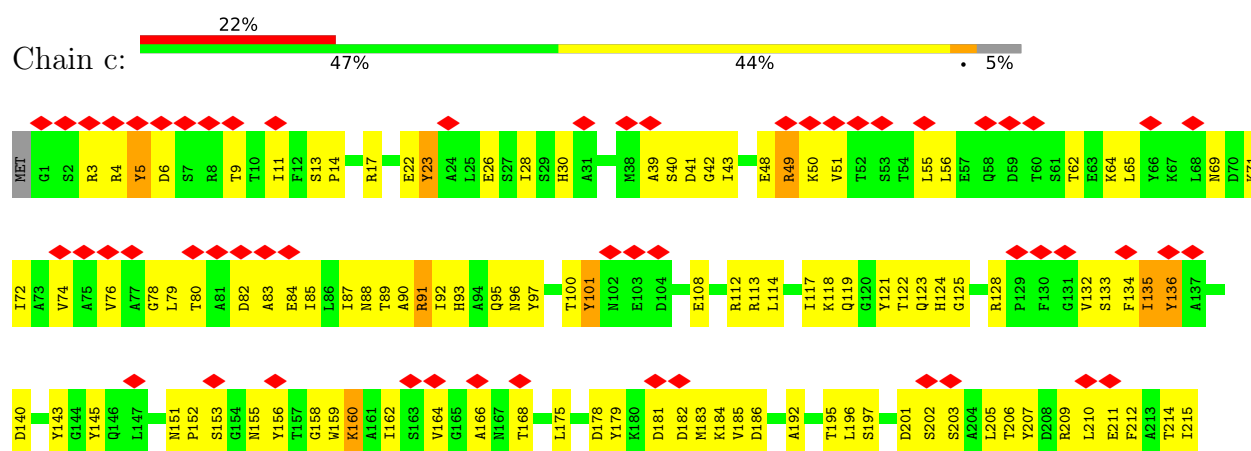
- Molecule 2: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-2

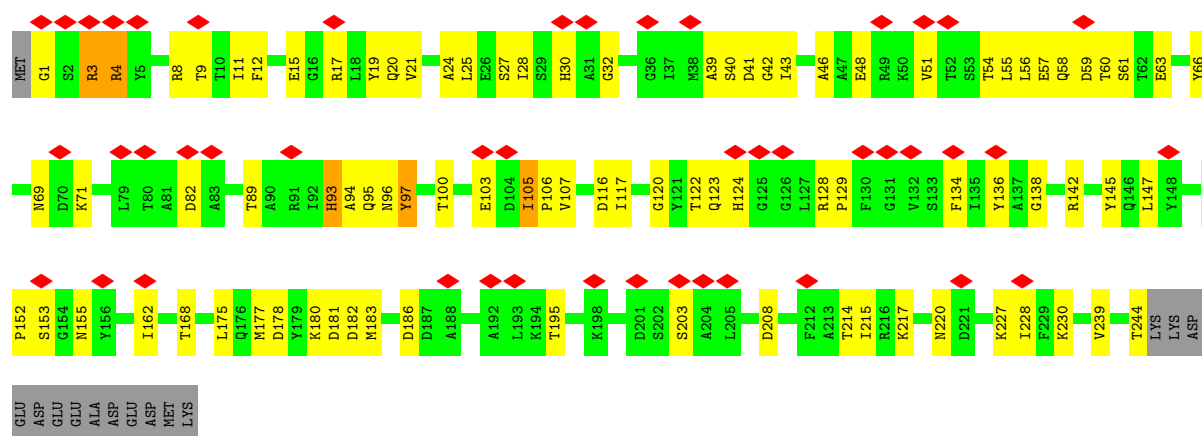


• Molecule 3: Proteasome subunit alpha type-3

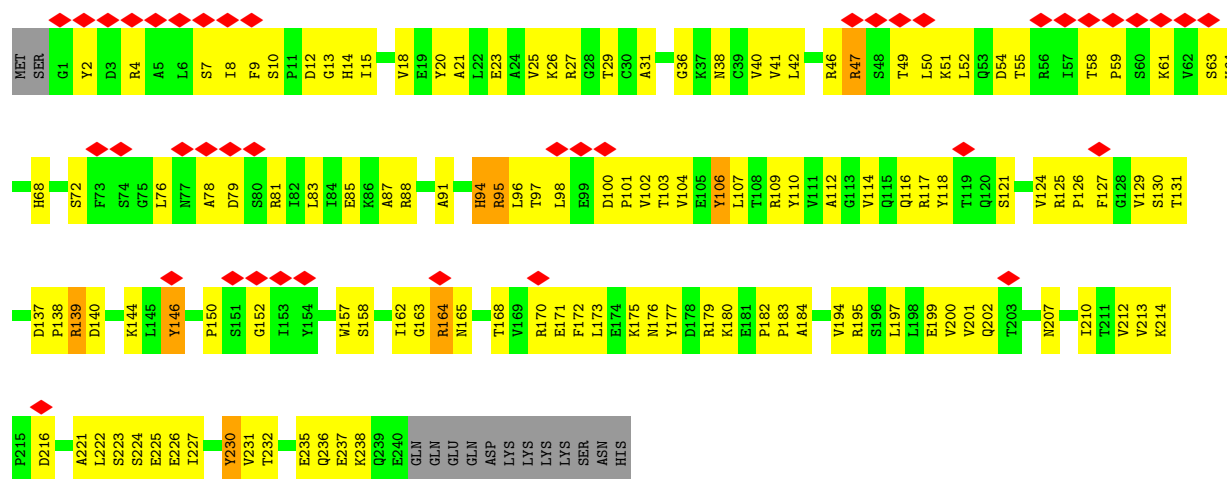




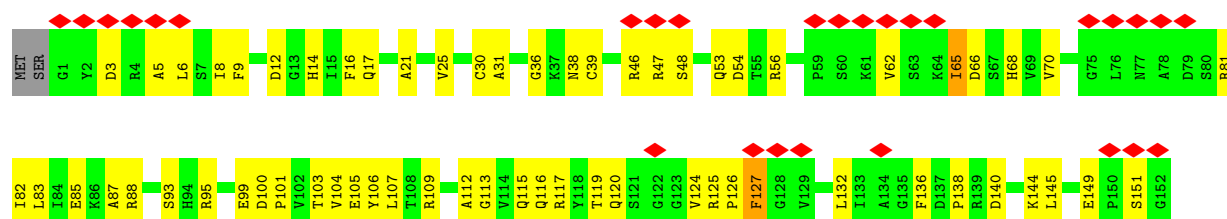
• Molecule 3: Proteasome subunit alpha type-3

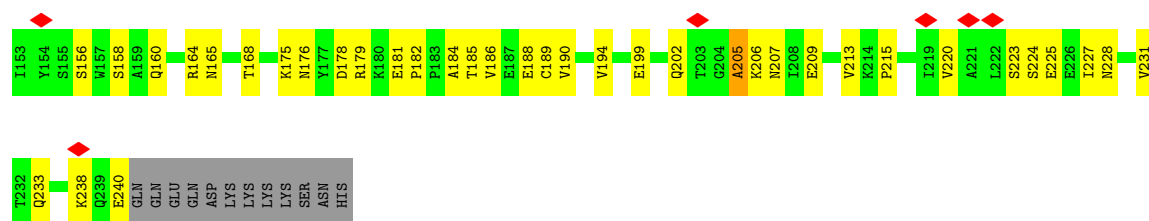


• Molecule 4: Proteasome subunit alpha type-4

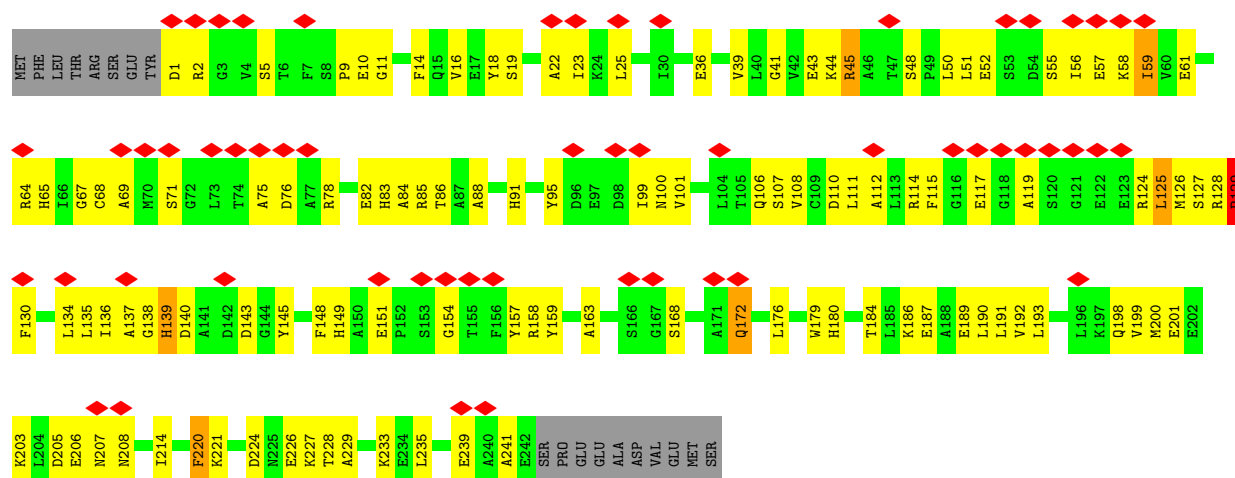


• Molecule 4: Proteasome subunit alpha type-4

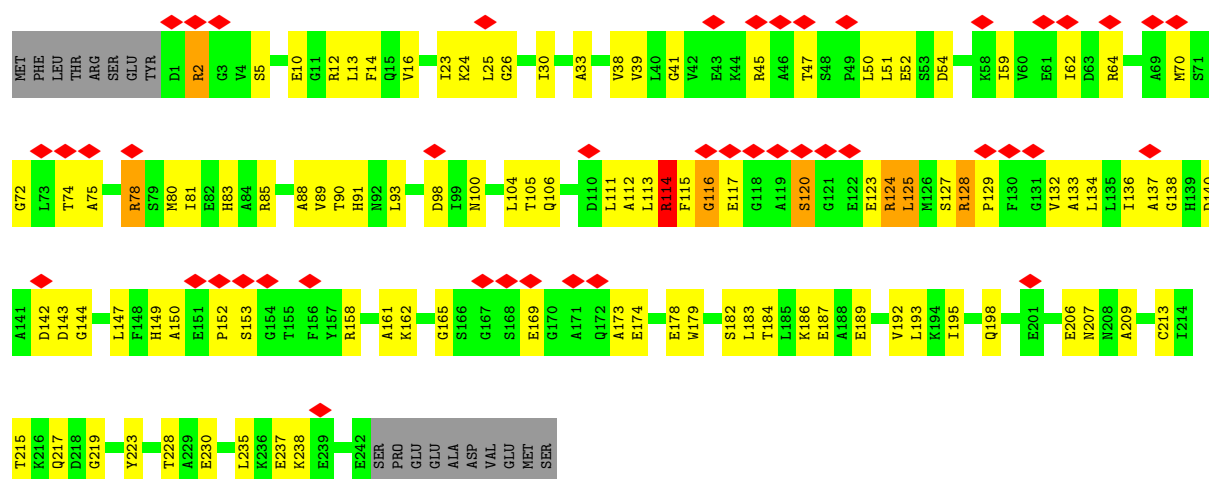




• Molecule 5: Proteasome subunit alpha type-5

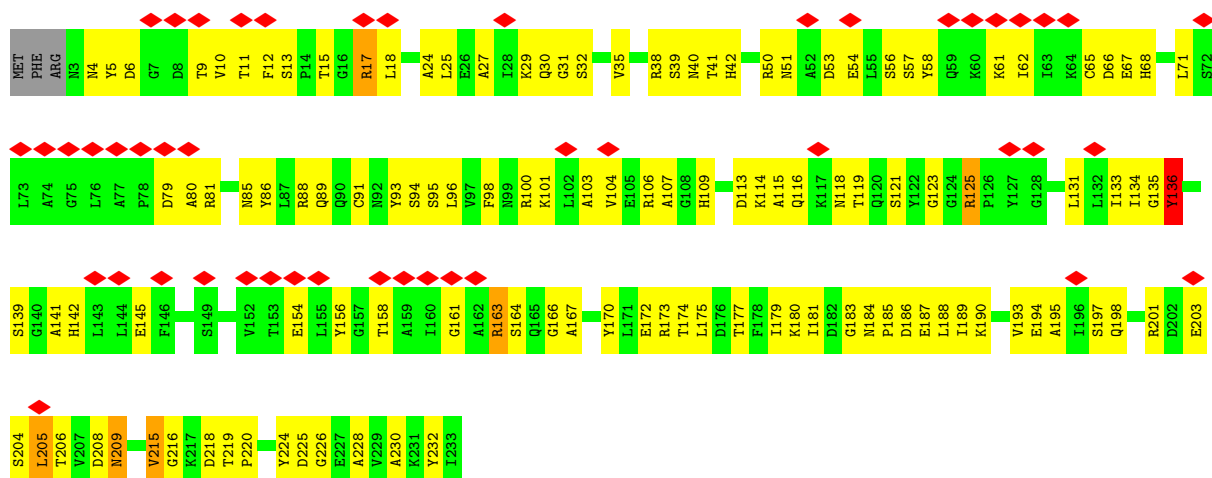


• Molecule 5: Proteasome subunit alpha type-5

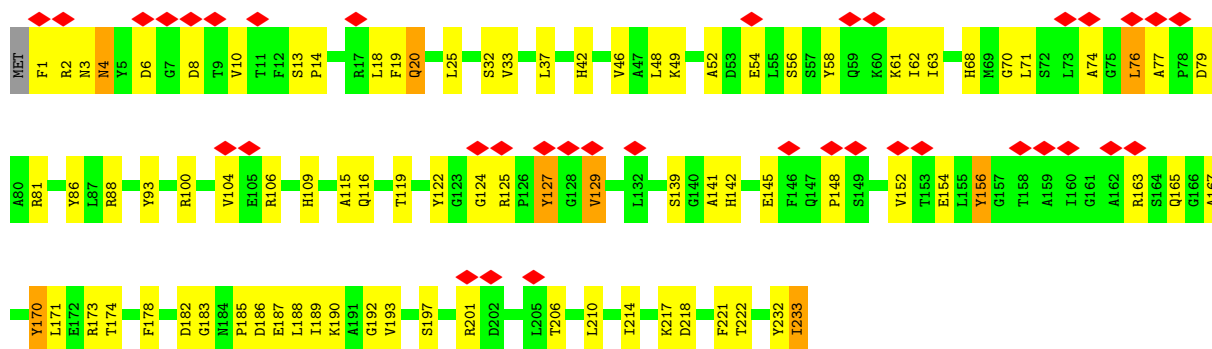


• Molecule 6: Proteasome subunit alpha type-6

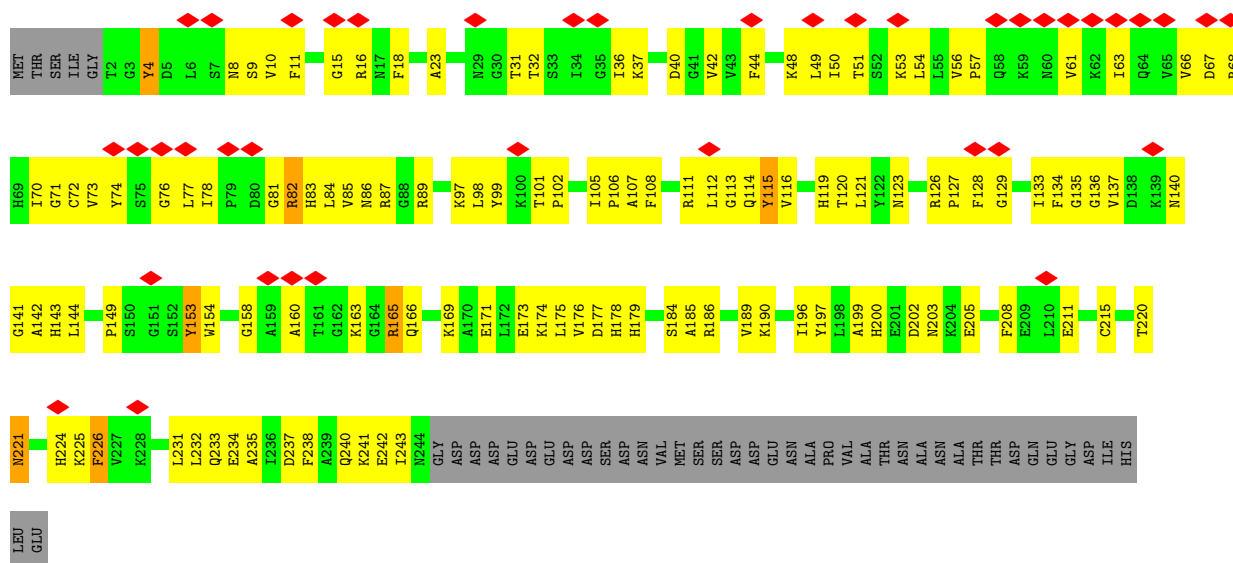




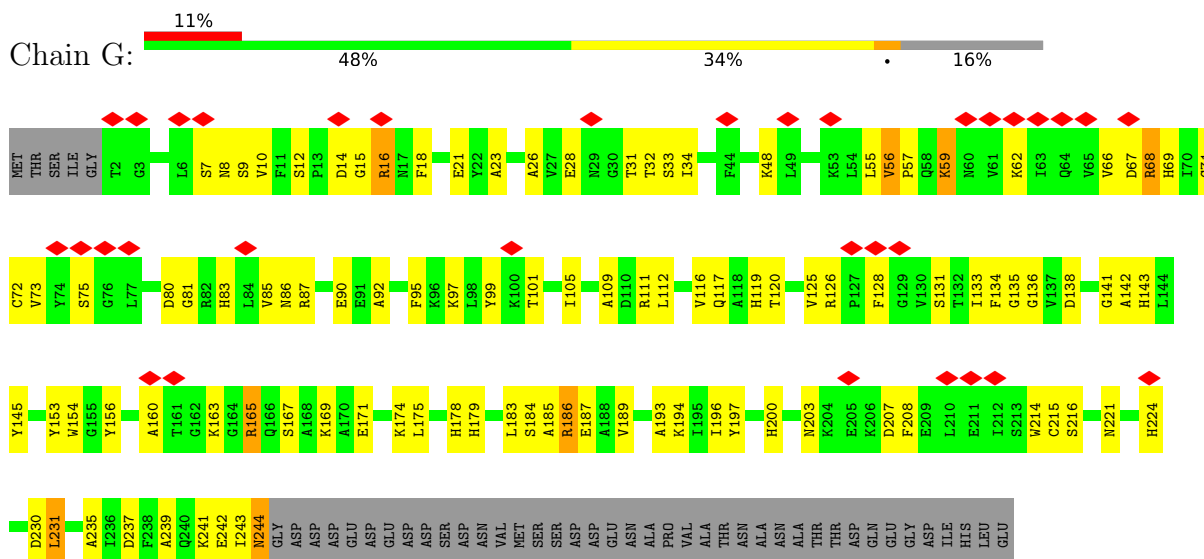
• Molecule 6: Proteasome subunit alpha type-6



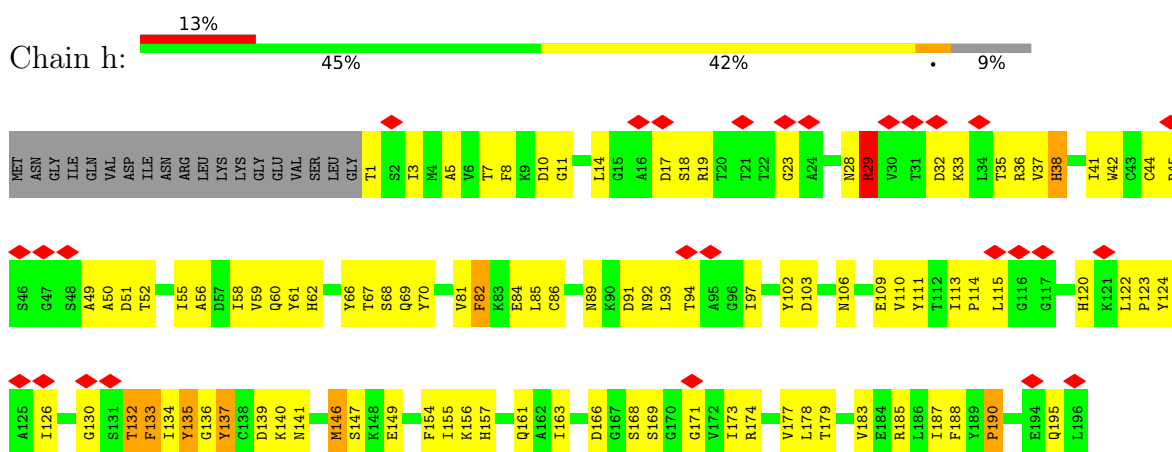
• Molecule 7: Probable proteasome subunit alpha type-7



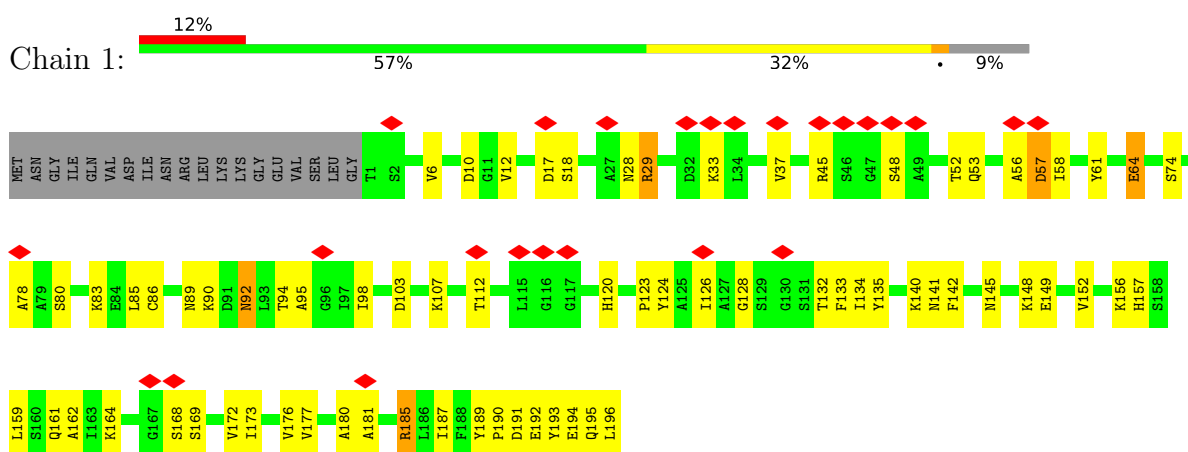
- Molecule 7: Probable proteasome subunit alpha type-7



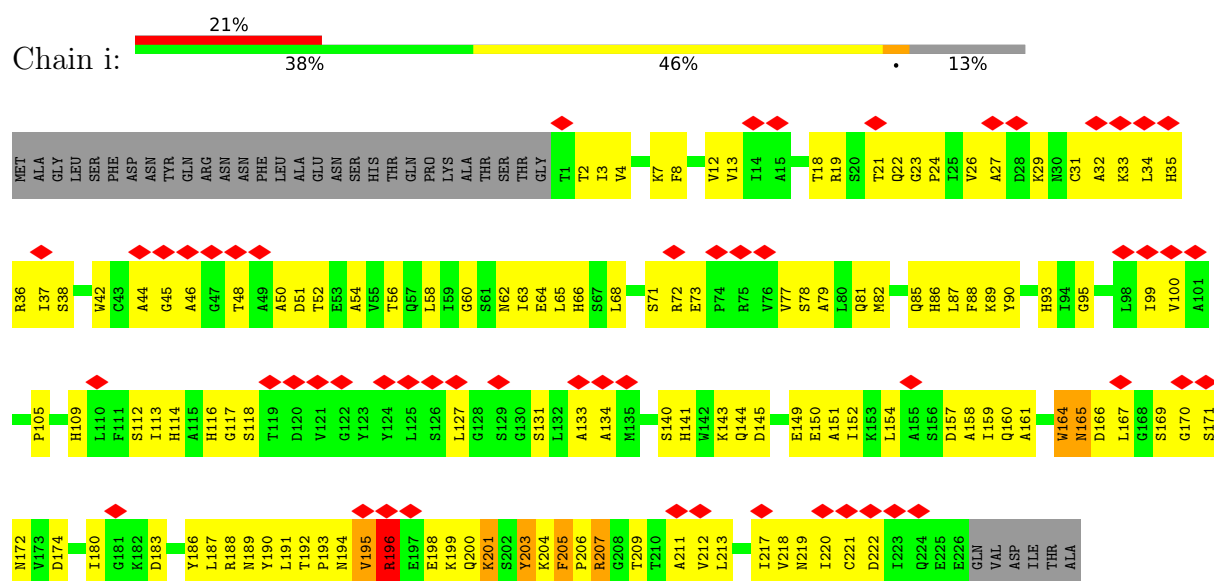
- Molecule 8: Proteasome subunit beta type-1



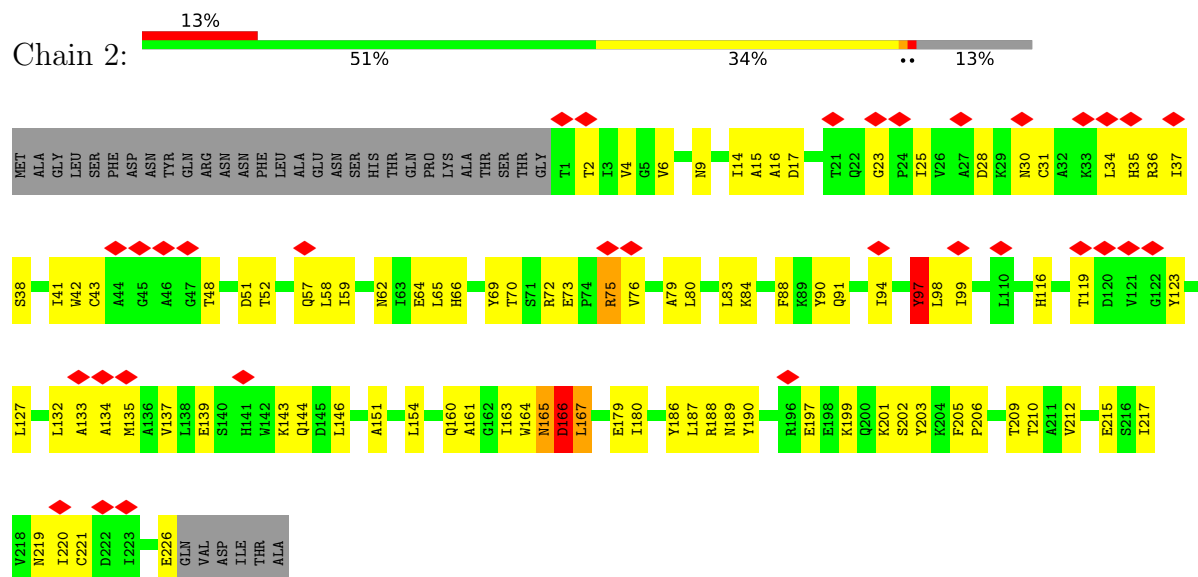
- Molecule 8: Proteasome subunit beta type-1



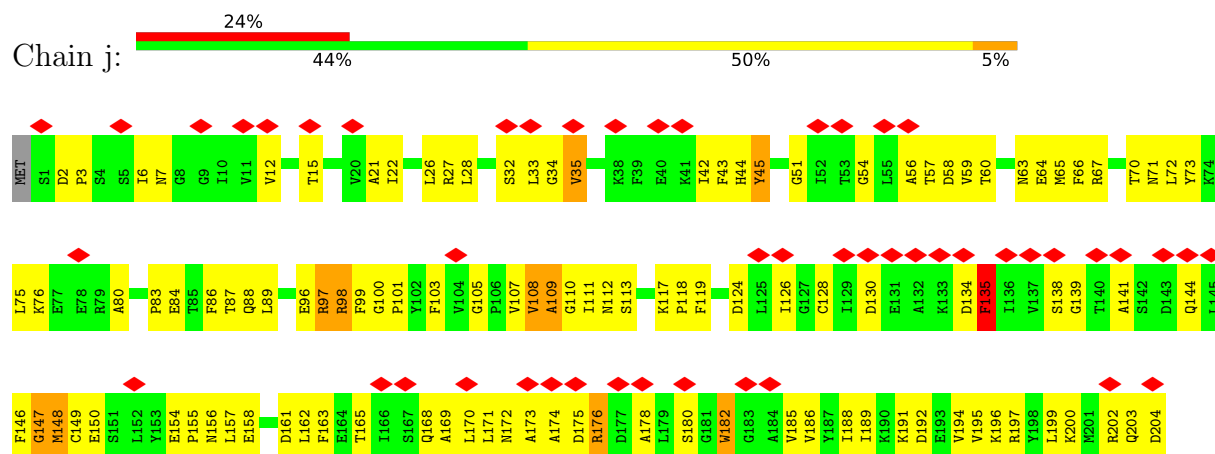
- Molecule 9: Proteasome subunit beta type-2



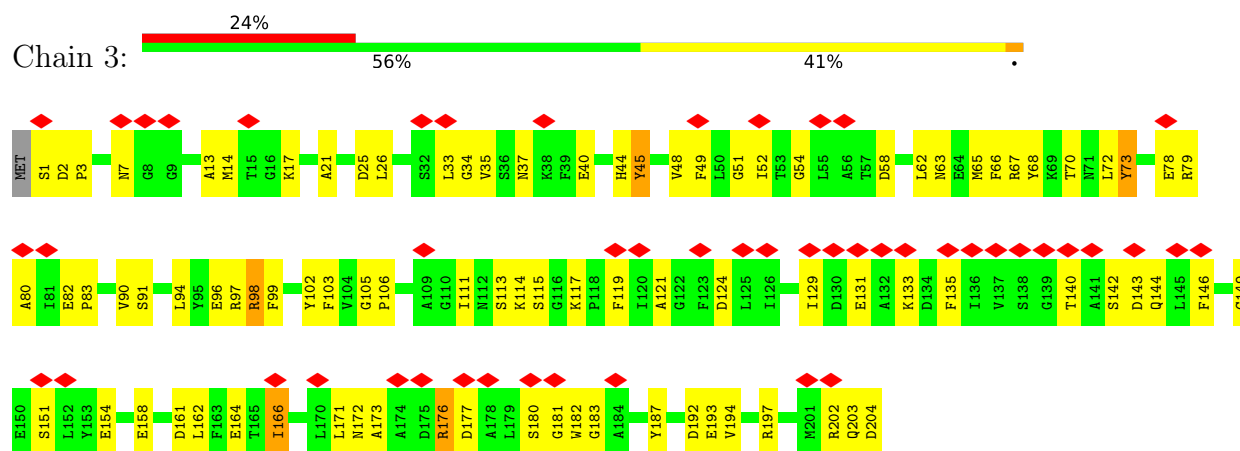
• Molecule 9: Proteasome subunit beta type-2



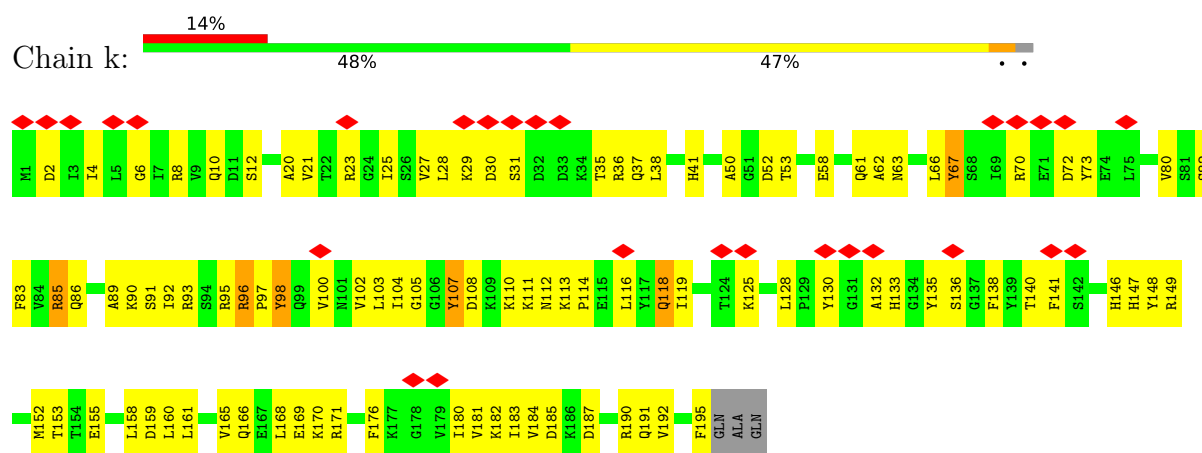
• Molecule 10: Proteasome subunit beta type-3



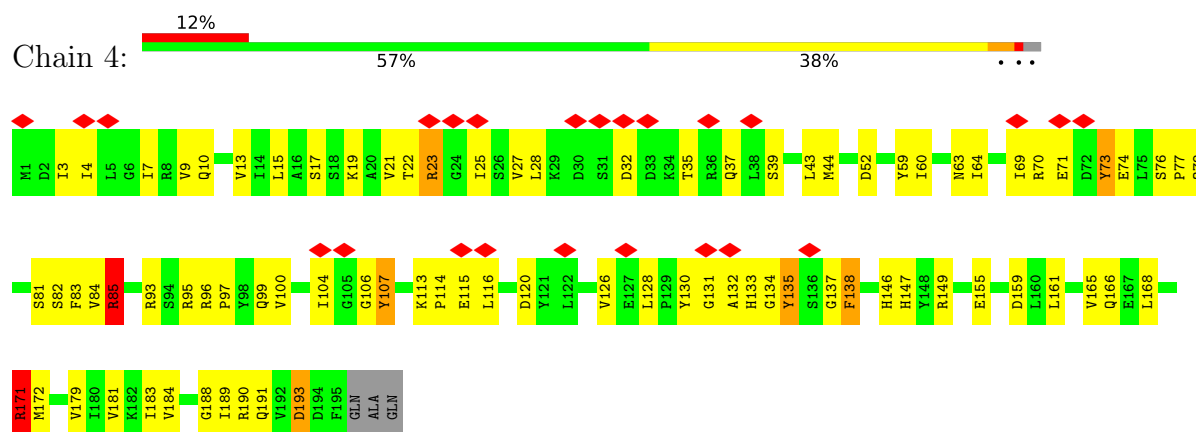
- Molecule 10: Proteasome subunit beta type-3



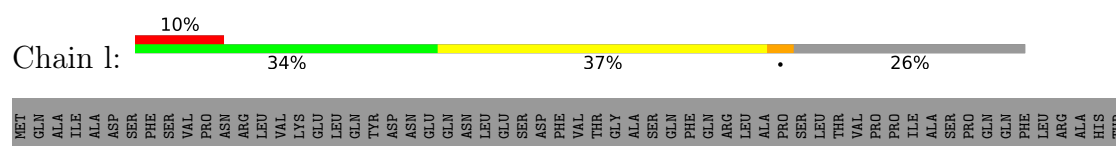
- Molecule 11: Proteasome subunit beta type-4

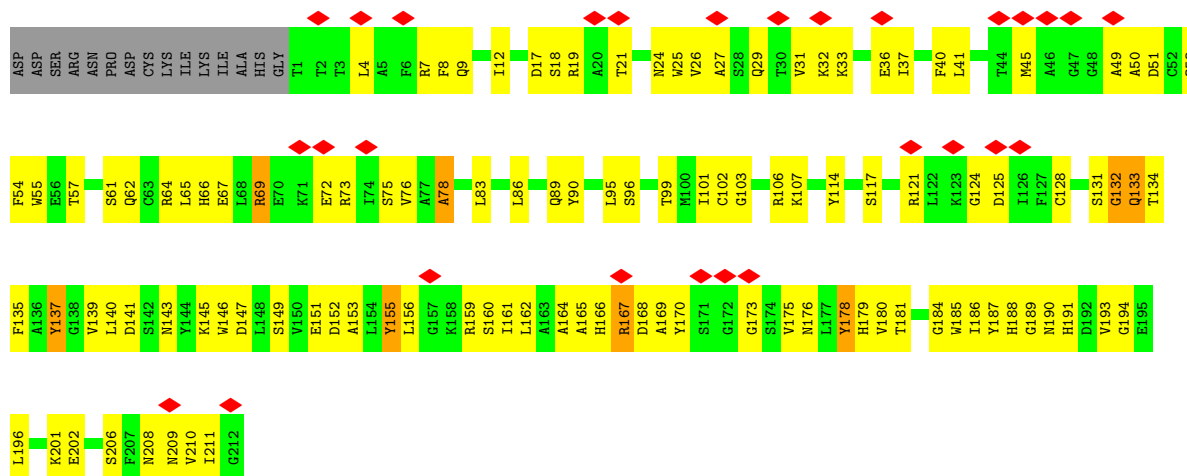


- Molecule 11: Proteasome subunit beta type-4

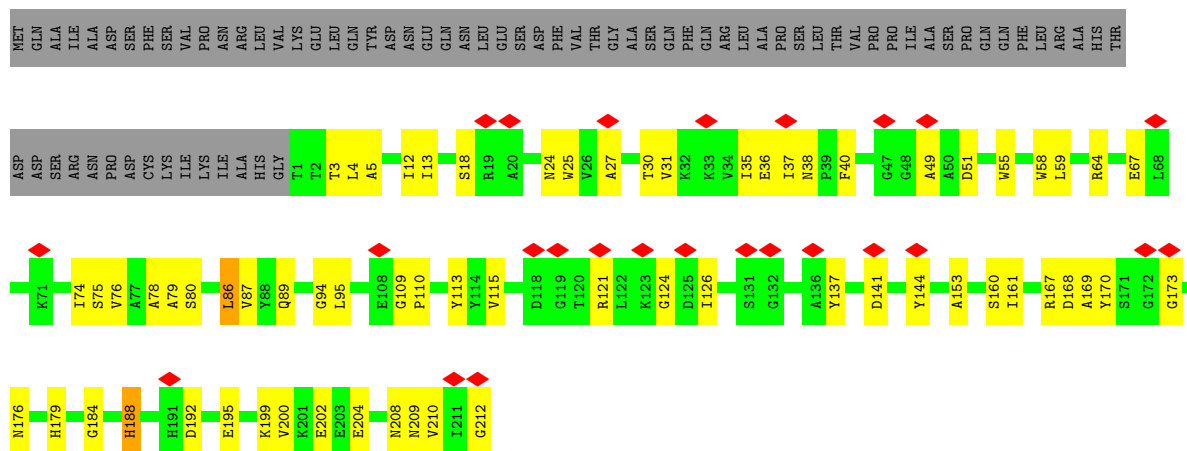


- Molecule 12: Proteasome subunit beta type-5

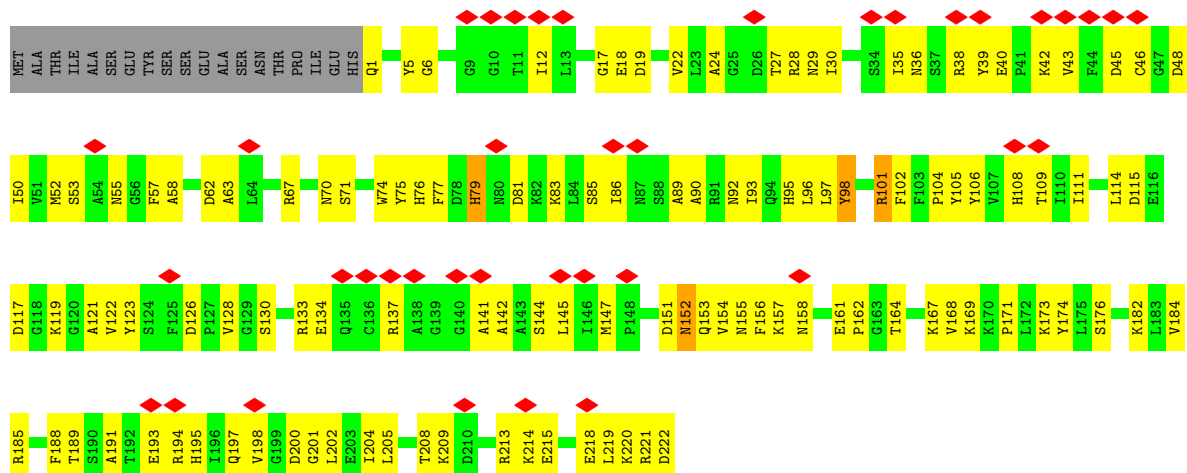
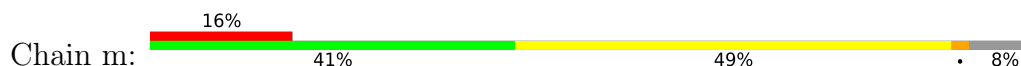




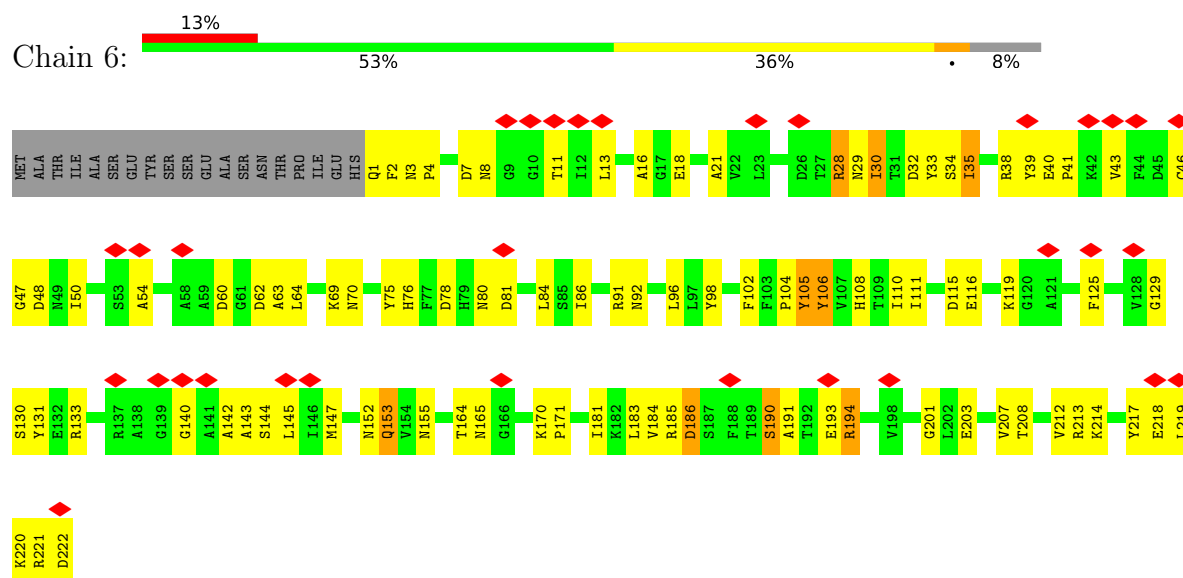
• Molecule 12: Proteasome subunit beta type-5



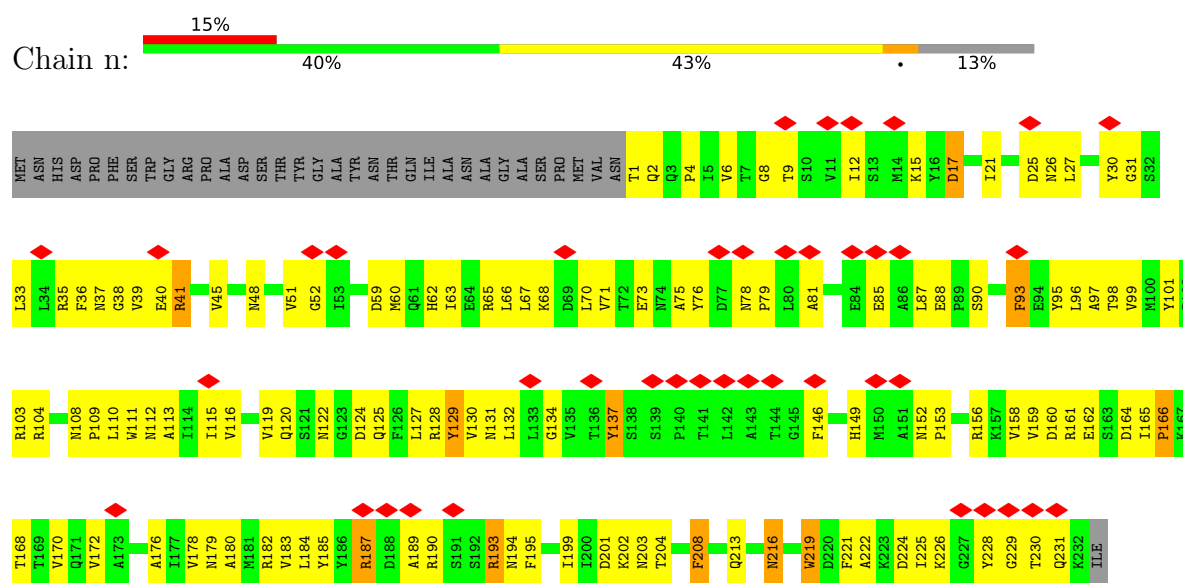
• Molecule 13: Proteasome subunit beta type-6



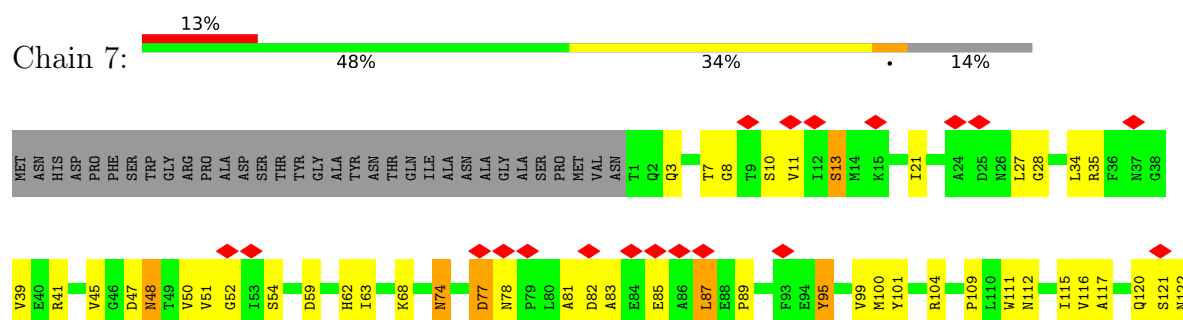
- Molecule 13: Proteasome subunit beta type-6

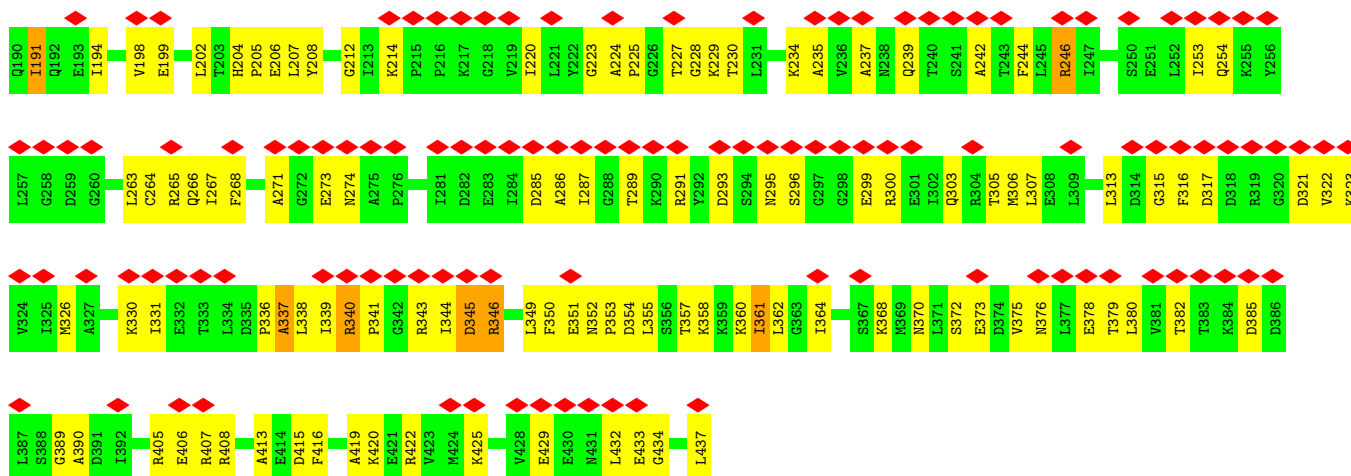


- Molecule 14: Proteasome subunit beta type-7

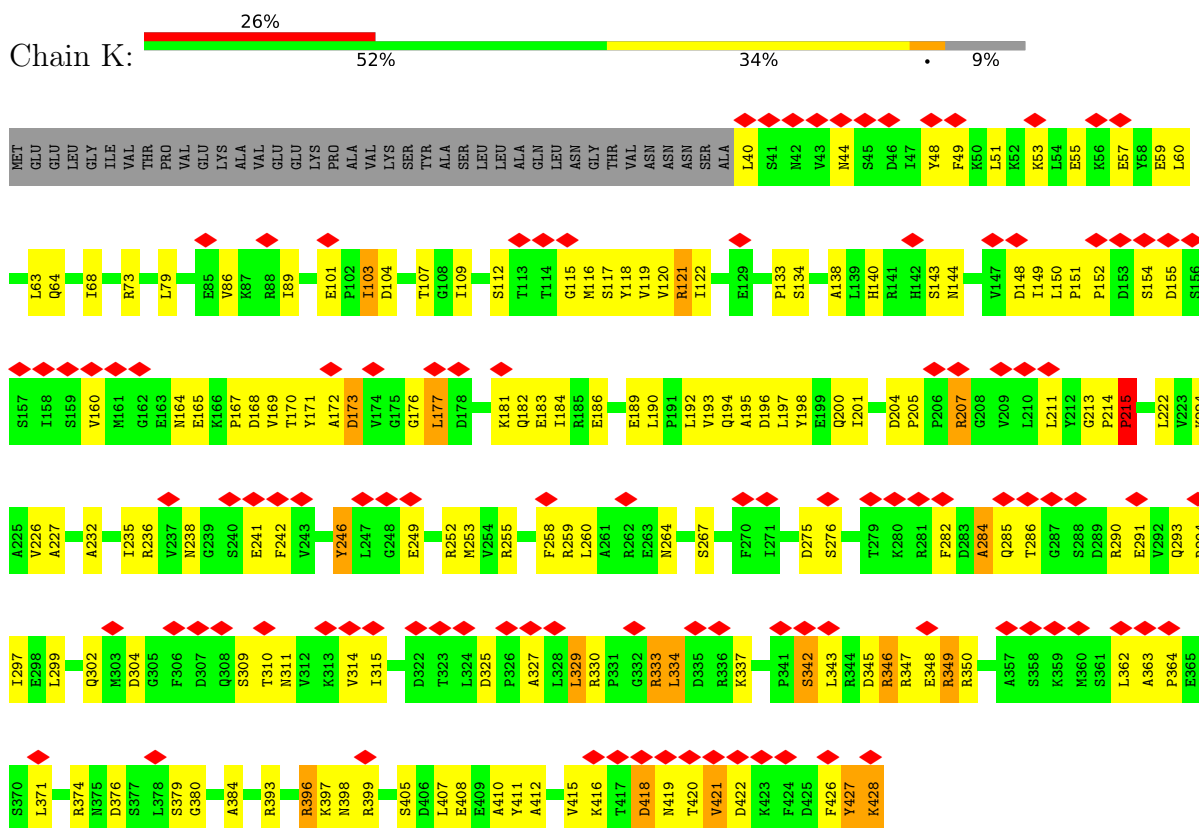


- Molecule 14: Proteasome subunit beta type-7

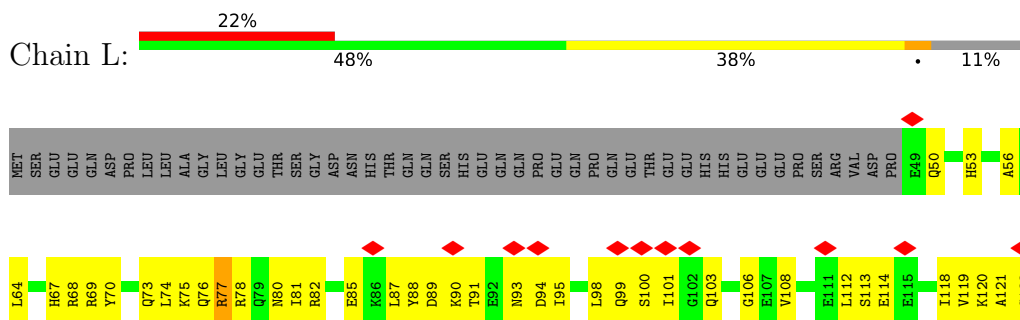




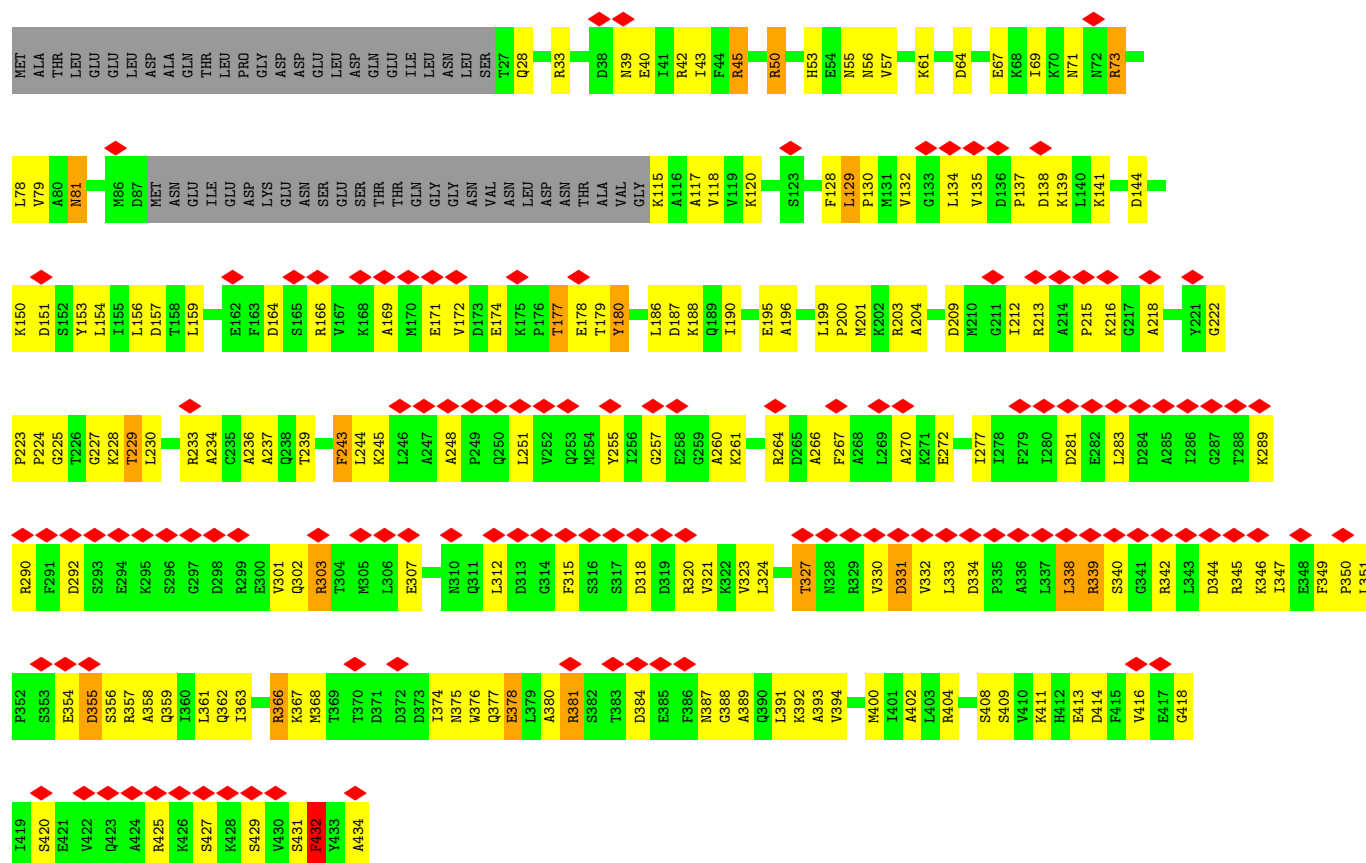
• Molecule 17: 26S protease regulatory subunit 6B homolog



• Molecule 18: 26S protease subunit RPT4

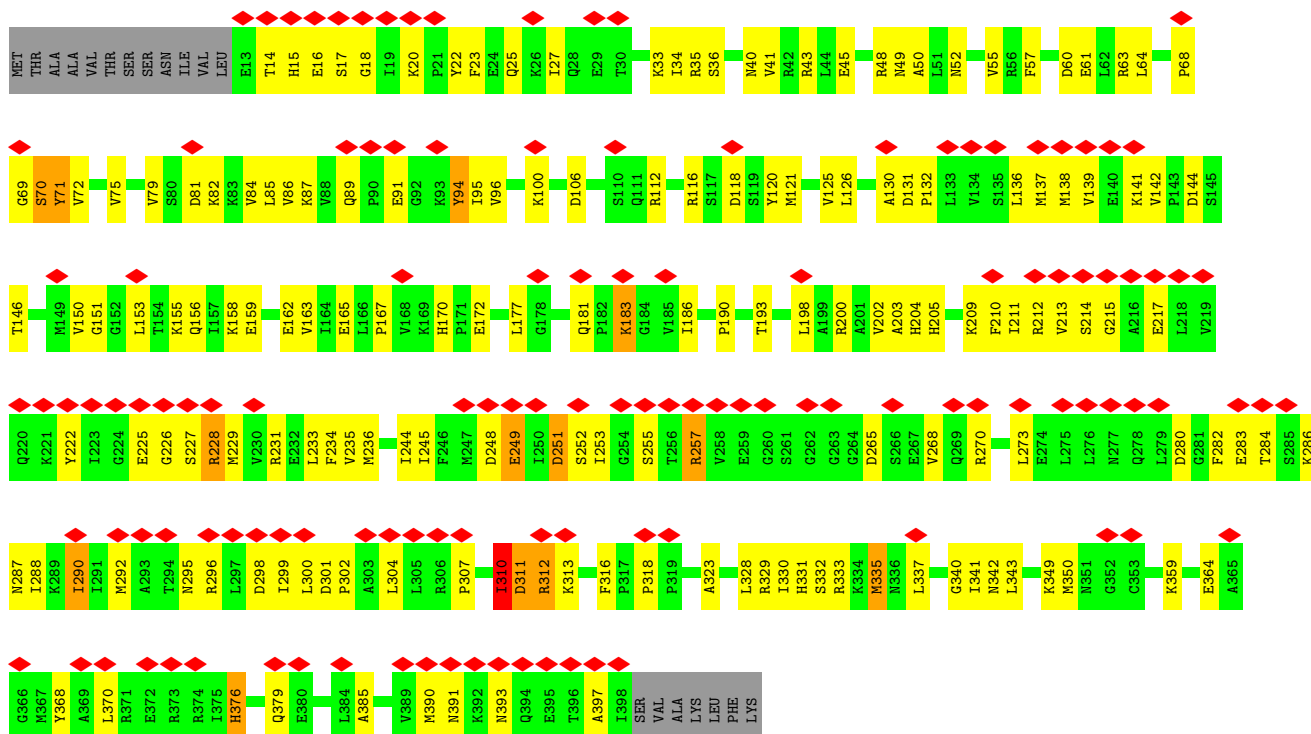


- Molecule 19: 26S protease regulatory subunit 6A

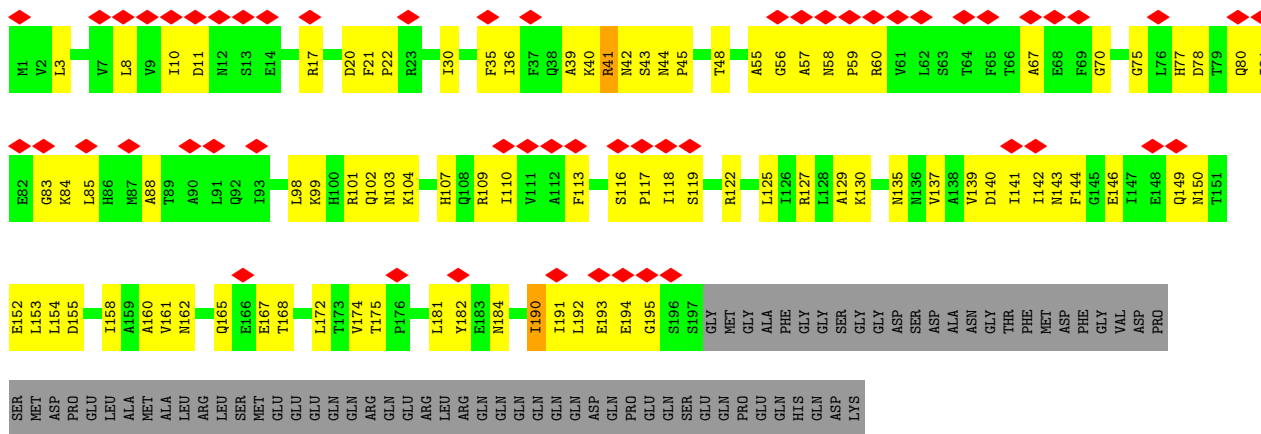


- Molecule 20: 26S protease regulatory subunit 8 homolog

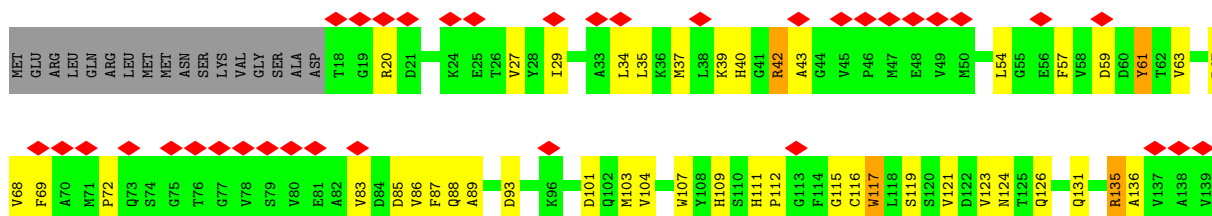


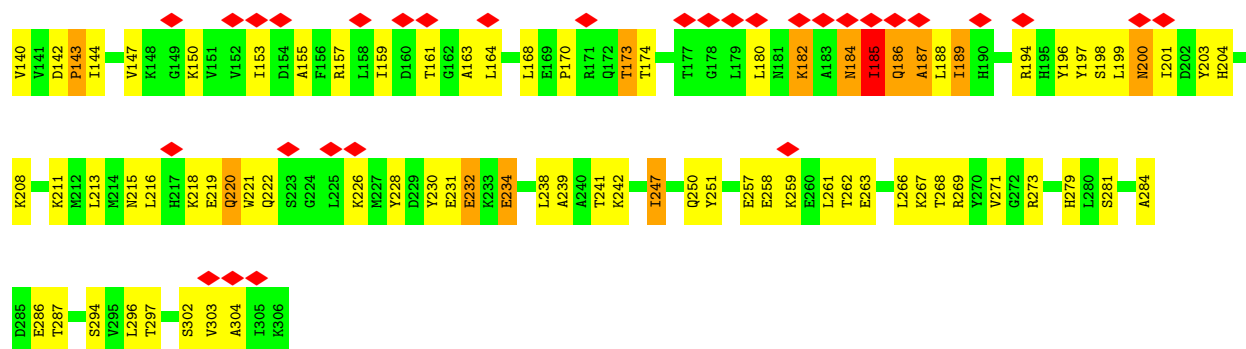


• Molecule 21: 26S proteasome regulatory subunit RPN10

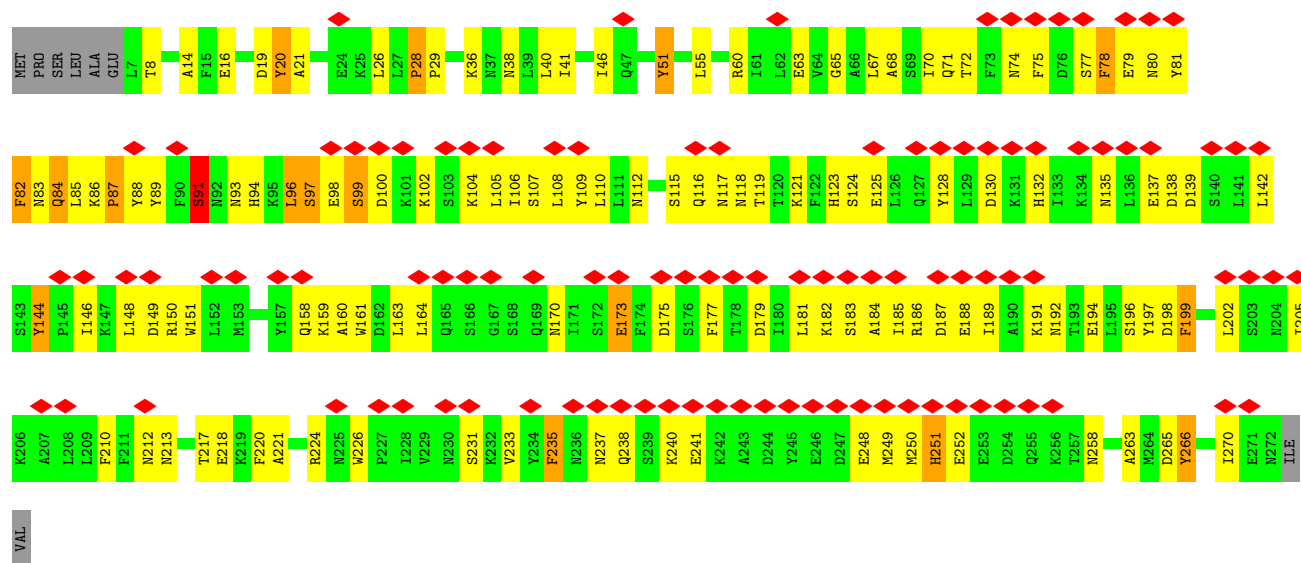
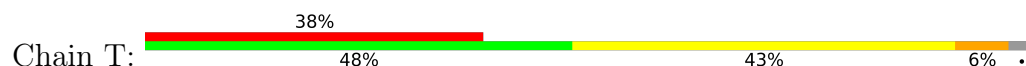


• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11

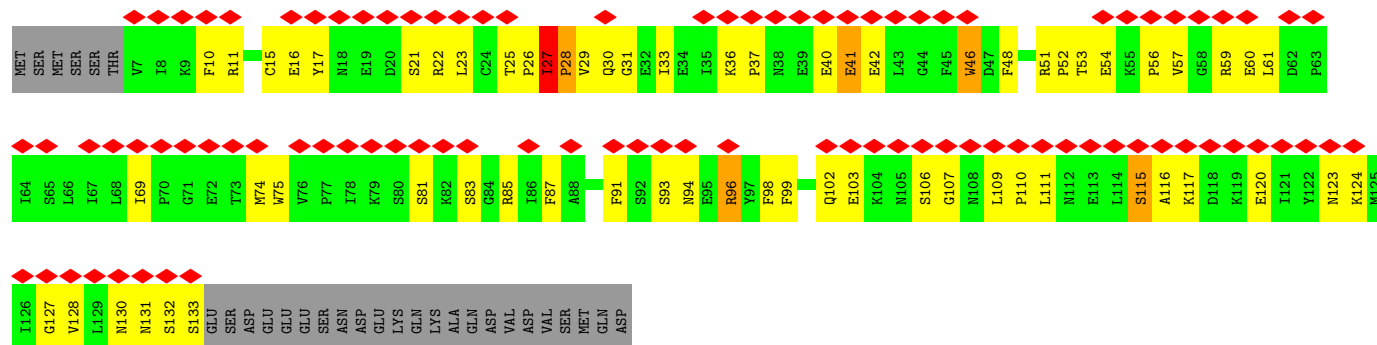




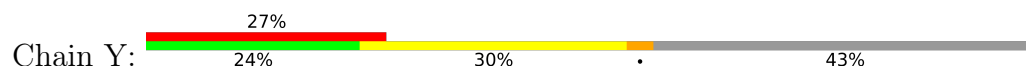
• Molecule 23: 26S proteasome regulatory subunit RPN12



• Molecule 24: 26S proteasome regulatory subunit RPN13



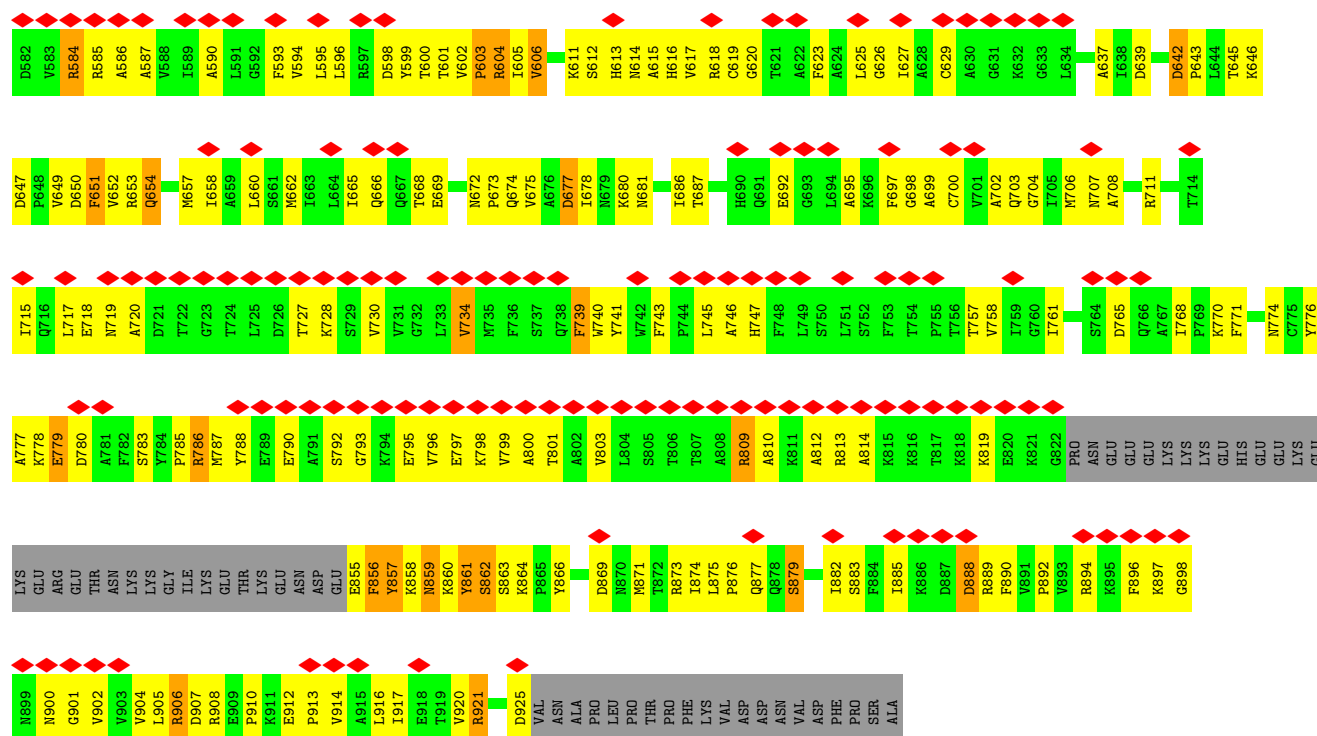
• Molecule 25: 26S proteasome complex subunit SEM1

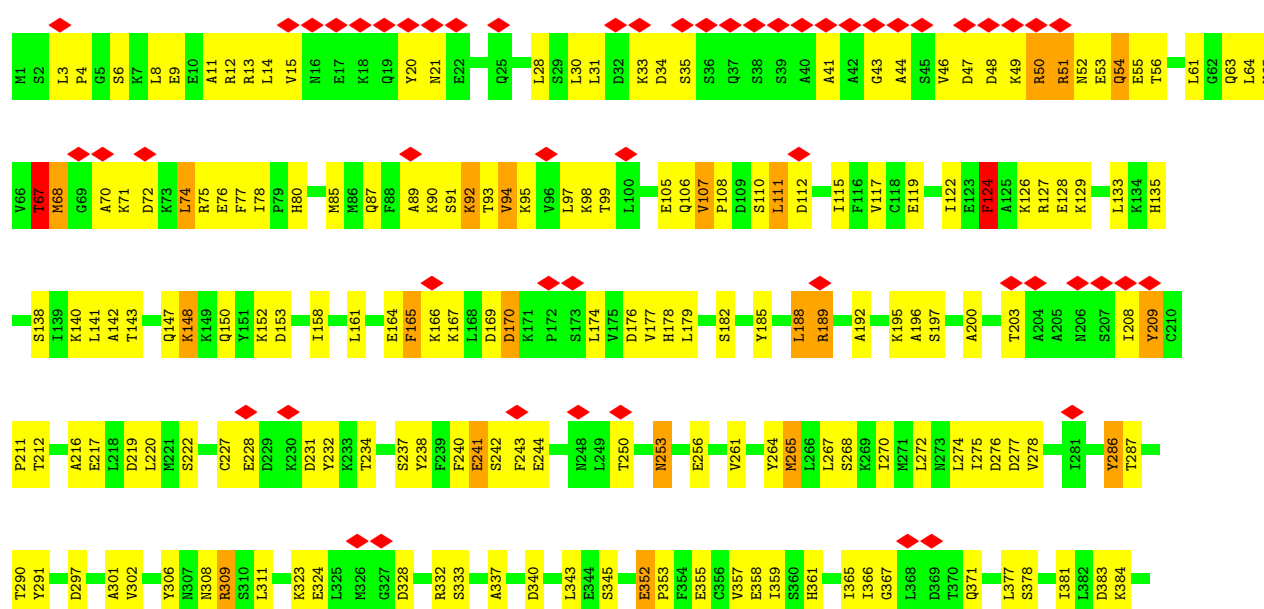


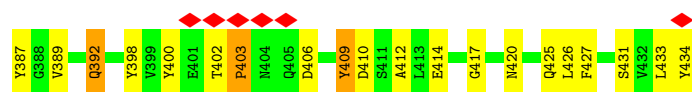
- Molecule 26: 26S proteasome regulatory subunit RPN1



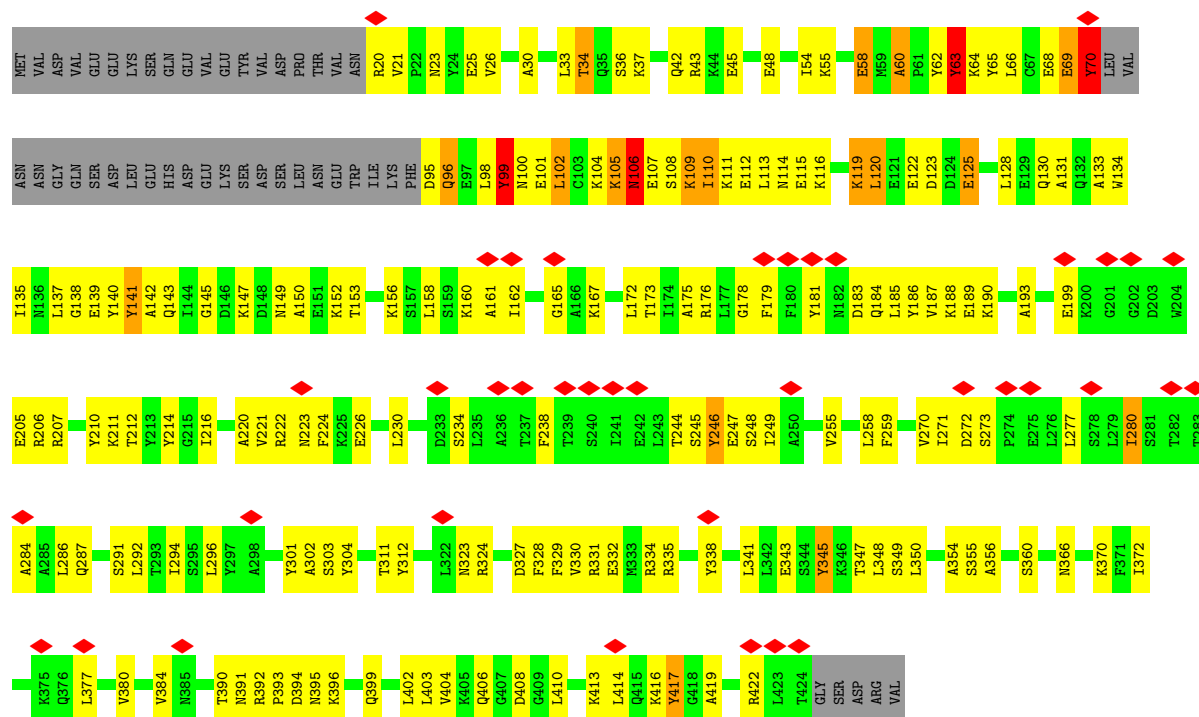
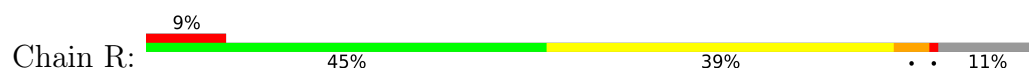




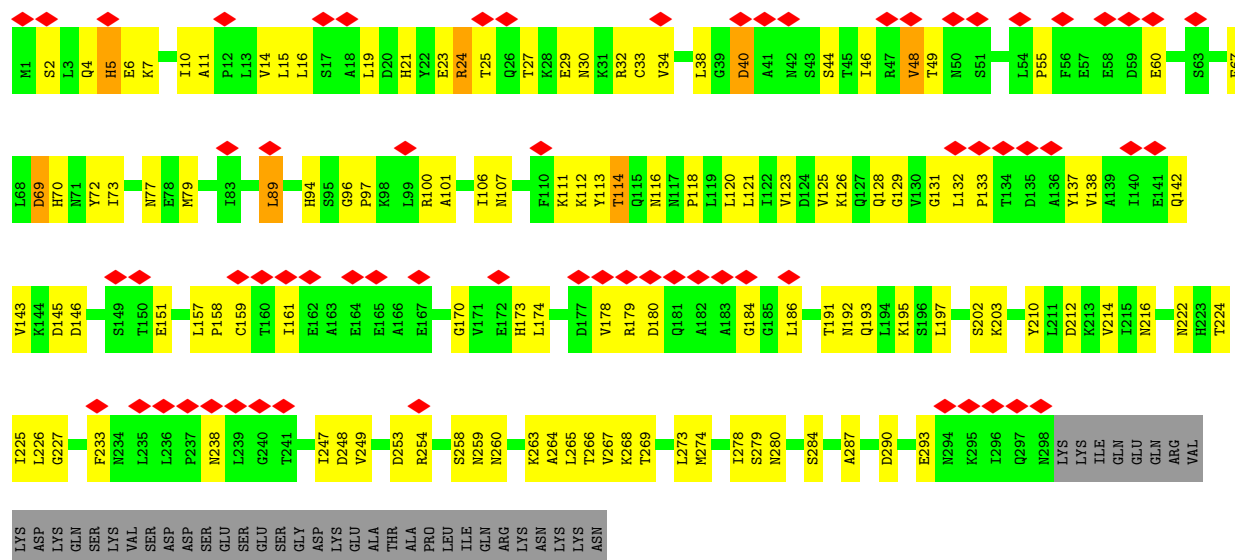




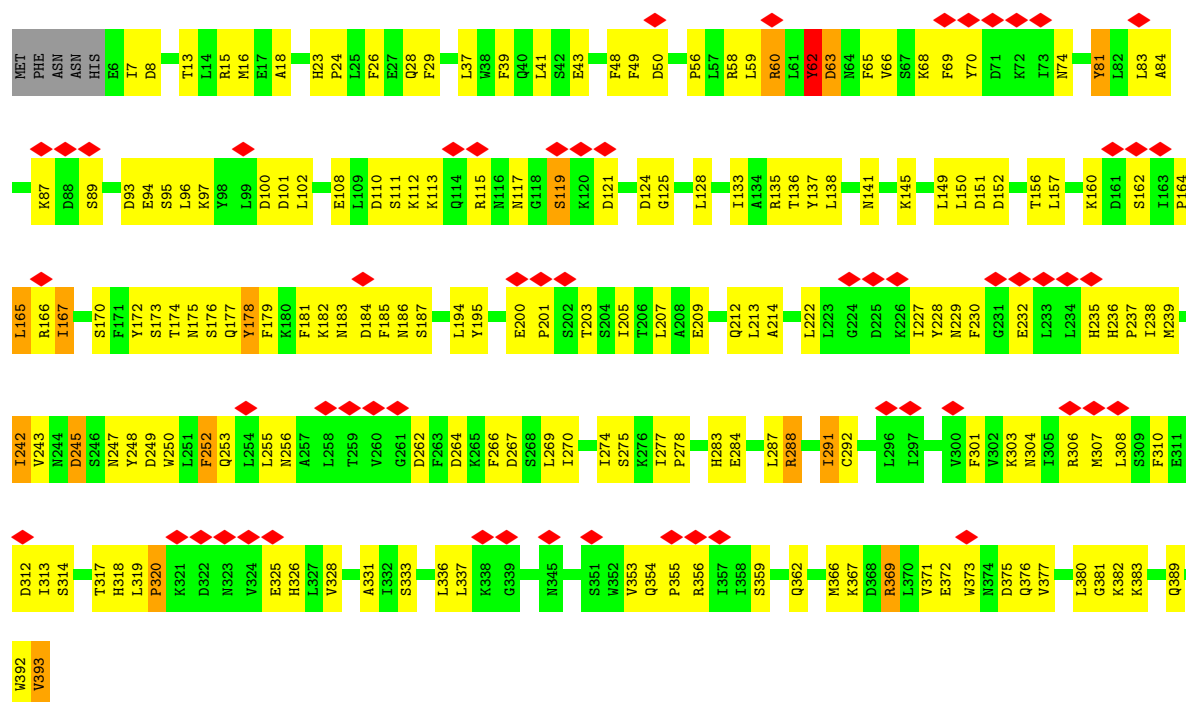
• Molecule 31: 26S proteasome regulatory subunit RPN7



• Molecule 32: 26S proteasome regulatory subunit RPN8



● Molecule 33: 26S proteasome regulatory subunit RPN9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67500	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	0.113	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	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, ADP, ANP

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	2.62	47/1945 (2.4%)	2.50	97/2634 (3.7%)
1	a	2.33	81/1945 (4.2%)	2.39	118/2634 (4.5%)
2	B	2.08	50/1952 (2.6%)	2.32	110/2642 (4.2%)
2	b	2.27	72/1952 (3.7%)	2.33	102/2642 (3.9%)
3	C	2.06	46/1934 (2.4%)	2.10	64/2618 (2.4%)
3	c	2.35	74/1934 (3.8%)	2.30	98/2618 (3.7%)
4	D	2.06	49/1910 (2.6%)	2.29	103/2586 (4.0%)
4	d	2.34	81/1910 (4.2%)	2.36	104/2586 (4.0%)
5	E	2.12	61/1886 (3.2%)	2.20	88/2541 (3.5%)
5	e	2.25	73/1886 (3.9%)	2.33	101/2541 (4.0%)
6	F	2.08	40/1823 (2.2%)	2.18	84/2463 (3.4%)
6	f	2.35	79/1800 (4.4%)	2.36	105/2433 (4.3%)
7	G	2.10	49/1932 (2.5%)	2.23	97/2609 (3.7%)
7	g	2.34	83/1932 (4.3%)	2.39	112/2609 (4.3%)
8	1	1.99	27/1541 (1.8%)	2.03	56/2087 (2.7%)
8	h	2.29	63/1541 (4.1%)	2.30	65/2087 (3.1%)
9	2	2.04	42/1750 (2.4%)	2.14	74/2373 (3.1%)
9	i	2.37	88/1750 (5.0%)	2.45	126/2373 (5.3%)
10	3	2.07	44/1611 (2.7%)	2.21	81/2174 (3.7%)
10	j	2.33	74/1611 (4.6%)	2.33	91/2174 (4.2%)
11	4	2.04	40/1589 (2.5%)	2.10	78/2142 (3.6%)
11	k	2.38	73/1589 (4.6%)	2.38	89/2142 (4.2%)
12	5	2.02	29/1681 (1.7%)	2.03	44/2274 (1.9%)
12	l	2.35	80/1681 (4.8%)	2.39	93/2274 (4.1%)
13	6	2.13	50/1795 (2.8%)	2.11	68/2420 (2.8%)
13	m	2.31	74/1795 (4.1%)	2.35	88/2420 (3.6%)
14	7	2.09	50/1821 (2.7%)	2.10	72/2470 (2.9%)
14	n	2.35	79/1846 (4.3%)	2.32	106/2503 (4.2%)
15	H	2.10	94/3014 (3.1%)	2.28	154/4058 (3.8%)
16	I	2.21	101/3061 (3.3%)	2.37	172/4121 (4.2%)
17	K	2.08	85/3121 (2.7%)	2.21	161/4213 (3.8%)
18	L	2.09	93/3128 (3.0%)	2.20	150/4204 (3.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	2.15	83/3023 (2.7%)	2.28	166/4070 (4.1%)
20	J	2.08	89/3073 (2.9%)	2.27	161/4129 (3.9%)
21	W	2.12	44/1557 (2.8%)	2.22	87/2111 (4.1%)
22	V	2.17	58/2309 (2.5%)	2.26	112/3115 (3.6%)
23	T	2.10	69/2235 (3.1%)	2.38	141/3017 (4.7%)
24	X	2.22	32/1058 (3.0%)	2.28	56/1432 (3.9%)
25	Y	2.23	16/438 (3.7%)	2.24	24/583 (4.1%)
26	Z	2.13	214/7122 (3.0%)	2.33	415/9645 (4.3%)
27	N	2.12	242/6994 (3.5%)	2.30	403/9455 (4.3%)
28	S	2.02	117/3966 (3.0%)	2.31	220/5355 (4.1%)
29	P	1.97	73/3663 (2.0%)	2.31	214/4940 (4.3%)
30	Q	2.03	95/3556 (2.7%)	2.27	176/4787 (3.7%)
31	R	2.10	76/3110 (2.4%)	2.40	207/4193 (4.9%)
32	U	2.02	63/2407 (2.6%)	2.13	97/3258 (3.0%)
33	O	2.13	91/3247 (2.8%)	2.35	188/4380 (4.3%)
All	All	2.16	3433/110424 (3.1%)	2.29	5818/149135 (3.9%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	5
11	4	0	6
11	k	0	5
12	5	0	2
12	l	0	7
13	6	0	6
13	m	0	6
14	7	0	4
14	n	0	5
15	H	0	7
16	I	0	7
17	K	0	12
18	L	0	10
19	M	0	14
20	J	0	8
21	W	0	1
22	V	0	3
23	T	0	12
24	X	0	2
25	Y	0	2
26	Z	0	13
27	N	0	13
28	S	0	7
29	P	0	8
30	Q	0	9
31	R	0	16
32	U	0	2
33	O	0	6
All	All	0	308

All (3433) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLN	CA-C	70.47	3.00	1.52
22	V	186	GLN	CA-CB	22.83	1.95	1.52
1	A	242	GLN	N-CA	-16.99	1.14	1.46
22	V	187	ALA	N-CA	-16.16	1.26	1.46
6	F	4	ASN	CA-CB	-16.14	1.26	1.53
6	f	161	GLY	CA-C	-12.88	1.38	1.52
1	a	78	ILE	CA-C	12.33	1.65	1.52
8	h	134	ILE	CA-C	-11.68	1.39	1.53
30	Q	434	TYR	C-O	-11.61	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	196	ALA	CA-C	-11.59	1.37	1.52
29	P	440	HIS	C-O	-11.59	1.00	1.23
4	D	240	GLU	C-O	-11.58	1.00	1.23
27	N	925	ASP	C-O	-11.58	1.00	1.23
25	Y	89	GLN	C-O	-11.58	1.00	1.23
7	G	244	ASN	C-O	-11.57	1.00	1.23
19	M	434	ALA	C-OXT	-11.57	1.00	1.23
9	2	226	GLU	C-O	-11.56	1.00	1.23
12	5	212	GLY	C-O	-11.56	1.00	1.23
16	I	437	LEU	C-O	-11.55	1.00	1.23
30	Q	434	TYR	C-OXT	-11.56	1.00	1.23
19	M	434	ALA	C-O	-11.55	1.00	1.23
3	C	244	THR	C-O	-11.55	1.00	1.23
6	F	233	ILE	C-O	-11.55	1.00	1.23
33	O	393	VAL	C-O	-11.55	1.00	1.23
24	X	133	SER	C-O	-11.55	1.00	1.23
28	S	492	LYS	C-O	-11.55	1.00	1.23
12	5	212	GLY	C-OXT	-11.54	1.00	1.23
17	K	428	LYS	C-O	-11.54	1.00	1.23
18	L	436	LYS	C-O	-11.54	1.00	1.23
6	F	233	ILE	C-OXT	-11.54	1.00	1.23
17	K	428	LYS	C-OXT	-11.54	1.00	1.23
14	7	229	GLY	C-O	-11.53	1.00	1.23
2	B	250	LEU	C-OXT	-11.53	1.00	1.23
33	O	393	VAL	C-OXT	-11.53	1.00	1.23
25	Y	89	GLN	C-OXT	-11.52	1.00	1.23
2	B	250	LEU	C-O	-11.52	1.00	1.23
13	6	222	ASP	C-OXT	-11.52	1.00	1.23
10	3	204	ASP	C-OXT	-11.51	1.00	1.23
16	I	437	LEU	C-OXT	-11.51	1.00	1.23
10	3	204	ASP	C-O	-11.50	1.00	1.23
13	6	222	ASP	C-O	-11.50	1.00	1.23
22	V	186	GLN	C-N	-11.24	1.19	1.33
27	N	768	ILE	N-CA	-11.21	1.36	1.46
22	V	187	ALA	C-N	-11.09	1.20	1.33
31	R	70	TYR	CA-CB	11.00	1.75	1.53
13	m	108	HIS	CA-C	-10.99	1.39	1.52
31	R	102	LEU	CA-C	-10.92	1.38	1.52
6	F	142	HIS	ND1-CE1	10.82	1.43	1.32
17	K	350	ARG	N-CA	-10.77	1.33	1.46
7	g	70	ILE	C-N	10.61	1.45	1.33
26	Z	263	ALA	N-CA	-10.60	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	111	ARG	NE-CZ	10.52	1.44	1.33
3	c	128	ARG	NE-CZ	10.52	1.44	1.33
17	K	207	ARG	C-N	10.38	1.48	1.33
2	B	148	TYR	CA-C	-10.15	1.40	1.52
26	Z	616	LEU	CA-C	-10.04	1.39	1.52
22	V	185	ILE	CA-CB	10.03	1.68	1.54
26	Z	730	ALA	CA-C	-10.02	1.39	1.52
31	R	106	ASN	CA-C	-9.99	1.39	1.52
13	m	171	PRO	CA-C	-9.98	1.41	1.52
33	O	318	HIS	ND1-CE1	9.96	1.42	1.32
16	I	97	GLU	CA-C	-9.93	1.40	1.52
24	X	23	LEU	CA-C	-9.80	1.40	1.52
21	W	57	ALA	CA-C	-9.77	1.40	1.52
27	N	908	ARG	C-N	9.77	1.42	1.33
10	j	86	PHE	N-CA	-9.69	1.34	1.46
10	j	42	ILE	N-CA	-9.69	1.34	1.46
9	i	86	HIS	ND1-CE1	9.68	1.42	1.32
11	k	21	VAL	CA-CB	-9.62	1.41	1.54
13	6	54	ALA	CA-C	-9.61	1.41	1.53
10	j	97	ARG	CD-NE	9.58	1.59	1.46
13	m	195	HIS	C-N	9.57	1.44	1.34
7	G	194	LYS	CA-C	-9.57	1.40	1.52
32	U	34	VAL	N-CA	-9.56	1.34	1.46
4	d	164	ARG	NE-CZ	9.53	1.43	1.33
12	l	4	LEU	CA-C	-9.52	1.40	1.52
10	3	202	ARG	CD-NE	9.50	1.59	1.46
19	M	281	ASP	CA-C	-9.48	1.41	1.52
14	7	143	ALA	CA-CB	-9.46	1.37	1.53
8	h	68	SER	N-CA	-9.41	1.34	1.46
16	I	267	ILE	CA-CB	-9.39	1.44	1.54
7	G	175	LEU	C-N	9.36	1.45	1.34
19	M	245	LYS	CA-CB	9.35	1.66	1.53
33	O	115	ARG	NE-CZ	9.34	1.43	1.33
31	R	69	GLU	CA-C	-9.32	1.39	1.52
11	k	20	ALA	CA-C	-9.31	1.40	1.53
19	M	404	ARG	CD-NE	9.29	1.59	1.46
6	F	42	HIS	ND1-CE1	9.28	1.41	1.32
12	l	167	ARG	CD-NE	9.24	1.59	1.46
12	l	191	HIS	C-N	9.24	1.45	1.33
17	K	252	ARG	NE-CZ	9.23	1.43	1.33
19	M	290	ARG	CD-NE	9.20	1.59	1.46
3	c	30	HIS	CB-CG	9.18	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	2	ARG	NE-CZ	9.17	1.43	1.33
29	P	263	HIS	CB-CG	9.12	1.62	1.50
15	H	275	ILE	CA-C	-9.11	1.41	1.52
5	e	2	ARG	NE-CZ	9.07	1.43	1.33
10	j	44	HIS	CA-C	-9.05	1.41	1.52
1	A	122	ARG	NE-CZ	9.04	1.43	1.33
17	K	60	LEU	CA-CB	9.03	1.67	1.53
7	G	72	CYS	CA-C	-9.01	1.41	1.52
22	V	68	VAL	C-N	9.01	1.45	1.33
5	e	82	GLU	N-CA	-9.00	1.35	1.46
25	Y	77	LEU	CA-C	-8.99	1.41	1.52
16	I	101	GLY	CA-C	-8.97	1.42	1.51
3	c	51	VAL	N-CA	-8.96	1.35	1.46
10	j	196	LYS	N-CA	-8.96	1.35	1.46
9	i	180	ILE	N-CA	-8.93	1.35	1.46
1	a	217	GLY	CA-C	-8.90	1.45	1.52
3	c	158	GLY	CA-C	-8.87	1.43	1.52
13	m	43	VAL	CA-C	-8.86	1.43	1.52
4	d	125	ARG	CD-NE	8.84	1.58	1.46
11	k	98	TYR	C-N	8.84	1.43	1.33
15	H	90	ARG	CD-NE	8.80	1.58	1.46
5	E	59	ILE	CA-C	-8.76	1.42	1.52
32	U	16	LEU	CA-C	-8.76	1.41	1.52
14	n	146	PHE	CA-C	-8.74	1.41	1.52
26	Z	769	ASN	CA-C	-8.72	1.45	1.53
27	N	408	LEU	CA-C	-8.72	1.41	1.52
10	3	34	GLY	CA-C	-8.71	1.46	1.52
27	N	798	LYS	N-CA	-8.71	1.35	1.46
13	m	117	ASP	N-CA	-8.70	1.35	1.46
14	7	51	VAL	C-N	8.70	1.39	1.33
9	i	112	SER	CA-C	-8.69	1.42	1.52
27	N	600	THR	N-CA	-8.66	1.36	1.46
13	m	157	LYS	N-CA	-8.66	1.35	1.46
7	g	135	GLY	CA-C	-8.66	1.43	1.51
8	h	126	ILE	CA-CB	-8.66	1.42	1.54
33	O	355	PRO	CA-C	-8.64	1.40	1.52
10	3	158	GLU	CA-C	-8.63	1.43	1.53
14	n	51	VAL	C-N	8.63	1.39	1.33
31	R	54	ILE	N-CA	-8.62	1.36	1.46
27	N	161	TYR	CA-C	-8.61	1.41	1.53
11	k	86	GLN	N-CA	-8.61	1.35	1.46
29	P	232	ARG	NE-CZ	8.60	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	O	262	ASP	CA-C	-8.59	1.42	1.52
7	G	56	VAL	CA-C	-8.57	1.46	1.53
11	k	119	ILE	CA-C	-8.56	1.41	1.52
26	Z	415	MET	C-N	8.55	1.45	1.33
4	d	109	ARG	NE-CZ	8.52	1.42	1.33
26	Z	120	SER	C-N	8.52	1.44	1.33
13	m	198	VAL	C-N	8.51	1.42	1.32
8	l	17	ASP	CA-C	-8.50	1.41	1.52
22	V	140	VAL	CA-C	-8.49	1.42	1.52
29	P	355	GLU	N-CA	-8.47	1.35	1.46
26	Z	269	TYR	N-CA	-8.47	1.35	1.46
10	j	194	VAL	CA-C	-8.45	1.41	1.52
4	d	195	ARG	NE-CZ	8.45	1.42	1.33
14	n	35	ARG	C-N	8.42	1.44	1.33
32	U	121	LEU	N-CA	-8.41	1.35	1.46
4	D	164	ARG	CD-NE	8.39	1.58	1.46
10	j	32	SER	CA-C	-8.38	1.41	1.52
1	A	42	THR	CA-C	-8.37	1.42	1.52
3	c	209	ARG	CD-NE	8.37	1.57	1.46
4	D	184	ALA	CA-C	-8.37	1.41	1.52
25	Y	20	LYS	N-CA	-8.36	1.35	1.46
16	I	390	ALA	CA-C	-8.34	1.42	1.52
11	k	83	PHE	C-N	8.34	1.44	1.33
30	Q	117	VAL	CA-C	-8.32	1.42	1.52
7	G	134	PHE	N-CA	-8.31	1.35	1.45
32	U	2	SER	N-CA	-8.30	1.35	1.46
21	W	41	ARG	NE-CZ	8.30	1.42	1.33
8	h	66	TYR	CA-C	-8.29	1.42	1.52
11	k	93	ARG	NE-CZ	8.29	1.42	1.33
17	K	399	ARG	NE-CZ	8.29	1.42	1.33
14	n	85	GLU	CA-C	-8.28	1.44	1.53
27	N	120	ASP	CA-C	-8.28	1.42	1.52
33	O	70	TYR	CA-CB	8.27	1.66	1.53
16	I	155	SER	CA-C	-8.25	1.42	1.52
16	I	370	ASN	CA-C	-8.24	1.42	1.52
13	m	221	ARG	NE-CZ	8.24	1.42	1.33
26	Z	78	SER	CA-C	-8.23	1.41	1.52
7	G	81	GLY	CA-C	-8.22	1.42	1.52
30	Q	409	TYR	CB-CG	-8.21	1.33	1.51
13	m	137	ARG	CA-C	-8.19	1.42	1.52
15	H	225	VAL	CA-CB	8.19	1.65	1.54
25	Y	86	ARG	NE-CZ	8.19	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	952	SER	CA-C	-8.19	1.42	1.52
11	4	7	ILE	CA-CB	-8.18	1.44	1.54
11	k	190	ARG	CD-NE	8.18	1.57	1.46
16	I	340	ARG	CD-NE	8.18	1.57	1.46
12	5	161	ILE	CA-C	-8.17	1.42	1.52
27	N	873	ARG	CZ-NH2	8.17	1.44	1.33
14	n	111	TRP	CA-CB	8.17	1.63	1.52
4	d	83	LEU	N-CA	-8.16	1.36	1.46
13	6	30	ILE	CA-C	-8.16	1.42	1.52
31	R	393	PRO	CA-C	-8.15	1.40	1.52
27	N	378	ASN	CA-C	-8.15	1.45	1.53
7	g	86	ASN	CA-C	-8.13	1.42	1.52
10	j	110	GLY	N-CA	-8.13	1.36	1.45
23	T	233	VAL	CA-CB	-8.13	1.44	1.54
31	R	112	GLU	CA-C	-8.11	1.42	1.52
5	e	99	ILE	CA-C	-8.11	1.42	1.52
13	6	38	ARG	CA-C	-8.09	1.42	1.52
22	V	119	SER	C-N	8.09	1.44	1.33
26	Z	553	ARG	NE-CZ	8.07	1.42	1.33
31	R	130	GLN	CA-CB	8.07	1.66	1.53
20	J	205	HIS	ND1-CE1	8.05	1.40	1.32
22	V	232	GLU	N-CA	-8.05	1.36	1.46
8	h	179	THR	CA-CB	-8.04	1.41	1.53
23	T	60	ARG	CZ-NH1	8.04	1.44	1.32
12	l	159	ARG	CD-NE	8.03	1.57	1.46
4	d	144	LYS	CA-C	-8.02	1.42	1.52
20	J	138	MET	CA-C	-8.02	1.42	1.52
26	Z	774	ARG	NE-CZ	8.01	1.41	1.33
27	N	232	LEU	N-CA	-8.01	1.35	1.46
20	J	310	ILE	CA-CB	-8.01	1.43	1.54
6	f	133	ILE	CA-CB	-8.00	1.44	1.54
17	K	107	THR	C-O	-7.98	1.14	1.23
8	1	185	ARG	CZ-NH2	7.97	1.43	1.33
23	T	132	HIS	CB-CG	7.96	1.61	1.50
26	Z	555	ALA	N-CA	-7.96	1.36	1.46
10	3	52	ILE	CA-C	-7.95	1.42	1.52
18	L	349	ILE	N-CA	-7.95	1.40	1.46
14	7	52	GLY	CA-C	-7.94	1.46	1.52
26	Z	352	LYS	C-N	7.93	1.42	1.33
22	V	67	ASP	CA-C	-7.93	1.42	1.52
11	4	70	ARG	NE-CZ	7.93	1.41	1.33
32	U	48	VAL	CA-CB	-7.93	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	58	ASP	CA-C	7.92	1.63	1.52
17	K	44	ASN	N-CA	-7.92	1.36	1.46
19	M	55	ASN	C-N	7.92	1.44	1.33
3	c	140	ASP	N-CA	-7.92	1.35	1.45
23	T	183	SER	CA-C	-7.91	1.42	1.52
24	X	96	ARG	NE-CZ	7.91	1.41	1.33
14	n	127	LEU	C-N	7.90	1.43	1.33
15	H	435	ARG	NE-CZ	7.90	1.41	1.33
3	c	114	LEU	CA-C	-7.90	1.42	1.52
5	E	217	GLN	N-CA	-7.89	1.36	1.46
12	5	209	ASN	CA-C	-7.89	1.42	1.52
29	P	75	LEU	N-CA	-7.89	1.36	1.46
33	O	74	ASN	CA-C	-7.88	1.42	1.52
5	E	209	ALA	C-N	7.88	1.44	1.33
5	E	51	LEU	CA-C	-7.87	1.42	1.52
16	I	433	GLU	N-CA	-7.87	1.36	1.46
26	Z	397	ASP	N-CA	-7.87	1.37	1.46
29	P	435	LYS	N-CA	-7.86	1.37	1.46
2	b	157	PHE	CA-C	7.86	1.61	1.52
7	g	71	GLY	N-CA	-7.86	1.35	1.46
14	7	77	ASP	CA-C	-7.86	1.42	1.52
7	g	231	LEU	CA-C	-7.85	1.42	1.52
19	M	139	LYS	CA-C	-7.85	1.42	1.52
18	L	348	GLU	CA-C	-7.84	1.43	1.52
13	m	133	ARG	NE-CZ	7.83	1.41	1.33
30	Q	196	ALA	CA-C	-7.82	1.42	1.52
5	e	193	LEU	N-CA	-7.81	1.36	1.46
9	i	141	HIS	ND1-CE1	7.81	1.40	1.32
15	H	313	ALA	CA-C	-7.81	1.43	1.52
24	X	75	TRP	CA-C	-7.81	1.43	1.52
18	L	153	LEU	CA-C	-7.81	1.46	1.53
5	e	130	PHE	CA-C	-7.80	1.43	1.52
7	G	179	HIS	ND1-CE1	7.80	1.40	1.32
5	E	153	SER	C-N	7.80	1.44	1.33
8	h	185	ARG	NE-CZ	7.80	1.41	1.33
11	k	187	ASP	C-N	7.79	1.42	1.33
28	S	435	LYS	N-CA	-7.79	1.36	1.46
26	Z	285	ALA	N-CA	-7.78	1.36	1.46
1	a	129	GLY	C-N	7.78	1.40	1.33
5	e	189	GLU	CA-C	-7.77	1.42	1.52
16	I	181	TYR	C-N	7.77	1.43	1.33
13	6	92	ASN	C-N	7.76	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	204	HIS	ND1-CE1	7.76	1.40	1.32
20	J	193	THR	CA-C	-7.76	1.42	1.52
31	R	26	VAL	CA-C	-7.75	1.43	1.52
27	N	921	ARG	NE-CZ	7.75	1.41	1.33
7	g	165	ARG	CD-NE	7.75	1.57	1.46
5	E	2	ARG	NE-CZ	7.75	1.41	1.33
20	J	130	ALA	CA-C	-7.75	1.43	1.52
12	5	78	ALA	CA-C	-7.74	1.42	1.52
26	Z	510	LEU	N-CA	-7.74	1.40	1.46
8	h	173	ILE	CA-C	-7.72	1.43	1.52
6	f	166	GLY	CA-C	-7.72	1.43	1.52
18	L	256	ILE	CA-C	-7.70	1.44	1.52
27	N	144	CYS	CA-C	-7.70	1.42	1.52
4	D	88	ARG	NE-CZ	7.70	1.41	1.33
11	k	149	ARG	CD-NE	7.69	1.57	1.46
28	S	320	ILE	CA-C	-7.68	1.42	1.52
26	Z	232	LYS	CA-C	-7.67	1.42	1.52
19	M	393	ALA	C-N	7.67	1.43	1.33
22	V	34	LEU	CA-C	-7.67	1.43	1.52
3	C	93	HIS	ND1-CE1	7.66	1.40	1.32
33	O	245	ASP	CA-C	-7.66	1.42	1.53
27	N	15	GLU	CA-CB	-7.65	1.41	1.53
18	L	53	HIS	CB-CG	7.65	1.60	1.50
4	d	179	ARG	CD-NE	7.64	1.56	1.46
11	k	102	VAL	N-CA	-7.64	1.37	1.46
13	6	153	GLN	CA-C	-7.64	1.42	1.52
2	b	184	GLU	CA-C	-7.63	1.43	1.52
6	f	203	GLU	C-N	7.63	1.44	1.33
8	h	42	TRP	CA-C	-7.63	1.43	1.52
26	Z	448	LYS	CA-C	-7.63	1.43	1.52
7	G	135	GLY	CA-C	-7.62	1.44	1.51
26	Z	370	SER	N-CA	7.62	1.56	1.46
33	O	150	LEU	N-CA	-7.61	1.36	1.46
23	T	112	ASN	N-CA	-7.61	1.37	1.46
33	O	58	ARG	CD-NE	7.61	1.56	1.46
7	g	165	ARG	CZ-NH1	7.60	1.43	1.32
12	5	74	ILE	N-CA	-7.60	1.38	1.46
23	T	150	ARG	N-CA	-7.60	1.37	1.46
7	G	112	LEU	C-N	7.60	1.43	1.33
11	k	93	ARG	CD-NE	7.59	1.56	1.46
7	g	76	GLY	CA-C	-7.59	1.43	1.52
5	e	48	SER	CA-CB	7.59	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	33	VAL	C-N	7.58	1.43	1.33
19	M	67	GLU	C-O	7.58	1.32	1.24
21	W	43	SER	N-CA	-7.57	1.37	1.46
14	7	225	ILE	C-N	7.56	1.44	1.33
16	I	132	ILE	CA-C	-7.56	1.43	1.52
27	N	619	CYS	CA-C	-7.56	1.43	1.52
32	U	129	GLY	N-CA	-7.56	1.34	1.45
2	b	107	THR	C-O	-7.55	1.15	1.24
5	E	5	SER	CA-C	-7.55	1.43	1.52
4	d	95	ARG	CZ-NH1	7.55	1.43	1.32
17	K	374	ARG	NE-CZ	7.55	1.41	1.33
13	m	30	ILE	CA-C	-7.54	1.43	1.52
1	A	54	LEU	CA-C	-7.54	1.43	1.52
26	Z	765	MET	CA-C	-7.52	1.43	1.52
13	m	185	ARG	CA-C	-7.52	1.43	1.52
9	2	206	PRO	CA-C	-7.52	1.43	1.52
9	2	217	ILE	N-CA	-7.51	1.37	1.46
10	j	32	SER	C-N	7.51	1.44	1.33
19	M	394	VAL	N-CA	-7.51	1.37	1.46
23	T	130	ASP	CA-C	-7.51	1.42	1.52
27	N	462	VAL	CA-C	-7.51	1.43	1.52
5	e	140	ASP	C-N	7.50	1.43	1.33
12	l	7	ARG	NE-CZ	7.50	1.41	1.33
16	I	70	LEU	N-CA	-7.50	1.37	1.46
27	N	81	TYR	N-CA	-7.50	1.36	1.46
5	E	14	PHE	CA-C	-7.50	1.43	1.52
28	S	255	SER	CA-C	-7.50	1.42	1.52
9	2	219	ASN	CA-C	-7.50	1.43	1.52
11	k	180	ILE	CA-C	-7.49	1.43	1.52
4	d	210	ILE	CA-C	-7.49	1.43	1.52
2	b	100	ILE	CA-CB	-7.48	1.44	1.54
32	U	161	ILE	CA-C	-7.48	1.43	1.52
3	c	85	ILE	CA-CB	-7.48	1.45	1.54
11	k	70	ARG	CA-C	-7.47	1.43	1.52
33	O	48	PHE	N-CA	-7.47	1.37	1.46
14	n	180	ALA	C-O	-7.47	1.15	1.24
30	Q	97	LEU	C-O	-7.47	1.15	1.24
3	c	166	ALA	C-N	7.46	1.43	1.33
2	B	207	ASP	C-N	7.46	1.44	1.33
6	F	186	ASP	CA-C	-7.46	1.43	1.52
22	V	116	CYS	C-N	7.46	1.43	1.33
15	H	420	ARG	NE-CZ	7.46	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	U	120	LEU	CA-C	-7.45	1.43	1.52
6	f	29	LYS	CA-C	-7.45	1.42	1.52
22	V	37	MET	CA-C	-7.45	1.43	1.52
7	g	116	VAL	CA-CB	-7.44	1.45	1.54
10	j	176	ARG	CA-CB	7.44	1.64	1.53
4	d	207	ASN	N-CA	-7.44	1.37	1.46
12	l	99	THR	CA-C	7.44	1.61	1.52
18	L	120	LYS	CA-C	-7.44	1.43	1.52
14	n	81	ALA	N-CA	-7.43	1.37	1.46
11	4	39	SER	N-CA	7.43	1.52	1.46
14	7	126	PHE	N-CA	-7.43	1.37	1.46
33	O	307	MET	N-CA	-7.43	1.37	1.46
8	h	178	LEU	CA-C	-7.43	1.43	1.53
27	N	474	SER	C-N	7.43	1.43	1.33
30	Q	129	LYS	CA-C	-7.43	1.43	1.52
19	M	391	LEU	CA-C	-7.43	1.43	1.52
11	k	155	GLU	C-N	7.42	1.44	1.34
20	J	251	ASP	CA-C	-7.42	1.42	1.52
5	E	134	LEU	CA-C	-7.42	1.43	1.52
21	W	10	ILE	CA-C	-7.42	1.43	1.52
24	X	81	SER	N-CA	-7.42	1.35	1.46
30	Q	12	ARG	CD-NE	7.42	1.56	1.46
21	W	165	GLN	N-CA	7.41	1.54	1.46
32	U	158	PRO	CA-C	-7.41	1.41	1.52
23	T	189	ILE	N-CA	-7.41	1.37	1.46
4	d	59	PRO	CA-CB	-7.41	1.44	1.53
9	i	42	TRP	CA-C	-7.41	1.44	1.52
30	Q	170	ASP	CA-C	-7.41	1.42	1.52
31	R	142	ALA	N-CA	-7.40	1.37	1.46
1	a	92	ALA	N-CA	-7.40	1.37	1.46
1	a	184	HIS	C-N	7.40	1.42	1.33
14	7	184	LEU	N-CA	-7.40	1.37	1.46
31	R	153	THR	CA-C	-7.40	1.43	1.52
3	C	123	GLN	CA-CB	7.39	1.65	1.53
22	V	135	ARG	CD-NE	7.39	1.56	1.46
5	E	47	THR	C-N	7.39	1.41	1.33
18	L	345	ARG	CD-NE	7.39	1.56	1.46
27	N	515	ARG	CA-C	-7.39	1.43	1.52
4	d	54	ASP	CA-CB	7.38	1.62	1.52
14	7	116	VAL	CA-C	-7.38	1.43	1.52
26	Z	163	GLU	N-CA	-7.38	1.37	1.46
30	Q	287	THR	CA-C	-7.38	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	179	HIS	ND1-CE1	7.37	1.40	1.32
14	n	103	ARG	NE-CZ	7.37	1.41	1.33
24	X	11	ARG	CD-NE	7.37	1.56	1.46
23	T	252	GLU	C-N	7.37	1.43	1.33
30	Q	65	TYR	CA-C	-7.36	1.43	1.52
13	6	214	LYS	CA-C	-7.36	1.43	1.52
2	b	18	LEU	CA-C	-7.36	1.43	1.53
9	i	2	THR	CA-C	-7.36	1.43	1.52
12	5	115	VAL	CA-C	-7.34	1.43	1.52
1	a	130	VAL	C-N	7.33	1.42	1.33
11	k	37	GLN	CA-C	-7.33	1.43	1.52
12	l	178	TYR	CA-C	-7.33	1.43	1.52
8	h	147	SER	CA-C	-7.32	1.43	1.52
26	Z	265	LEU	N-CA	-7.32	1.37	1.46
26	Z	454	GLY	CA-C	7.32	1.60	1.52
2	b	207	ASP	CA-CB	7.32	1.66	1.53
13	6	32	ASP	CA-C	-7.32	1.46	1.53
24	X	54	GLU	CA-CB	7.32	1.67	1.53
1	a	5	ARG	CZ-NH1	7.31	1.43	1.32
16	I	205	PRO	N-CA	-7.31	1.38	1.47
6	f	50	ARG	CD-NE	7.31	1.56	1.46
14	n	103	ARG	CD-NE	7.30	1.56	1.46
27	N	614	ASN	N-CA	-7.30	1.36	1.46
7	g	78	ILE	CA-CB	7.29	1.58	1.54
9	i	174	ASP	CA-CB	7.29	1.65	1.53
18	L	103	GLN	C-N	7.29	1.43	1.33
1	a	72	MET	CA-C	-7.29	1.43	1.52
6	f	173	ARG	NE-CZ	7.29	1.41	1.33
27	N	163	LEU	CA-C	-7.28	1.42	1.52
7	g	113	GLY	CA-C	-7.27	1.44	1.52
3	C	162	ILE	N-CA	-7.26	1.38	1.46
5	e	201	GLU	N-CA	-7.26	1.36	1.46
27	N	15	GLU	CG-CD	-7.26	1.33	1.52
12	l	167	ARG	CZ-NH1	7.26	1.43	1.32
33	O	291	ILE	CB-CG1	-7.26	1.39	1.53
28	S	193	THR	CA-C	-7.25	1.43	1.52
27	N	859	ASN	CA-CB	7.25	1.64	1.53
10	j	51	GLY	CA-C	-7.25	1.45	1.52
26	Z	438	LYS	CA-CB	7.24	1.65	1.53
2	b	138	GLY	N-CA	-7.24	1.37	1.45
14	n	31	GLY	CA-C	-7.24	1.42	1.52
33	O	128	LEU	CA-C	-7.24	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	103	ASN	CA-C	-7.23	1.43	1.52
26	Z	297	VAL	N-CA	7.23	1.55	1.46
17	K	73	ARG	CD-NE	7.23	1.56	1.46
28	S	369	GLN	CA-C	-7.23	1.43	1.52
26	Z	961	GLU	CA-C	-7.22	1.44	1.52
27	N	493	GLY	C-N	7.22	1.44	1.33
8	h	174	ARG	CD-NE	7.21	1.56	1.46
27	N	397	SER	CA-C	-7.21	1.43	1.52
16	I	244	PHE	C-O	-7.21	1.15	1.24
30	Q	80	HIS	ND1-CE1	7.21	1.39	1.32
3	c	185	VAL	CA-C	-7.21	1.43	1.52
24	X	15	CYS	N-CA	-7.21	1.36	1.46
5	E	161	ALA	N-CA	-7.20	1.37	1.46
7	g	87	ARG	NE-CZ	7.19	1.41	1.33
26	Z	728	LYS	CA-C	7.19	1.62	1.52
2	B	99	ARG	NE-CZ	7.19	1.41	1.33
30	Q	164	GLU	CA-C	-7.18	1.42	1.52
27	N	474	SER	CA-CB	7.18	1.64	1.53
5	E	230	GLU	N-CA	-7.18	1.37	1.46
22	V	187	ALA	CA-C	-7.18	1.43	1.52
28	S	343	LEU	N-CA	-7.18	1.40	1.46
22	V	42	ARG	CA-C	-7.18	1.43	1.52
27	N	801	THR	CA-C	-7.18	1.43	1.52
5	e	84	ALA	CA-CB	7.17	1.64	1.53
29	P	172	GLU	CA-C	7.17	1.62	1.52
2	B	223	GLY	C-N	7.17	1.43	1.33
17	K	267	SER	C-N	7.17	1.42	1.33
14	n	149	HIS	ND1-CE1	7.17	1.39	1.32
5	E	129	PRO	CA-C	-7.16	1.44	1.52
9	2	41	ILE	CA-C	-7.16	1.43	1.52
12	l	89	GLN	CA-C	-7.16	1.43	1.52
28	S	160	ARG	NE-CZ	7.15	1.41	1.33
9	2	64	GLU	N-CA	-7.15	1.37	1.46
5	E	162	LYS	C-N	7.14	1.43	1.33
27	N	873	ARG	NE-CZ	7.14	1.41	1.33
13	m	137	ARG	CD-NE	7.14	1.56	1.46
23	T	63	GLU	C-N	7.14	1.42	1.33
15	H	169	GLU	C-N	7.14	1.43	1.33
4	d	94	HIS	ND1-CE1	7.13	1.39	1.32
14	7	45	VAL	N-CA	-7.13	1.37	1.46
1	a	172	ASN	C-N	7.13	1.43	1.33
17	K	211	LEU	CA-C	-7.13	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	73	ARG	CZ-NH2	7.13	1.42	1.33
2	b	7	PHE	N-CA	-7.13	1.37	1.46
12	l	124	GLY	CA-C	-7.12	1.41	1.51
27	N	594	VAL	N-CA	-7.12	1.38	1.46
8	h	36	ARG	NE-CZ	7.12	1.40	1.33
27	N	149	GLU	CA-C	-7.11	1.44	1.52
6	F	163	ARG	CA-C	-7.11	1.44	1.53
7	g	111	ARG	CZ-NH2	7.11	1.42	1.33
22	V	187	ALA	CA-CB	7.10	1.64	1.53
26	Z	707	LYS	CA-C	-7.10	1.43	1.52
9	i	201	LYS	CA-C	7.10	1.61	1.52
21	W	181	LEU	CA-C	7.10	1.61	1.52
10	3	176	ARG	NE-CZ	7.10	1.40	1.33
27	N	395	ALA	N-CA	-7.10	1.41	1.47
9	2	25	ILE	CA-C	-7.10	1.44	1.52
6	f	56	SER	CA-CB	7.09	1.64	1.53
16	I	98	GLU	CA-C	-7.09	1.43	1.52
30	Q	108	PRO	N-CA	7.09	1.55	1.46
27	N	813	ARG	CD-NE	7.09	1.56	1.46
9	2	189	ASN	CA-C	-7.09	1.45	1.53
13	m	208	THR	CA-C	-7.08	1.43	1.52
28	S	347	HIS	ND1-CE1	7.08	1.39	1.32
1	A	186	ASN	N-CA	-7.08	1.37	1.46
19	M	429	SER	C-N	7.08	1.43	1.33
27	N	237	LEU	N-CA	-7.08	1.37	1.46
28	S	307	LEU	N-CA	-7.08	1.37	1.46
9	i	172	ASN	N-CA	-7.08	1.37	1.46
26	Z	790	MET	CA-C	-7.07	1.44	1.52
15	H	341	ASP	CA-CB	7.07	1.64	1.53
12	l	7	ARG	CD-NE	7.07	1.56	1.46
29	P	370	ASP	CA-CB	7.07	1.64	1.53
30	Q	377	LEU	CA-C	-7.07	1.43	1.52
28	S	431	VAL	C-N	7.06	1.42	1.33
33	O	39	PHE	CA-C	-7.06	1.43	1.52
14	n	85	GLU	CA-CB	7.06	1.58	1.53
3	c	91	ARG	NE-CZ	7.05	1.40	1.33
31	R	176	ARG	N-CA	7.05	1.54	1.46
27	N	233	ASN	CA-CB	7.05	1.64	1.53
19	M	345	ARG	CA-C	-7.05	1.43	1.52
13	m	213	ARG	CZ-NH2	7.05	1.42	1.33
17	K	380	GLY	CA-C	-7.04	1.43	1.52
2	b	160	LYS	CA-CB	7.04	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	194	ARG	NE-CZ	7.04	1.40	1.33
9	i	191	LEU	CA-C	-7.04	1.44	1.52
1	A	5	ARG	CA-C	-7.04	1.43	1.52
11	4	28	LEU	CA-C	-7.04	1.44	1.52
2	B	246	ARG	NE-CZ	7.04	1.40	1.33
6	f	42	HIS	CE1-NE2	-7.03	1.25	1.32
23	T	224	ARG	NE-CZ	7.03	1.40	1.33
13	m	89	ALA	N-CA	-7.03	1.37	1.46
22	V	173	THR	C-N	7.03	1.42	1.33
19	M	387	ASN	CA-CB	7.02	1.63	1.53
33	O	292	CYS	CA-C	-7.02	1.44	1.52
13	6	29	ASN	C-N	7.02	1.42	1.33
29	P	10	ASP	CA-CB	7.02	1.64	1.53
32	U	106	ILE	CA-CB	-7.02	1.45	1.54
5	E	150	ALA	CA-C	-7.01	1.44	1.52
16	I	263	LEU	N-CA	-7.01	1.37	1.46
6	f	24	ALA	C-O	-7.01	1.16	1.24
15	H	324	GLY	C-N	7.01	1.42	1.33
16	I	322	VAL	CA-C	-7.01	1.43	1.52
24	X	40	GLU	CA-CB	7.01	1.63	1.53
17	K	227	ALA	N-CA	-7.00	1.37	1.46
4	d	85	GLU	N-CA	-7.00	1.38	1.46
5	E	72	GLY	CA-C	-7.00	1.42	1.51
18	L	106	GLY	N-CA	-7.00	1.39	1.44
4	d	195	ARG	CZ-NH1	6.99	1.42	1.32
5	e	36	GLU	CA-C	-6.99	1.43	1.52
10	j	158	GLU	CA-C	-6.99	1.44	1.52
2	b	179	TRP	C-O	-6.99	1.15	1.23
19	M	431	SER	CA-C	-6.99	1.44	1.52
1	a	195	GLU	CA-CB	6.99	1.64	1.53
6	f	190	LYS	C-N	6.98	1.43	1.34
11	k	168	LEU	CA-C	-6.98	1.43	1.52
2	b	62	SER	N-CA	-6.97	1.37	1.46
5	e	239	GLU	CA-C	-6.97	1.43	1.52
14	7	206	LEU	CA-C	-6.97	1.44	1.52
16	I	330	LYS	CA-C	-6.97	1.44	1.52
12	l	208	ASN	N-CA	-6.97	1.37	1.46
19	M	359	GLN	CA-C	-6.97	1.43	1.52
17	K	396	ARG	CD-NE	6.97	1.56	1.46
29	P	298	SER	C-N	6.97	1.42	1.33
10	3	48	VAL	CA-C	-6.96	1.44	1.52
18	L	69	ARG	N-CA	-6.96	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	761	ILE	CA-C	-6.96	1.44	1.52
21	W	8	LEU	CA-C	-6.96	1.43	1.52
1	a	71	GLY	N-CA	-6.95	1.37	1.44
4	D	151	SER	C-N	6.95	1.42	1.33
5	e	112	ALA	CA-C	-6.95	1.43	1.52
16	I	130	VAL	CA-C	-6.95	1.43	1.53
8	h	41	ILE	CA-CB	6.95	1.62	1.54
12	l	64	ARG	N-CA	-6.95	1.38	1.46
21	W	190	ILE	N-CA	-6.95	1.37	1.46
20	J	94	TYR	CA-C	-6.95	1.44	1.52
2	b	208	THR	CA-C	-6.95	1.44	1.52
4	d	163	GLY	CA-C	-6.94	1.43	1.52
13	6	2	PHE	N-CA	-6.94	1.37	1.46
17	K	224	LYS	CA-C	-6.94	1.43	1.52
33	O	113	LYS	CA-C	-6.94	1.43	1.52
5	e	158	ARG	NE-CZ	6.94	1.40	1.33
32	U	249	VAL	CA-C	-6.94	1.44	1.52
6	f	206	THR	C-N	6.93	1.41	1.33
18	L	77	ARG	NE-CZ	6.93	1.40	1.33
28	S	211	ARG	NE-CZ	6.92	1.40	1.33
1	a	144	SER	C-N	6.92	1.42	1.33
21	W	80	GLN	N-CA	-6.92	1.38	1.46
27	N	912	GLU	N-CA	-6.92	1.36	1.46
30	Q	150	GLN	CA-CB	6.92	1.61	1.52
12	5	5	ALA	CA-C	-6.91	1.43	1.52
20	J	236	MET	C-O	-6.91	1.15	1.24
27	N	653	ARG	NE-CZ	6.91	1.40	1.33
1	a	49	LYS	CA-C	-6.91	1.44	1.52
11	k	149	ARG	CZ-NH1	6.90	1.42	1.32
7	g	120	THR	C-N	6.90	1.43	1.33
17	K	346	ARG	N-CA	-6.90	1.38	1.46
6	f	204	SER	CA-C	6.90	1.61	1.52
28	S	196	ARG	CA-C	-6.90	1.43	1.52
8	h	29	ARG	CZ-NH1	6.90	1.42	1.32
8	h	14	LEU	C-N	6.89	1.41	1.33
18	L	156	MET	C-N	6.89	1.42	1.33
7	g	81	GLY	CA-C	-6.89	1.44	1.52
21	W	17	ARG	NE-CZ	6.89	1.40	1.33
17	K	109	ILE	CA-C	-6.88	1.44	1.52
2	b	236	ARG	CZ-NH1	6.88	1.42	1.32
16	I	145	CYS	CA-C	-6.88	1.43	1.53
18	L	261	ARG	CA-C	6.88	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	211	ILE	CA-CB	-6.88	1.47	1.54
27	N	786	ARG	CZ-NH1	6.88	1.42	1.32
29	P	26	SER	CA-CB	6.88	1.64	1.53
12	l	40	PHE	N-CA	-6.87	1.40	1.46
16	I	408	ARG	NE-CZ	6.87	1.40	1.33
19	M	42	ARG	NE-CZ	6.87	1.40	1.33
14	n	194	ASN	C-N	6.87	1.42	1.33
26	Z	948	TRP	C-N	6.87	1.42	1.33
5	E	104	LEU	N-CA	-6.87	1.38	1.46
19	M	195	GLU	C-O	-6.87	1.16	1.24
27	N	389	TYR	CA-C	-6.87	1.43	1.52
1	a	139	GLU	N-CA	-6.87	1.38	1.46
26	Z	95	THR	N-CA	-6.87	1.36	1.46
3	c	232	GLN	CA-CB	6.86	1.64	1.53
4	d	163	GLY	C-N	6.86	1.42	1.33
18	L	69	ARG	CD-NE	6.86	1.55	1.46
20	J	60	ASP	N-CA	-6.86	1.37	1.46
26	Z	928	ARG	NE-CZ	6.86	1.40	1.33
6	f	30	GLN	CA-CB	6.86	1.64	1.53
23	T	186	ARG	CD-NE	6.86	1.55	1.46
28	S	175	SER	CA-CB	6.86	1.64	1.53
15	H	346	ARG	CD-NE	6.85	1.55	1.46
19	M	342	ARG	CA-C	-6.85	1.44	1.53
1	a	3	TYR	N-CA	-6.85	1.38	1.46
13	m	90	ALA	CA-C	-6.85	1.43	1.52
27	N	681	ASN	C-N	6.85	1.43	1.33
11	k	67	TYR	CA-C	-6.85	1.44	1.52
5	E	114	ARG	NE-CZ	6.85	1.40	1.33
19	M	355	ASP	N-CA	-6.84	1.37	1.46
4	D	56	ARG	NE-CZ	6.84	1.40	1.33
27	N	241	LEU	N-CA	-6.84	1.38	1.46
1	a	50	VAL	CA-C	6.84	1.60	1.52
33	O	264	ASP	CA-C	-6.84	1.44	1.52
2	b	83	ARG	CD-NE	6.83	1.55	1.46
15	H	293	GLU	C-N	6.83	1.43	1.33
30	Q	128	GLU	N-CA	-6.83	1.38	1.46
10	j	202	ARG	NE-CZ	6.83	1.40	1.33
12	l	69	ARG	CA-C	-6.83	1.44	1.52
26	Z	249	MET	CA-C	-6.83	1.44	1.52
27	N	394	ARG	CD-NE	6.83	1.55	1.46
33	O	266	PHE	CA-C	-6.83	1.44	1.52
33	O	366	MET	C-N	6.83	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	213	LEU	CA-C	-6.82	1.44	1.52
16	I	375	VAL	C-O	6.82	1.31	1.23
2	B	220	ASP	CA-C	-6.82	1.44	1.52
12	5	12	ILE	CA-C	6.82	1.60	1.52
14	7	13	SER	CA-C	-6.82	1.43	1.52
4	d	236	GLN	C-N	6.82	1.43	1.34
18	L	417	LYS	CA-C	-6.82	1.44	1.52
28	S	134	ILE	N-CA	-6.81	1.38	1.46
11	k	105	GLY	C-N	6.81	1.42	1.33
22	V	273	ARG	CA-C	-6.81	1.44	1.52
23	T	36	LYS	CA-C	-6.81	1.44	1.52
26	Z	820	ALA	CA-C	-6.81	1.44	1.52
26	Z	17	GLN	CA-C	-6.81	1.44	1.52
18	L	361	PHE	N-CA	-6.81	1.38	1.46
23	T	159	LYS	N-CA	-6.80	1.38	1.46
4	d	42	LEU	C-N	6.80	1.38	1.33
23	T	138	ASP	CA-C	6.80	1.59	1.53
18	L	122	SER	C-N	6.80	1.43	1.34
30	Q	377	LEU	C-N	6.80	1.42	1.33
3	c	118	LYS	CA-C	-6.80	1.44	1.52
33	O	356	ARG	CD-NE	6.79	1.55	1.46
28	S	88	PHE	CA-C	-6.79	1.44	1.52
3	C	147	LEU	C-N	6.79	1.42	1.33
6	F	70	GLY	CA-C	-6.79	1.44	1.51
29	P	107	SER	CA-C	6.79	1.61	1.52
14	7	161	ARG	CD-NE	6.79	1.55	1.46
3	c	90	ALA	C-O	-6.79	1.15	1.24
5	E	106	GLN	N-CA	-6.78	1.38	1.46
16	I	167	MET	CA-C	-6.78	1.43	1.52
4	d	42	LEU	CB-CG	6.78	1.67	1.53
26	Z	295	ARG	NE-CZ	6.78	1.40	1.33
10	j	170	LEU	CA-CB	6.78	1.64	1.53
27	N	310	ASP	N-CA	-6.78	1.37	1.46
26	Z	238	ASP	CA-C	-6.77	1.43	1.52
10	j	128	CYS	CA-C	-6.77	1.44	1.52
28	S	160	ARG	CZ-NH2	6.77	1.42	1.33
6	f	17	ARG	NE-CZ	6.77	1.40	1.33
11	k	4	ILE	N-CA	-6.77	1.38	1.46
1	a	65	CYS	N-CA	-6.77	1.38	1.46
19	M	120	LYS	CA-C	-6.76	1.44	1.52
20	J	162	GLU	C-N	6.76	1.42	1.33
26	Z	326	VAL	CA-CB	-6.76	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	221	PHE	CA-C	-6.76	1.43	1.52
23	T	117	ASN	CA-C	-6.76	1.44	1.53
5	e	55	SER	C-N	6.75	1.41	1.33
11	k	191	GLN	C-N	6.75	1.41	1.33
4	D	16	PHE	CA-C	-6.75	1.44	1.52
7	G	75	SER	C-N	6.75	1.41	1.33
1	A	65	CYS	CA-CB	6.75	1.61	1.53
3	C	151	ASN	N-CA	-6.75	1.38	1.45
1	a	7	ILE	C-N	6.74	1.42	1.33
9	2	35	HIS	ND1-CE1	6.74	1.39	1.32
27	N	629	CYS	C-O	6.74	1.32	1.23
17	K	238	ASN	CA-C	-6.74	1.44	1.52
15	H	224	VAL	N-CA	-6.74	1.38	1.46
12	l	185	TRP	CA-CB	6.73	1.64	1.53
5	E	192	VAL	N-CA	-6.73	1.38	1.46
14	n	6	VAL	CA-C	-6.73	1.44	1.52
2	B	139	HIS	ND1-CE1	6.73	1.39	1.32
1	A	189	SER	N-CA	-6.73	1.37	1.46
4	d	162	ILE	N-CA	-6.72	1.39	1.46
7	g	23	ALA	C-N	6.72	1.42	1.33
5	E	30	ILE	CA-CB	-6.72	1.46	1.54
18	L	404	ARG	CA-C	6.72	1.61	1.52
3	c	41	ASP	N-CA	-6.72	1.38	1.46
9	i	78	SER	C-N	6.71	1.42	1.33
28	S	338	MET	CA-C	-6.71	1.43	1.52
25	Y	85	LYS	N-CA	-6.71	1.38	1.46
3	c	93	HIS	CA-C	-6.71	1.44	1.52
31	R	245	SER	N-CA	-6.71	1.37	1.45
26	Z	844	ALA	C-N	6.71	1.42	1.33
4	d	130	SER	C-N	6.71	1.43	1.33
29	P	44	LYS	CA-CB	6.71	1.62	1.53
30	Q	63	GLN	C-N	6.71	1.43	1.33
3	c	178	ASP	CA-C	-6.70	1.43	1.52
9	i	186	TYR	CA-CB	6.70	1.62	1.53
9	i	38	SER	CA-C	6.70	1.58	1.52
23	T	40	LEU	C-O	-6.70	1.16	1.24
24	X	93	SER	CA-C	-6.70	1.45	1.53
1	a	183	ASP	N-CA	-6.70	1.38	1.46
3	c	49	ARG	CZ-NH2	6.70	1.42	1.33
1	A	188	GLU	N-CA	-6.70	1.38	1.46
4	d	41	VAL	CA-C	-6.70	1.44	1.52
5	e	221	LYS	CA-C	-6.70	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	12	ILE	C-N	6.70	1.41	1.33
4	D	9	PHE	CA-C	-6.70	1.44	1.52
21	W	40	LYS	CA-C	-6.70	1.44	1.52
22	V	27	VAL	N-CA	6.69	1.54	1.46
9	i	207	ARG	NE-CZ	6.69	1.40	1.33
30	Q	11	ALA	CA-C	-6.69	1.44	1.52
32	U	121	LEU	CA-C	-6.69	1.44	1.52
12	l	151	GLU	CA-C	-6.68	1.44	1.52
1	a	89	LYS	C-O	-6.68	1.16	1.24
19	M	169	ALA	C-N	6.67	1.42	1.33
33	O	37	LEU	CA-C	-6.67	1.44	1.52
4	d	15	ILE	CA-C	-6.67	1.45	1.52
14	n	15	LYS	CA-C	-6.67	1.44	1.52
19	M	132	VAL	C-N	6.67	1.42	1.33
26	Z	239	GLU	N-CA	-6.67	1.38	1.46
3	c	48	GLU	CA-C	-6.66	1.44	1.52
28	S	457	PRO	CA-C	-6.66	1.41	1.52
26	Z	968	ASP	CA-C	-6.66	1.44	1.52
24	X	27	ILE	CA-CB	-6.66	1.48	1.54
26	Z	622	HIS	CA-C	-6.66	1.44	1.52
28	S	269	GLU	CA-C	-6.66	1.44	1.52
7	G	141	GLY	CA-C	-6.65	1.43	1.52
23	T	128	TYR	N-CA	-6.65	1.38	1.46
28	S	199	GLU	CA-C	-6.65	1.44	1.52
29	P	202	LYS	CA-C	-6.65	1.44	1.52
33	O	227	ILE	CA-C	6.65	1.59	1.53
12	l	106	ARG	NE-CZ	6.65	1.40	1.33
27	N	901	GLY	C-N	6.65	1.41	1.33
14	n	128	ARG	CA-C	-6.65	1.44	1.52
1	A	60	VAL	CA-C	-6.65	1.44	1.52
20	J	61	GLU	CA-C	-6.64	1.44	1.52
5	e	125	LEU	CA-CB	6.64	1.64	1.53
15	H	90	ARG	CZ-NH2	6.64	1.42	1.33
22	V	239	ALA	C-N	6.64	1.42	1.33
5	e	208	ASN	CA-C	6.63	1.61	1.53
14	n	4	PRO	CA-C	-6.63	1.45	1.52
8	h	41	ILE	CA-C	-6.63	1.44	1.52
11	4	23	ARG	NE-CZ	6.63	1.40	1.33
20	J	311	ASP	N-CA	6.63	1.54	1.46
16	I	168	VAL	C-N	6.62	1.41	1.33
1	a	111	ARG	CD-NE	6.62	1.55	1.46
2	b	224	TYR	N-CA	-6.62	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	351	ARG	CZ-NH2	6.62	1.42	1.33
13	m	79	HIS	ND1-CE1	6.62	1.39	1.32
1	A	26	THR	CA-C	-6.61	1.44	1.52
5	E	78	ARG	CD-NE	6.61	1.55	1.46
15	H	51	GLN	CA-CB	6.61	1.63	1.53
16	I	405	ARG	N-CA	6.61	1.54	1.46
27	N	353	LEU	CA-C	-6.61	1.44	1.52
30	Q	76	GLU	CA-CB	6.61	1.64	1.53
29	P	344	ARG	CA-C	-6.61	1.44	1.52
31	R	284	ALA	CA-C	-6.61	1.44	1.52
27	N	340	HIS	ND1-CE1	6.61	1.39	1.32
23	T	144	TYR	CA-CB	6.60	1.63	1.53
2	B	220	ASP	CA-CB	6.60	1.63	1.53
17	K	121	ARG	CZ-NH2	6.60	1.42	1.33
30	Q	107	VAL	CA-CB	-6.60	1.45	1.54
29	P	115	ARG	NE-CZ	6.60	1.40	1.33
32	U	11	ALA	N-CA	-6.60	1.36	1.45
4	D	8	ILE	N-CA	-6.60	1.38	1.46
1	a	126	ARG	CA-C	-6.59	1.46	1.52
21	W	117	PRO	C-N	6.59	1.41	1.33
17	K	155	ASP	N-CA	-6.59	1.36	1.46
27	N	498	ILE	C-N	6.59	1.42	1.33
28	S	86	SER	C-O	-6.59	1.16	1.24
15	H	300	THR	N-CA	-6.59	1.38	1.46
9	i	190	TYR	CA-C	6.58	1.61	1.52
16	I	171	MET	C-N	6.58	1.42	1.33
18	L	108	VAL	CA-C	-6.58	1.44	1.52
20	J	379	GLN	N-CA	6.58	1.54	1.46
14	n	224	ASP	CA-C	-6.58	1.44	1.52
27	N	34	GLN	CA-C	6.58	1.61	1.52
27	N	271	GLU	N-CA	-6.58	1.38	1.46
20	J	212	ARG	NE-CZ	6.58	1.40	1.33
14	n	170	VAL	CA-CB	-6.58	1.46	1.54
16	I	433	GLU	CA-C	-6.58	1.44	1.52
2	B	238	LEU	CA-C	-6.57	1.44	1.52
14	7	41	ARG	CD-NE	6.57	1.55	1.46
27	N	511	GLY	CA-C	-6.57	1.43	1.51
1	a	87	ARG	CZ-NH2	6.57	1.42	1.33
7	g	185	ALA	N-CA	-6.57	1.38	1.46
18	L	100	SER	CA-C	-6.57	1.44	1.52
26	Z	60	ASP	CA-CB	6.56	1.64	1.53
10	j	103	PHE	CA-C	-6.56	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	26	LYS	N-CA	-6.56	1.38	1.46
12	l	156	LEU	C-N	6.56	1.42	1.33
22	V	20	ARG	CZ-NH1	6.56	1.42	1.32
26	Z	601	VAL	CA-C	-6.56	1.44	1.52
26	Z	121	ILE	CA-C	-6.56	1.44	1.52
26	Z	214	HIS	N-CA	-6.56	1.38	1.46
8	l	56	ALA	C-N	6.56	1.42	1.33
15	H	354	ALA	N-CA	-6.56	1.38	1.46
6	f	25	LEU	CA-C	-6.55	1.43	1.52
32	U	7	LYS	CA-C	-6.55	1.44	1.52
3	C	103	GLU	CA-C	-6.55	1.44	1.52
7	g	82	ARG	CD-NE	6.55	1.55	1.46
9	i	192	THR	N-CA	-6.55	1.40	1.46
17	K	255	ARG	CD-NE	6.55	1.55	1.46
26	Z	205	LEU	CA-C	-6.55	1.44	1.52
32	U	19	LEU	CA-C	-6.55	1.44	1.52
27	N	529	GLN	CA-C	6.54	1.59	1.53
26	Z	292	ASP	N-CA	-6.54	1.38	1.46
3	c	124	HIS	ND1-CE1	6.54	1.39	1.32
6	f	145	GLU	CA-C	-6.54	1.44	1.52
22	V	204	HIS	ND1-CE1	6.54	1.39	1.32
27	N	135	SER	CA-C	-6.54	1.44	1.52
31	R	205	GLU	CA-CB	6.54	1.63	1.53
1	a	155	VAL	CA-C	6.53	1.60	1.52
6	f	38	ARG	NE-CZ	6.53	1.40	1.33
2	B	240	SER	N-CA	-6.53	1.38	1.46
7	g	42	VAL	N-CA	-6.53	1.38	1.46
11	k	182	LYS	CA-CB	6.53	1.65	1.53
25	Y	26	LYS	N-CA	-6.53	1.38	1.46
11	k	100	VAL	CA-C	-6.53	1.44	1.52
20	J	112	ARG	NE-CZ	6.53	1.40	1.33
24	X	85	ARG	NE-CZ	6.53	1.40	1.33
14	n	62	HIS	CD2-NE2	6.53	1.45	1.37
17	K	167	PRO	N-CA	-6.53	1.39	1.47
10	j	76	LYS	C-N	6.53	1.43	1.33
10	3	33	LEU	C-N	6.53	1.37	1.33
16	I	161	GLN	N-CA	-6.53	1.38	1.46
6	F	210	LEU	CA-CB	6.52	1.62	1.53
19	M	225	GLY	CA-C	-6.52	1.43	1.51
29	P	99	LYS	N-CA	-6.52	1.38	1.46
27	N	459	ASN	CA-C	-6.52	1.44	1.52
7	g	136	GLY	N-CA	-6.51	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	102	VAL	CA-CB	-6.51	1.46	1.54
11	k	107	TYR	CA-CB	6.51	1.62	1.53
15	H	153	ALA	CA-C	-6.51	1.44	1.52
19	M	216	LYS	N-CA	-6.51	1.38	1.46
30	Q	308	ASN	CA-C	-6.51	1.44	1.52
27	N	627	ILE	N-CA	-6.51	1.38	1.46
7	G	8	ASN	C-N	6.51	1.42	1.33
15	H	245	GLY	CA-C	-6.51	1.47	1.52
2	b	134	LEU	CA-C	-6.51	1.45	1.52
22	V	54	LEU	N-CA	-6.51	1.38	1.46
1	A	151	ALA	CA-C	-6.50	1.44	1.52
3	C	138	GLY	CA-C	6.50	1.58	1.52
4	D	82	ILE	C-N	6.50	1.42	1.33
31	R	60	ALA	C-O	-6.50	1.18	1.24
33	O	13	THR	CA-C	-6.50	1.44	1.52
14	n	182	ARG	CZ-NH1	6.50	1.41	1.32
14	n	41	ARG	NE-CZ	6.50	1.40	1.33
8	l	94	THR	CA-C	-6.50	1.46	1.53
14	7	137	TYR	CA-C	-6.50	1.44	1.52
20	J	313	LYS	C-N	6.50	1.41	1.33
30	Q	352	GLU	C-N	6.50	1.38	1.33
28	S	261	HIS	CB-CG	-6.49	1.41	1.50
3	c	26	GLU	CA-C	-6.49	1.44	1.52
26	Z	405	ASN	N-CA	-6.49	1.38	1.46
11	4	116	LEU	N-CA	-6.49	1.38	1.46
1	a	126	ARG	CD-NE	6.49	1.55	1.46
22	V	194	ARG	NE-CZ	6.49	1.40	1.33
8	h	84	GLU	CA-C	-6.49	1.44	1.52
30	Q	412	ALA	CA-C	-6.49	1.44	1.52
26	Z	843	ASP	CA-CB	6.49	1.63	1.53
16	I	118	ALA	N-CA	-6.48	1.37	1.45
13	m	204	ILE	CA-C	-6.48	1.44	1.52
13	6	221	ARG	CZ-NH2	6.48	1.41	1.33
32	U	226	LEU	CA-CB	6.48	1.63	1.53
26	Z	798	ARG	CZ-NH1	6.47	1.41	1.32
4	d	46	ARG	NE-CZ	6.47	1.40	1.33
16	I	343	ARG	CD-NE	6.47	1.55	1.46
22	V	116	CYS	CA-C	-6.47	1.44	1.52
26	Z	760	HIS	ND1-CE1	6.47	1.39	1.32
2	b	240	SER	N-CA	-6.47	1.38	1.46
6	f	100	ARG	CZ-NH2	6.46	1.41	1.33
13	m	98	TYR	N-CA	-6.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	200	GLN	N-CA	-6.46	1.38	1.46
29	P	15	GLN	CA-C	-6.46	1.44	1.52
16	I	291	ARG	CA-C	-6.46	1.45	1.52
4	d	138	PRO	C-N	6.46	1.42	1.33
8	h	169	SER	C-N	6.46	1.40	1.33
17	K	259	ARG	NE-CZ	6.46	1.40	1.33
15	H	273	ARG	CD-NE	6.46	1.55	1.46
9	i	13	VAL	N-CA	-6.46	1.38	1.46
3	C	57	GLU	CA-CB	6.46	1.61	1.52
33	O	222	LEU	CA-C	-6.46	1.44	1.52
20	J	313	LYS	CA-CB	6.46	1.66	1.53
29	P	196	ALA	N-CA	-6.46	1.38	1.46
5	e	154	GLY	C-N	6.45	1.42	1.33
15	H	78	PRO	N-CD	6.45	1.56	1.47
9	2	135	MET	C-N	6.45	1.42	1.33
16	I	385	ASP	N-CA	-6.45	1.37	1.46
2	B	218	ASN	CA-C	-6.45	1.47	1.52
7	G	126	ARG	CD-NE	6.45	1.55	1.46
10	3	78	GLU	CA-C	6.45	1.61	1.53
25	Y	86	ARG	CD-NE	6.45	1.55	1.46
26	Z	237	VAL	CA-CB	-6.45	1.47	1.54
16	I	274	ASN	C-N	6.45	1.42	1.33
28	S	214	MET	C-N	6.45	1.42	1.33
28	S	372	LEU	N-CA	-6.45	1.38	1.46
30	Q	13	ARG	CZ-NH1	6.45	1.41	1.32
6	F	165	GLN	CA-C	-6.44	1.44	1.52
14	7	210	LYS	CA-C	-6.44	1.44	1.52
5	e	114	ARG	CD-NE	6.44	1.55	1.46
6	f	4	ASN	CA-C	-6.44	1.44	1.52
21	W	161	VAL	N-CA	-6.44	1.38	1.46
4	d	95	ARG	CD-NE	6.43	1.55	1.46
26	Z	616	LEU	N-CA	-6.43	1.38	1.46
28	S	459	GLN	N-CA	-6.43	1.38	1.46
4	d	170	ARG	CZ-NH2	6.43	1.41	1.33
9	i	32	ALA	N-CA	-6.43	1.37	1.46
26	Z	593	HIS	ND1-CE1	6.43	1.39	1.32
33	O	336	LEU	CA-C	-6.43	1.44	1.52
17	K	327	ALA	N-CA	-6.43	1.38	1.46
1	a	122	ARG	CA-C	-6.42	1.44	1.52
19	M	389	ALA	CA-C	-6.42	1.44	1.52
27	N	443	LEU	C-O	-6.42	1.15	1.24
28	S	459	GLN	C-N	6.42	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	54	SER	CA-C	-6.42	1.44	1.52
6	f	218	ASP	C-N	6.42	1.39	1.33
6	f	115	ALA	CA-C	-6.42	1.44	1.52
30	Q	256	GLU	CA-C	6.42	1.61	1.52
12	l	61	SER	C-N	6.41	1.42	1.33
10	3	62	LEU	CA-C	-6.41	1.44	1.52
29	P	54	SER	C-N	6.41	1.42	1.33
30	Q	309	ARG	CA-C	-6.41	1.44	1.52
6	f	163	ARG	CA-C	-6.41	1.45	1.53
3	c	5	TYR	C-N	6.41	1.42	1.33
3	c	175	LEU	C-N	6.41	1.42	1.34
9	i	85	GLN	N-CA	-6.41	1.38	1.46
29	P	157	ALA	CA-C	-6.41	1.44	1.52
8	h	132	THR	CA-C	-6.41	1.44	1.52
7	g	115	TYR	C-O	-6.40	1.16	1.24
12	l	176	ASN	CA-C	-6.40	1.45	1.52
4	D	175	LYS	N-CA	6.40	1.54	1.46
23	T	184	ALA	C-N	6.40	1.41	1.33
27	N	536	ILE	N-CA	-6.40	1.38	1.46
29	P	29	GLN	C-N	6.40	1.42	1.33
32	U	151	GLU	CA-C	-6.40	1.45	1.52
10	j	144	GLN	CA-C	-6.40	1.44	1.52
6	F	129	VAL	N-CA	-6.40	1.38	1.46
27	N	28	ILE	N-CA	-6.40	1.38	1.46
7	G	135	GLY	N-CA	-6.39	1.39	1.45
17	K	207	ARG	CD-NE	6.39	1.55	1.46
18	L	327	THR	C-N	6.38	1.42	1.33
27	N	796	VAL	N-CA	-6.38	1.39	1.46
6	F	173	ARG	NE-CZ	6.38	1.40	1.33
18	L	216	LYS	CA-C	-6.38	1.44	1.52
28	S	314	ASN	CA-C	-6.38	1.44	1.52
6	F	2	ARG	C-N	6.38	1.40	1.32
17	K	117	SER	CA-C	-6.38	1.45	1.52
23	T	40	LEU	C-N	6.38	1.41	1.33
27	N	788	TYR	CA-C	-6.38	1.44	1.52
32	U	132	LEU	CA-C	-6.38	1.44	1.52
2	B	19	GLY	CA-C	-6.37	1.45	1.52
16	I	177	PRO	CA-C	-6.37	1.44	1.52
12	5	121	ARG	CA-C	-6.37	1.45	1.52
27	N	270	LEU	CA-CB	6.37	1.63	1.53
29	P	374	SER	C-O	-6.37	1.16	1.24
7	G	186	ARG	CZ-NH2	6.37	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	51	ARG	C-N	6.37	1.39	1.33
31	R	296	LEU	N-CA	-6.37	1.38	1.46
5	e	69	ALA	CA-C	-6.36	1.45	1.52
7	G	165	ARG	CD-NE	6.36	1.55	1.46
26	Z	217	GLU	CA-C	-6.36	1.45	1.52
28	S	469	ASN	N-CA	-6.36	1.38	1.46
4	d	179	ARG	CZ-NH1	6.36	1.41	1.32
16	I	362	LEU	N-CA	-6.36	1.38	1.46
11	k	96	ARG	CA-C	-6.36	1.45	1.52
14	n	109	PRO	N-CA	-6.36	1.39	1.47
20	J	156	GLN	CA-CB	6.36	1.63	1.53
23	T	132	HIS	ND1-CE1	6.35	1.39	1.32
4	D	109	ARG	CD-NE	6.35	1.55	1.46
26	Z	709	LYS	CA-C	-6.35	1.44	1.52
6	f	114	LYS	CA-CB	6.35	1.63	1.53
6	f	39	SER	N-CA	-6.34	1.38	1.46
6	f	96	LEU	CA-CB	6.34	1.63	1.53
31	R	329	PHE	CA-CB	6.34	1.63	1.53
9	i	105	PRO	N-CA	-6.34	1.39	1.47
14	n	96	LEU	N-CA	-6.34	1.38	1.46
23	T	106	ILE	CA-C	-6.34	1.44	1.52
22	V	231	GLU	CA-CB	6.34	1.63	1.53
22	V	144	ILE	CA-C	-6.34	1.44	1.52
26	Z	303	ASP	CA-C	6.34	1.60	1.52
2	b	246	ARG	NE-CZ	6.33	1.40	1.33
9	i	204	LYS	N-CA	-6.33	1.38	1.46
22	V	89	ALA	N-CA	-6.33	1.38	1.46
26	Z	60	ASP	N-CA	-6.33	1.38	1.46
8	l	194	GLU	C-N	6.33	1.42	1.33
26	Z	730	ALA	C-N	6.33	1.41	1.33
29	P	220	TYR	CA-CB	6.33	1.63	1.53
30	Q	141	LEU	N-CA	-6.33	1.38	1.46
6	f	173	ARG	CD-NE	6.33	1.55	1.46
26	Z	90	LYS	C-N	6.33	1.42	1.33
15	H	409	ARG	N-CA	-6.33	1.38	1.46
28	S	121	VAL	N-CA	-6.33	1.39	1.46
1	a	80	ASP	N-CA	-6.33	1.38	1.46
2	B	39	ALA	N-CA	-6.33	1.37	1.45
2	B	245	ASP	N-CA	-6.33	1.38	1.46
30	Q	220	LEU	CA-CB	6.33	1.63	1.53
26	Z	136	ARG	NE-CZ	6.32	1.40	1.33
17	K	236	ARG	NE-CZ	6.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	605	ILE	C-N	6.32	1.40	1.34
29	P	232	ARG	CD-NE	6.32	1.55	1.46
26	Z	826	ARG	NE-CZ	6.32	1.40	1.33
26	Z	88	PRO	C-N	6.32	1.42	1.33
2	b	189	ILE	CA-CB	-6.32	1.47	1.54
5	E	124	ARG	CD-NE	6.31	1.55	1.46
11	4	149	ARG	CA-C	6.31	1.58	1.52
27	N	565	ASN	CA-C	-6.31	1.44	1.52
27	N	579	SER	C-N	6.31	1.42	1.33
29	P	363	LEU	CA-C	-6.31	1.44	1.52
13	6	28	ARG	CZ-NH2	6.31	1.41	1.33
12	l	27	ALA	N-CA	-6.31	1.38	1.46
12	5	208	ASN	CA-CB	6.31	1.64	1.53
2	B	23	TYR	N-CA	-6.31	1.38	1.46
29	P	267	PHE	C-N	6.31	1.42	1.33
8	h	32	ASP	N-CA	-6.31	1.39	1.46
9	2	98	LEU	C-N	6.31	1.41	1.33
27	N	874	ILE	C-N	6.31	1.42	1.33
2	b	10	THR	N-CA	-6.30	1.38	1.46
7	g	233	GLN	N-CA	-6.30	1.38	1.46
2	B	106	PRO	N-CA	-6.30	1.39	1.47
14	n	187	ARG	CZ-NH1	6.30	1.41	1.32
27	N	646	LYS	C-N	6.30	1.42	1.33
2	B	210	GLU	CA-C	-6.30	1.45	1.52
13	6	40	GLU	N-CA	-6.30	1.37	1.46
18	L	210	VAL	CA-C	-6.30	1.44	1.52
18	L	321	THR	N-CA	-6.29	1.38	1.46
32	U	70	HIS	ND1-CE1	6.29	1.38	1.32
1	a	225	PHE	N-CA	-6.29	1.38	1.45
10	j	168	GLN	C-O	-6.29	1.16	1.24
28	S	227	ASN	N-CA	-6.29	1.38	1.46
32	U	131	GLY	CA-C	-6.29	1.46	1.52
21	W	190	ILE	CA-C	-6.28	1.44	1.52
26	Z	214	HIS	CG-CD2	6.28	1.42	1.35
16	I	422	ARG	CD-NE	6.28	1.55	1.46
27	N	606	VAL	N-CA	-6.28	1.38	1.46
27	N	879	SER	CA-C	-6.28	1.44	1.52
28	S	279	ILE	N-CA	-6.28	1.39	1.46
4	d	104	VAL	CA-CB	-6.28	1.46	1.54
31	R	114	ASN	CA-CB	6.28	1.64	1.53
32	U	192	ASN	N-CA	-6.28	1.38	1.46
9	i	159	ILE	N-CA	-6.28	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	164	PRO	N-CA	-6.28	1.39	1.47
15	H	172	MET	C-N	6.28	1.41	1.33
5	e	50	LEU	C-N	6.27	1.42	1.33
27	N	544	GLU	N-CA	-6.27	1.38	1.46
13	m	38	ARG	CD-NE	6.27	1.55	1.46
19	M	355	ASP	CA-C	-6.27	1.44	1.52
26	Z	829	GLN	CA-CB	6.27	1.63	1.53
14	n	161	ARG	CZ-NH1	6.27	1.41	1.32
8	l	142	PHE	CA-CB	6.27	1.63	1.53
14	7	109	PRO	N-CA	-6.27	1.39	1.46
32	U	248	ASP	N-CA	-6.27	1.38	1.46
1	a	56	ASP	CA-C	6.26	1.60	1.52
9	i	169	SER	CA-C	-6.26	1.44	1.53
21	W	43	SER	CA-C	-6.26	1.44	1.52
19	M	408	SER	CA-C	-6.26	1.44	1.52
20	J	100	LYS	C-O	-6.26	1.16	1.24
29	P	380	ILE	C-N	6.26	1.42	1.33
4	d	235	GLU	N-CA	-6.26	1.38	1.46
11	k	118	GLN	N-CA	-6.26	1.38	1.46
10	j	155	PRO	CA-CB	6.26	1.62	1.53
15	H	86	GLY	CA-C	-6.26	1.44	1.52
16	I	361	ILE	CA-C	6.26	1.60	1.52
27	N	533	ASP	N-CA	-6.26	1.38	1.46
30	Q	276	ASP	CA-C	-6.26	1.44	1.52
11	k	8	ARG	CZ-NH1	6.25	1.41	1.32
27	N	88	ARG	CZ-NH1	6.25	1.41	1.32
8	h	178	LEU	CA-CB	6.25	1.61	1.53
10	j	169	ALA	N-CA	-6.25	1.39	1.46
3	C	105	ILE	CA-C	6.25	1.60	1.52
6	F	68	HIS	ND1-CE1	6.25	1.38	1.32
26	Z	298	PHE	CA-C	-6.25	1.44	1.52
11	k	83	PHE	N-CA	-6.25	1.39	1.46
4	D	138	PRO	CA-C	-6.25	1.45	1.52
26	Z	779	ALA	CA-C	-6.25	1.44	1.52
16	I	188	GLU	C-O	-6.25	1.16	1.24
11	k	50	ALA	C-N	6.24	1.42	1.33
27	N	757	THR	C-N	6.24	1.41	1.33
14	n	9	THR	C-N	6.24	1.41	1.33
24	X	109	LEU	C-N	6.24	1.41	1.33
31	R	395	ASN	CA-CB	6.24	1.62	1.53
2	b	115	ALA	C-N	6.24	1.42	1.33
8	h	29	ARG	CD-NE	6.24	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	98	PHE	CA-C	-6.24	1.45	1.52
9	2	188	ARG	N-CA	-6.24	1.38	1.46
11	k	104	ILE	C-N	6.23	1.38	1.33
12	5	184	GLY	CA-C	-6.23	1.44	1.52
14	n	164	ASP	N-CA	-6.23	1.37	1.46
27	N	625	LEU	N-CA	-6.23	1.38	1.46
16	I	346	ARG	CD-NE	6.23	1.54	1.46
26	Z	828	ALA	C-N	6.23	1.42	1.33
2	B	183	LEU	N-CA	-6.23	1.38	1.46
18	L	161	ARG	C-O	-6.23	1.16	1.23
21	W	39	ALA	CA-C	6.23	1.60	1.52
31	R	115	GLU	C-N	6.23	1.41	1.33
2	b	243	ILE	N-CA	-6.23	1.39	1.46
14	n	202	LYS	C-N	6.22	1.42	1.33
12	5	80	SER	C-N	6.22	1.42	1.33
27	N	303	LEU	CA-C	-6.22	1.44	1.52
11	k	66	LEU	C-N	6.22	1.42	1.33
13	m	218	GLU	CA-C	6.22	1.60	1.52
19	M	53	HIS	CA-CB	6.22	1.63	1.53
27	N	162	ARG	CD-NE	6.22	1.54	1.46
27	N	490	LEU	CA-C	6.22	1.61	1.52
33	O	320	PRO	C-N	6.22	1.42	1.33
12	5	89	GLN	N-CA	-6.22	1.38	1.46
4	D	70	VAL	CA-C	-6.22	1.45	1.52
5	E	111	LEU	CA-C	-6.22	1.44	1.52
16	I	229	LYS	CA-C	-6.22	1.45	1.52
13	m	83	LYS	CA-C	-6.21	1.44	1.52
10	3	3	PRO	N-CA	-6.21	1.39	1.47
26	Z	136	ARG	CZ-NH1	6.21	1.41	1.32
5	e	56	ILE	N-CA	-6.21	1.39	1.46
15	H	289	ARG	CA-C	-6.21	1.44	1.52
28	S	219	LYS	CA-C	-6.21	1.44	1.52
5	e	158	ARG	CD-NE	6.21	1.54	1.46
8	h	146	MET	CA-C	-6.21	1.45	1.52
9	i	151	ALA	C-N	6.21	1.41	1.33
22	V	101	ASP	CA-CB	6.21	1.63	1.53
2	B	4	ARG	CD-NE	6.20	1.54	1.46
3	C	136	TYR	N-CA	-6.20	1.38	1.46
23	T	149	ASP	CA-C	-6.20	1.44	1.52
20	J	141	LYS	CA-C	-6.20	1.44	1.52
22	V	303	VAL	C-N	6.20	1.42	1.33
7	g	101	THR	CA-C	-6.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	174	LEU	CA-C	-6.20	1.44	1.52
10	j	175	ASP	C-N	6.20	1.42	1.33
10	j	97	ARG	CA-C	-6.20	1.45	1.52
5	e	233	LYS	C-N	6.20	1.42	1.34
14	n	33	LEU	CA-CB	6.20	1.61	1.53
5	E	213	CYS	N-CA	-6.19	1.38	1.45
4	D	117	ARG	NE-CZ	6.19	1.39	1.33
7	G	116	VAL	N-CA	-6.19	1.39	1.46
13	6	91	ARG	NE-CZ	6.19	1.39	1.33
21	W	98	LEU	CA-CB	6.19	1.63	1.53
2	b	87	ASP	CA-C	-6.19	1.44	1.52
8	h	84	GLU	C-O	-6.19	1.17	1.24
12	l	189	GLY	CA-C	6.19	1.58	1.52
3	c	11	ILE	CA-C	-6.19	1.45	1.52
10	j	76	LYS	C-O	-6.19	1.16	1.24
18	L	324	ILE	CA-C	-6.19	1.45	1.52
26	Z	410	THR	C-N	6.19	1.42	1.33
12	l	131	SER	C-N	6.19	1.41	1.33
18	L	258	GLU	C-N	6.19	1.42	1.33
4	d	184	ALA	C-N	6.18	1.41	1.33
6	f	65	CYS	N-CA	-6.18	1.38	1.46
2	B	123	GLN	N-CA	-6.18	1.38	1.46
30	Q	99	THR	C-N	6.18	1.42	1.33
30	Q	381	ILE	N-CA	-6.18	1.39	1.46
12	l	45	MET	CA-CB	6.18	1.63	1.53
10	3	73	TYR	C-N	6.18	1.42	1.33
2	b	128	ARG	CD-NE	6.18	1.54	1.46
26	Z	413	ASP	N-CA	-6.18	1.38	1.46
11	k	10	GLN	C-N	6.18	1.43	1.33
28	S	466	LYS	N-CA	-6.18	1.38	1.46
7	g	111	ARG	NE-CZ	6.18	1.39	1.33
9	i	188	ARG	CZ-NH1	6.18	1.41	1.32
10	j	202	ARG	N-CA	-6.18	1.38	1.46
6	f	201	ARG	CD-NE	6.17	1.54	1.46
14	n	27	LEU	C-N	6.17	1.42	1.33
7	g	186	ARG	NE-CZ	6.17	1.39	1.33
20	J	106	ASP	C-N	6.17	1.41	1.33
3	c	84	GLU	CA-C	-6.17	1.44	1.52
17	K	59	GLU	CA-C	6.17	1.60	1.52
17	K	138	ALA	CA-C	-6.17	1.45	1.52
7	G	92	ALA	C-N	6.17	1.42	1.33
15	H	361	LEU	N-CA	6.17	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	1	ASP	N-CA	6.17	1.57	1.46
18	L	392	ARG	CZ-NH1	6.17	1.41	1.32
28	S	318	CYS	C-N	6.17	1.42	1.33
33	O	392	TRP	CA-C	-6.17	1.46	1.52
17	K	260	LEU	N-CA	-6.16	1.38	1.46
32	U	60	GLU	C-N	6.16	1.42	1.33
30	Q	200	ALA	C-O	6.16	1.31	1.24
1	a	154	TYR	C-N	6.15	1.39	1.33
6	F	106	ARG	CA-C	-6.15	1.44	1.52
7	g	82	ARG	NE-CZ	6.15	1.39	1.33
14	n	156	ARG	NE-CZ	6.15	1.39	1.33
27	N	36	TRP	N-CA	-6.15	1.38	1.46
27	N	810	ALA	C-N	6.15	1.42	1.33
8	h	81	VAL	CA-CB	-6.15	1.46	1.54
33	O	178	TYR	N-CA	-6.15	1.39	1.46
1	a	12	PRO	N-CA	-6.15	1.39	1.47
7	G	111	ARG	NE-CZ	6.15	1.39	1.33
12	5	173	GLY	CA-C	-6.15	1.47	1.53
31	R	131	ALA	N-CA	-6.15	1.39	1.46
32	U	193	GLN	N-CA	6.15	1.53	1.46
32	U	267	VAL	CA-CB	-6.15	1.46	1.54
21	W	119	SER	C-N	6.15	1.42	1.33
8	h	55	ILE	CA-C	-6.14	1.45	1.52
18	L	213	LYS	CA-CB	6.14	1.62	1.53
18	L	209	ARG	N-CA	-6.14	1.39	1.46
30	Q	357	VAL	CA-C	6.14	1.59	1.52
26	Z	832	ARG	NE-CZ	6.14	1.39	1.33
6	f	185	PRO	CA-CB	6.14	1.62	1.53
15	H	257	THR	C-N	6.14	1.42	1.33
27	N	164	ASP	CA-C	-6.14	1.44	1.52
28	S	478	SER	CA-C	-6.14	1.44	1.52
29	P	115	ARG	C-N	6.14	1.41	1.33
4	d	232	THR	N-CA	-6.14	1.39	1.46
14	n	38	GLY	C-N	6.14	1.40	1.33
2	b	139	HIS	C-O	-6.13	1.16	1.23
12	l	102	CYS	N-CA	-6.13	1.38	1.46
13	m	101	ARG	NE-CZ	6.13	1.39	1.33
3	C	59	ASP	CA-C	-6.13	1.45	1.52
27	N	571	LEU	CA-C	-6.13	1.45	1.52
4	d	25	VAL	C-N	6.13	1.42	1.33
9	i	85	GLN	CA-CB	6.13	1.63	1.53
9	2	62	ASN	N-CA	-6.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	175	VAL	CA-C	-6.13	1.45	1.52
24	X	22	ARG	NE-CZ	6.13	1.39	1.33
9	i	71	SER	CA-C	-6.12	1.45	1.53
20	J	63	ARG	CZ-NH2	6.12	1.41	1.33
6	f	205	LEU	C-N	6.12	1.38	1.33
7	g	224	HIS	C-O	6.12	1.31	1.24
12	l	64	ARG	CD-NE	6.12	1.54	1.46
15	H	438	ALA	CA-CB	6.12	1.61	1.53
26	Z	533	VAL	CA-CB	-6.12	1.46	1.54
1	a	40	ASP	CA-C	-6.12	1.44	1.52
2	b	75	TYR	CA-C	-6.12	1.44	1.52
11	k	89	ALA	CA-C	-6.12	1.45	1.52
6	F	188	LEU	CA-C	-6.12	1.45	1.52
33	O	372	GLU	N-CA	-6.12	1.39	1.46
26	Z	618	GLN	N-CA	-6.12	1.39	1.46
22	V	182	LYS	CA-C	-6.12	1.45	1.52
26	Z	962	ARG	CA-C	-6.12	1.44	1.52
3	c	229	PHE	C-N	6.11	1.42	1.33
20	J	335	MET	CA-CB	6.11	1.63	1.53
27	N	687	THR	C-N	6.11	1.41	1.33
9	i	85	GLN	CA-C	-6.11	1.45	1.52
9	i	196	ARG	CD-NE	6.11	1.54	1.46
8	h	62	HIS	ND1-CE1	6.11	1.38	1.32
7	G	214	TRP	NE1-CE2	6.11	1.44	1.37
26	Z	914	LEU	CA-C	-6.11	1.45	1.52
5	e	203	LYS	CA-C	-6.11	1.44	1.52
12	l	96	SER	C-N	6.11	1.41	1.33
16	I	313	LEU	CA-C	-6.11	1.45	1.52
28	S	379	LEU	C-N	6.11	1.42	1.33
11	k	125	LYS	CA-C	-6.11	1.45	1.52
13	6	110	ILE	CA-C	-6.11	1.45	1.52
14	7	82	ASP	CA-CB	6.11	1.63	1.53
18	L	267	PHE	N-CA	-6.11	1.38	1.46
26	Z	907	GLY	CA-C	-6.11	1.46	1.52
27	N	43	LEU	C-O	-6.11	1.18	1.24
18	L	409	HIS	CA-C	-6.10	1.45	1.52
26	Z	243	GLN	C-N	6.10	1.42	1.33
19	M	363	ILE	N-CA	-6.10	1.39	1.46
30	Q	8	LEU	C-N	6.10	1.41	1.33
9	i	192	THR	C-O	-6.10	1.18	1.24
13	6	207	VAL	N-CA	-6.10	1.38	1.46
16	I	191	ILE	N-CA	-6.10	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	270	ARG	NE-CZ	6.10	1.39	1.33
9	2	154	LEU	C-N	6.10	1.42	1.33
21	W	167	GLU	N-CA	-6.10	1.38	1.45
23	T	123	HIS	N-CA	-6.10	1.38	1.46
27	N	480	ALA	CA-C	-6.10	1.44	1.52
4	d	76	LEU	CA-C	-6.09	1.44	1.52
11	k	103	LEU	CA-C	-6.09	1.45	1.52
26	Z	849	ARG	CD-NE	6.09	1.54	1.46
28	S	430	GLY	CA-C	-6.09	1.43	1.51
1	a	15	ARG	NE-CZ	6.09	1.39	1.33
5	E	117	GLU	N-CA	-6.09	1.38	1.46
12	5	59	LEU	CA-C	-6.09	1.45	1.52
26	Z	138	ARG	CZ-NH1	6.09	1.41	1.32
26	Z	364	ASN	CA-C	-6.09	1.44	1.52
17	K	284	ALA	CA-C	6.09	1.58	1.52
4	d	118	TYR	CA-CB	6.09	1.63	1.53
15	H	370	ARG	N-CA	-6.09	1.38	1.46
26	Z	365	SER	C-N	6.09	1.42	1.33
27	N	158	LEU	N-CA	-6.09	1.39	1.46
7	G	66	VAL	CA-C	-6.08	1.44	1.52
20	J	79	VAL	N-CA	-6.08	1.39	1.46
23	T	100	ASP	C-N	6.08	1.42	1.34
26	Z	773	ARG	CZ-NH1	6.08	1.41	1.32
12	l	188	HIS	CG-CD2	6.08	1.42	1.35
4	D	145	LEU	CA-C	-6.08	1.45	1.52
5	E	147	LEU	N-CA	-6.08	1.38	1.46
18	L	341	GLY	CA-C	-6.08	1.43	1.51
12	l	169	ALA	C-N	6.07	1.42	1.33
27	N	155	GLY	N-CA	6.07	1.53	1.45
6	F	214	ILE	N-CA	-6.07	1.39	1.46
30	Q	152	LYS	CA-C	-6.07	1.45	1.52
1	a	189	SER	C-N	6.07	1.42	1.33
4	d	117	ARG	NE-CZ	6.07	1.39	1.33
10	j	109	ALA	CA-C	-6.07	1.44	1.52
33	O	125	GLY	CA-C	-6.07	1.45	1.52
2	b	234	ARG	CD-NE	6.07	1.54	1.46
10	j	176	ARG	NE-CZ	6.07	1.39	1.33
8	l	173	ILE	CA-C	-6.07	1.45	1.52
3	c	184	LYS	CA-CB	6.07	1.62	1.53
17	K	290	ARG	NE-CZ	6.06	1.39	1.33
9	i	200	GLN	CA-C	-6.06	1.45	1.52
17	K	367	ASP	C-N	6.06	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	91	GLU	C-N	6.06	1.40	1.33
31	R	406	GLN	C-N	6.06	1.42	1.34
7	g	200	HIS	CB-CG	6.06	1.58	1.50
9	2	166	ASP	N-CA	-6.06	1.38	1.46
13	m	105	TYR	CA-C	-6.06	1.45	1.52
2	B	132	VAL	CA-C	-6.06	1.45	1.52
11	4	130	TYR	C-N	6.06	1.42	1.33
18	L	303	ARG	NE-CZ	6.06	1.39	1.33
18	L	334	ASP	CA-C	6.06	1.57	1.52
9	i	221	CYS	C-N	6.05	1.41	1.33
6	f	98	PHE	CA-C	-6.05	1.44	1.52
15	H	194	SER	CA-CB	6.05	1.63	1.53
26	Z	927	VAL	N-CA	-6.05	1.39	1.46
29	P	324	GLU	C-N	6.05	1.42	1.33
32	U	15	LEU	C-N	6.05	1.41	1.33
5	e	106	GLN	CA-CB	6.05	1.62	1.53
6	f	91	CYS	CA-C	-6.05	1.45	1.52
15	H	373	ARG	CD-NE	6.05	1.54	1.46
20	J	41	VAL	N-CA	-6.05	1.39	1.46
28	S	117	SER	C-N	6.05	1.42	1.33
4	d	87	ALA	N-CA	-6.05	1.39	1.46
23	T	68	ALA	N-CA	6.05	1.53	1.46
12	l	210	VAL	CA-CB	-6.04	1.46	1.53
1	A	194	VAL	CA-CB	-6.04	1.47	1.54
29	P	401	ASN	CA-C	-6.04	1.46	1.53
26	Z	933	VAL	C-N	6.04	1.41	1.33
33	O	145	LYS	N-CA	-6.04	1.39	1.46
7	G	26	ALA	CA-C	-6.04	1.45	1.52
13	6	18	GLU	N-CA	-6.04	1.39	1.46
18	L	82	ARG	N-CA	-6.04	1.39	1.46
14	n	63	ILE	N-CA	-6.04	1.38	1.46
15	H	420	ARG	CZ-NH2	6.04	1.41	1.33
10	j	80	ALA	CA-C	-6.04	1.45	1.52
16	I	306	MET	CA-C	-6.04	1.45	1.52
25	Y	82	ASP	CA-C	-6.04	1.45	1.52
28	S	266	SER	CA-CB	6.04	1.63	1.53
6	f	224	TYR	C-N	6.03	1.41	1.33
8	h	32	ASP	CA-C	-6.03	1.45	1.53
13	6	39	TYR	CA-C	-6.03	1.45	1.52
20	J	139	VAL	CA-CB	-6.03	1.47	1.54
28	S	18	LEU	CA-C	-6.03	1.40	1.52
19	M	53	HIS	CA-C	-6.03	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	201	GLU	C-N	6.03	1.41	1.33
30	Q	420	ASN	C-O	-6.03	1.17	1.24
27	N	493	GLY	CA-C	-6.03	1.45	1.51
28	S	407	ILE	CA-C	6.03	1.60	1.52
33	O	66	VAL	C-N	6.03	1.42	1.33
33	O	89	SER	CA-CB	6.03	1.62	1.53
6	f	163	ARG	CZ-NH1	6.03	1.41	1.32
7	G	163	LYS	CA-CB	6.03	1.62	1.53
9	2	201	LYS	N-CA	-6.03	1.39	1.46
21	W	143	ASN	CA-C	-6.03	1.45	1.52
3	C	58	GLN	CA-CB	6.02	1.63	1.53
19	M	81	ASN	CA-C	-6.02	1.45	1.52
27	N	678	ILE	CA-C	-6.02	1.45	1.52
33	O	124	ASP	C-O	6.02	1.31	1.24
3	c	42	GLY	C-N	6.02	1.42	1.33
16	I	432	LEU	CA-C	-6.02	1.45	1.52
20	J	49	ASN	CA-C	-6.02	1.45	1.52
26	Z	458	SER	CA-CB	6.02	1.62	1.53
2	b	82	TYR	CA-CB	6.02	1.62	1.53
10	3	96	GLU	N-CA	-6.02	1.39	1.46
26	Z	909	ARG	CZ-NH1	6.02	1.41	1.32
28	S	468	ALA	CA-C	-6.02	1.45	1.52
12	5	204	GLU	C-N	6.02	1.41	1.33
29	P	364	ARG	NE-CZ	6.02	1.39	1.33
23	T	98	GLU	C-O	6.01	1.31	1.23
33	O	326	HIS	ND1-CE1	6.01	1.38	1.32
10	3	66	PHE	CA-C	-6.01	1.45	1.52
33	O	380	LEU	C-N	6.01	1.41	1.33
1	a	120	THR	C-N	6.01	1.42	1.33
10	j	126	ILE	N-CA	6.01	1.53	1.46
16	I	289	THR	N-CA	-6.01	1.37	1.46
31	R	324	ARG	CZ-NH1	6.01	1.41	1.32
20	J	332	SER	CA-C	6.01	1.60	1.52
26	Z	287	ARG	CZ-NH2	6.01	1.41	1.33
7	G	32	THR	CA-C	-6.01	1.45	1.52
29	P	178	GLN	CA-C	-6.01	1.45	1.52
16	I	300	ARG	CA-C	-6.00	1.44	1.52
4	d	88	ARG	CZ-NH2	6.00	1.41	1.33
10	j	101	PRO	N-CA	-6.00	1.39	1.47
3	C	8	ARG	CZ-NH2	6.00	1.41	1.33
18	L	144	VAL	CA-C	-6.00	1.45	1.52
31	R	99	TYR	CA-C	-6.00	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	70	ASN	C-N	6.00	1.41	1.33
6	f	51	ASN	C-N	6.00	1.41	1.33
7	G	62	LYS	C-N	6.00	1.40	1.33
13	6	69	LYS	CA-C	-6.00	1.45	1.52
19	M	187	ASP	C-N	6.00	1.41	1.33
27	N	313	LEU	C-N	6.00	1.42	1.33
27	N	356	LEU	C-N	6.00	1.41	1.33
2	B	90	ARG	CZ-NH2	6.00	1.41	1.33
3	C	39	ALA	CA-C	-6.00	1.45	1.52
26	Z	580	GLN	N-CA	-6.00	1.38	1.46
27	N	420	THR	CA-C	-6.00	1.45	1.52
14	7	41	ARG	N-CA	-5.99	1.40	1.46
31	R	128	LEU	N-CA	-5.99	1.38	1.46
13	m	213	ARG	NE-CZ	5.99	1.39	1.33
18	L	332	THR	CA-C	-5.99	1.45	1.52
22	V	109	HIS	CA-C	-5.99	1.45	1.52
3	C	227	LYS	N-CA	-5.99	1.39	1.46
32	U	290	ASP	CA-C	-5.99	1.45	1.52
7	G	160	ALA	C-N	5.98	1.41	1.33
28	S	284	LEU	CA-CB	5.98	1.62	1.53
7	g	226	PHE	CA-C	-5.98	1.45	1.52
3	C	93	HIS	C-N	5.98	1.41	1.33
9	i	203	TYR	N-CA	-5.98	1.38	1.46
27	N	126	LYS	CA-C	5.98	1.60	1.52
18	L	81	ILE	N-CA	-5.98	1.39	1.46
5	E	124	ARG	CZ-NH1	5.98	1.41	1.32
11	4	165	VAL	N-CA	-5.98	1.39	1.46
14	7	162	GLU	C-N	5.98	1.41	1.33
26	Z	593	HIS	N-CA	-5.98	1.40	1.46
27	N	381	GLU	CA-CB	5.98	1.63	1.53
9	i	189	ASN	CA-C	-5.98	1.45	1.53
12	l	73	ARG	CZ-NH1	5.97	1.41	1.32
13	m	122	VAL	CA-C	-5.97	1.45	1.52
14	n	88	GLU	CA-C	-5.97	1.45	1.52
3	C	162	ILE	C-N	5.97	1.41	1.33
3	C	15	GLU	C-N	5.97	1.41	1.33
26	Z	545	SER	N-CA	-5.97	1.38	1.46
27	N	390	LEU	CA-C	-5.97	1.46	1.53
29	P	233	GLU	N-CA	-5.97	1.38	1.46
3	c	216	ARG	NE-CZ	5.97	1.39	1.33
3	C	17	ARG	CZ-NH2	5.97	1.41	1.33
6	f	86	TYR	CA-C	-5.97	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	37	LYS	CA-C	-5.97	1.45	1.52
18	L	394	CYS	C-N	5.97	1.42	1.33
27	N	98	VAL	C-O	5.97	1.31	1.24
27	N	813	ARG	NE-CZ	5.97	1.39	1.33
30	Q	261	VAL	C-N	5.97	1.41	1.33
33	O	275	SER	N-CA	-5.97	1.39	1.46
8	h	85	LEU	N-CA	-5.96	1.39	1.46
4	D	179	ARG	CZ-NH2	5.96	1.41	1.33
15	H	158	GLY	N-CA	-5.96	1.36	1.45
23	T	102	LYS	CA-C	5.96	1.60	1.52
27	N	908	ARG	NE-CZ	5.96	1.39	1.33
14	7	78	ASN	N-CA	-5.96	1.37	1.45
32	U	258	SER	N-CA	-5.96	1.39	1.46
9	2	64	GLU	CA-C	-5.96	1.45	1.52
8	1	56	ALA	N-CA	5.96	1.53	1.46
14	n	184	LEU	N-CA	-5.96	1.39	1.46
33	O	287	LEU	C-N	5.96	1.41	1.33
2	b	90	ARG	NE-CZ	5.96	1.39	1.33
6	F	145	GLU	CA-C	-5.96	1.45	1.52
15	H	192	ASP	N-CA	-5.95	1.37	1.46
22	V	302	SER	CA-CB	5.95	1.62	1.53
26	Z	196	SER	C-O	-5.95	1.17	1.24
1	a	104	PRO	CA-CB	-5.95	1.45	1.53
5	E	33	ALA	CA-C	-5.95	1.45	1.52
14	n	190	ARG	CD-NE	5.95	1.54	1.46
3	C	186	ASP	CA-C	-5.95	1.45	1.52
10	3	13	ALA	C-N	5.95	1.40	1.33
14	7	136	THR	C-N	5.95	1.40	1.33
24	X	15	CYS	C-N	5.94	1.41	1.33
30	Q	30	LEU	CA-C	-5.94	1.45	1.52
19	M	427	SER	C-N	5.94	1.41	1.33
26	Z	446	GLU	C-N	5.94	1.41	1.34
26	Z	604	GLY	N-CA	-5.94	1.38	1.45
29	P	396	PRO	N-CA	-5.94	1.40	1.47
2	b	240	SER	CA-CB	5.94	1.62	1.53
18	L	191	ARG	NE-CZ	5.94	1.39	1.33
22	V	93	ASP	CA-CB	5.94	1.63	1.53
24	X	21	SER	C-N	5.94	1.42	1.33
28	S	234	ILE	N-CA	-5.94	1.39	1.46
16	I	339	ILE	N-CA	-5.94	1.39	1.46
20	J	35	ARG	NE-CZ	5.94	1.39	1.33
27	N	133	LEU	N-CA	-5.94	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	62	ASN	CA-CB	5.93	1.62	1.53
3	c	6	ASP	CA-C	-5.93	1.45	1.52
3	c	156	TYR	CA-C	-5.93	1.45	1.52
11	k	171	ARG	CD-NE	5.93	1.54	1.46
2	b	239	THR	CA-C	-5.93	1.45	1.52
12	l	53	GLN	N-CA	-5.93	1.39	1.46
14	n	108	ASN	CA-C	5.93	1.60	1.52
26	Z	81	SER	CA-C	-5.93	1.45	1.52
5	E	235	LEU	C-N	5.93	1.41	1.33
13	6	78	ASP	CA-C	-5.93	1.44	1.52
27	N	602	VAL	N-CA	-5.93	1.39	1.46
27	N	740	TRP	NE1-CE2	5.93	1.44	1.37
8	h	49	ALA	N-CA	-5.93	1.39	1.46
1	a	82	ARG	CA-C	-5.93	1.45	1.52
7	g	16	ARG	CD-NE	5.93	1.54	1.46
27	N	499	HIS	N-CA	-5.93	1.39	1.46
27	N	519	VAL	N-CA	-5.93	1.39	1.46
3	c	215	ILE	C-N	5.92	1.41	1.33
7	g	140	ASN	C-N	5.92	1.40	1.33
15	H	97	LEU	CA-C	-5.92	1.45	1.52
3	c	223	GLU	CA-C	-5.92	1.45	1.52
14	n	103	ARG	N-CA	-5.92	1.39	1.46
12	5	202	GLU	CA-C	-5.92	1.45	1.52
17	K	249	GLU	N-CA	-5.92	1.38	1.46
3	c	3	ARG	CZ-NH2	5.92	1.41	1.33
3	c	41	ASP	C-N	5.92	1.40	1.32
12	l	149	SER	CA-C	-5.92	1.45	1.52
6	F	217	LYS	N-CA	-5.92	1.39	1.46
18	L	248	ALA	N-CA	-5.92	1.38	1.46
1	a	75	ASN	N-CA	-5.92	1.39	1.46
27	N	15	GLU	N-CA	-5.91	1.38	1.46
13	m	152	ASN	C-N	5.91	1.42	1.33
22	V	239	ALA	C-O	-5.91	1.17	1.24
27	N	896	PHE	CA-CB	5.91	1.63	1.53
31	R	26	VAL	N-CA	-5.91	1.39	1.46
27	N	604	ARG	CZ-NH1	5.91	1.41	1.32
12	5	192	ASP	N-CA	-5.91	1.38	1.46
23	T	218	GLU	C-N	5.91	1.41	1.33
27	N	246	LYS	CA-C	-5.91	1.45	1.52
11	k	36	ARG	NE-CZ	5.90	1.39	1.33
7	g	178	HIS	C-N	5.90	1.39	1.33
9	i	220	ILE	CA-CB	-5.90	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	156	TYR	N-CA	-5.90	1.38	1.46
19	M	358	ALA	CA-C	-5.90	1.45	1.52
28	S	446	THR	C-N	5.90	1.41	1.33
9	i	180	ILE	CA-CB	-5.90	1.46	1.54
26	Z	202	ARG	N-CA	-5.90	1.39	1.46
26	Z	704	GLU	CA-C	-5.90	1.44	1.52
6	f	183	GLY	C-N	5.89	1.38	1.33
26	Z	169	VAL	CA-C	-5.89	1.45	1.52
7	g	42	VAL	CA-C	-5.89	1.45	1.52
20	J	151	GLY	CA-C	-5.89	1.40	1.52
29	P	409	SER	C-O	-5.89	1.17	1.24
7	g	84	LEU	CA-C	-5.89	1.45	1.52
14	7	51	VAL	N-CA	-5.89	1.39	1.46
3	C	124	HIS	ND1-CE1	5.89	1.38	1.32
26	Z	448	LYS	C-N	5.89	1.41	1.33
9	i	46	ALA	N-CA	-5.89	1.37	1.46
1	A	44	VAL	CA-C	-5.89	1.45	1.52
5	E	39	VAL	N-CA	-5.89	1.39	1.46
14	7	201	ASP	N-CA	-5.89	1.38	1.45
29	P	173	MET	N-CA	-5.89	1.39	1.46
3	c	237	ILE	N-CA	-5.88	1.38	1.46
10	3	129	ILE	CA-C	-5.88	1.46	1.53
1	a	37	ARG	NE-CZ	5.88	1.39	1.33
1	a	45	ILE	CA-CB	-5.88	1.46	1.55
27	N	210	SER	CA-CB	5.88	1.62	1.53
4	d	36	GLY	N-CA	-5.88	1.36	1.44
19	M	156	LEU	C-N	5.88	1.40	1.33
23	T	192	ASN	CA-C	-5.88	1.45	1.52
26	Z	583	ASP	C-N	5.88	1.40	1.33
28	S	394	ILE	CA-C	-5.88	1.45	1.52
7	g	48	LYS	CA-C	-5.88	1.45	1.52
11	4	171	ARG	NE-CZ	5.87	1.39	1.33
26	Z	757	SER	CA-CB	5.87	1.63	1.53
10	3	37	ASN	N-CA	5.87	1.52	1.46
17	K	397	LYS	CA-C	-5.87	1.44	1.52
28	S	165	PRO	N-CA	-5.87	1.39	1.47
5	e	45	ARG	CD-NE	5.87	1.54	1.46
11	k	165	VAL	N-CA	-5.87	1.39	1.46
15	H	392	HIS	CG-CD2	5.87	1.42	1.35
28	S	192	GLU	CA-CB	-5.87	1.44	1.53
30	Q	359	ILE	CA-C	-5.87	1.44	1.52
33	O	135	ARG	CD-NE	5.87	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	79	ALA	CA-C	-5.87	1.45	1.52
18	L	76	GLN	N-CA	-5.87	1.39	1.46
1	a	48	LYS	CA-C	-5.87	1.45	1.52
8	h	67	THR	CA-C	-5.87	1.45	1.52
13	m	29	ASN	C-O	-5.87	1.17	1.24
14	7	202	LYS	CA-C	-5.87	1.44	1.52
26	Z	36	GLU	N-CA	-5.87	1.38	1.46
27	N	255	ALA	CA-CB	5.87	1.62	1.53
4	d	96	LEU	CA-C	-5.86	1.45	1.52
9	i	26	VAL	C-N	5.86	1.41	1.33
20	J	253	ILE	N-CA	-5.86	1.38	1.46
9	i	211	ALA	CA-C	-5.86	1.45	1.52
28	S	275	TYR	CA-C	-5.86	1.45	1.52
1	a	184	HIS	N-CA	-5.86	1.38	1.45
21	W	56	GLY	C-O	5.86	1.31	1.23
31	R	107	GLU	N-CA	-5.86	1.39	1.46
13	m	137	ARG	CZ-NH2	5.86	1.41	1.33
3	C	41	ASP	C-N	5.85	1.39	1.33
15	H	452	SER	CA-C	-5.85	1.45	1.52
6	f	88	ARG	CZ-NH1	5.85	1.41	1.32
17	K	349	ARG	NE-CZ	5.85	1.39	1.33
26	Z	748	LEU	CA-CB	5.85	1.62	1.53
27	N	613	HIS	CB-CG	5.85	1.58	1.50
11	k	130	TYR	N-CA	-5.85	1.38	1.46
12	l	41	LEU	CA-C	-5.85	1.45	1.52
12	l	69	ARG	NE-CZ	5.85	1.39	1.33
13	m	97	LEU	CA-C	-5.85	1.45	1.52
1	A	68	ARG	NE-CZ	5.85	1.39	1.33
16	I	84	PRO	CA-C	-5.85	1.44	1.52
17	K	426	PHE	CA-CB	5.85	1.63	1.53
26	Z	743	ILE	CA-C	-5.85	1.45	1.52
1	A	28	GLN	CA-C	-5.85	1.44	1.52
27	N	615	ALA	N-CA	-5.85	1.39	1.46
11	k	53	THR	N-CA	-5.85	1.39	1.46
6	f	186	ASP	N-CA	-5.84	1.39	1.46
26	Z	124	MET	CA-C	-5.84	1.45	1.52
31	R	138	GLY	CA-C	-5.84	1.43	1.51
31	R	176	ARG	CZ-NH1	5.84	1.41	1.32
2	B	157	PHE	C-N	-5.84	1.26	1.33
3	c	74	VAL	N-CA	-5.84	1.39	1.46
13	m	173	LYS	C-N	5.84	1.41	1.33
3	C	142	ARG	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	206	ILE	C-N	5.84	1.41	1.33
27	N	487	LEU	CA-CB	5.84	1.62	1.53
16	I	246	ARG	C-N	5.84	1.40	1.33
10	j	98	ARG	CZ-NH1	5.83	1.41	1.32
22	V	297	THR	CA-C	-5.83	1.45	1.52
26	Z	518	LEU	CA-C	5.83	1.59	1.53
31	R	165	GLY	CA-C	-5.83	1.45	1.52
2	b	214	ILE	N-CA	-5.83	1.39	1.46
6	f	136	TYR	CA-C	-5.83	1.45	1.52
11	k	95	ARG	CZ-NH2	5.83	1.41	1.33
1	a	157	TYR	CA-C	-5.83	1.45	1.52
3	c	108	GLU	C-N	5.83	1.41	1.33
1	A	217	GLY	CA-C	5.83	1.56	1.52
27	N	47	GLU	C-N	5.83	1.41	1.33
1	a	74	VAL	C-O	5.83	1.29	1.24
7	g	49	LEU	N-CA	-5.83	1.39	1.46
14	n	35	ARG	CD-NE	5.83	1.54	1.46
19	M	409	SER	N-CA	-5.83	1.38	1.46
3	c	11	ILE	C-N	5.82	1.41	1.33
8	h	155	ILE	N-CA	-5.82	1.39	1.46
9	2	189	ASN	C-N	5.82	1.41	1.33
15	H	173	ARG	NE-CZ	5.82	1.39	1.33
27	N	297	ASP	CA-C	-5.82	1.45	1.52
1	a	68	ARG	CZ-NH1	5.82	1.41	1.32
2	b	245	ASP	CA-CB	5.82	1.62	1.53
11	k	70	ARG	CZ-NH2	5.82	1.41	1.33
17	K	294	ARG	NE-CZ	5.82	1.39	1.33
15	H	285	GLY	CA-C	-5.82	1.43	1.51
21	W	41	ARG	CA-C	-5.82	1.45	1.52
28	S	460	VAL	N-CA	-5.82	1.39	1.46
31	R	100	ASN	CA-C	-5.82	1.45	1.52
15	H	434	ARG	NE-CZ	5.82	1.39	1.33
11	k	6	GLY	C-N	5.82	1.41	1.33
27	N	447	SER	CA-CB	5.82	1.62	1.53
6	f	35	VAL	C-N	5.82	1.40	1.33
11	k	128	LEU	N-CA	-5.82	1.41	1.45
20	J	302	PRO	N-CA	-5.82	1.40	1.47
23	T	135	ASN	N-CA	-5.82	1.41	1.46
29	P	257	TRP	NE1-CE2	-5.82	1.31	1.37
29	P	285	GLN	N-CA	5.82	1.53	1.46
31	R	112	GLU	N-CA	5.82	1.53	1.46
1	a	239	ILE	CA-CB	-5.81	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	10	VAL	CA-C	-5.81	1.44	1.52
14	7	21	ILE	N-CA	-5.81	1.39	1.46
20	J	25	GLN	CA-C	-5.81	1.45	1.52
27	N	198	THR	C-N	5.81	1.41	1.33
31	R	419	ALA	C-N	5.81	1.41	1.33
1	A	105	CYS	CA-C	-5.81	1.45	1.52
16	I	161	GLN	C-N	5.81	1.41	1.33
14	n	26	ASN	C-N	5.81	1.40	1.33
4	d	109	ARG	CZ-NH1	5.81	1.40	1.32
14	7	111	TRP	CA-CB	5.81	1.60	1.52
18	L	164	ASP	C-N	5.81	1.41	1.33
18	L	314	GLY	CA-C	5.81	1.60	1.51
27	N	285	ALA	N-CA	-5.81	1.39	1.46
27	N	563	GLY	CA-C	-5.81	1.43	1.51
4	D	88	ARG	N-CA	-5.81	1.39	1.46
19	M	416	VAL	CA-CB	-5.81	1.47	1.54
14	n	101	TYR	N-CA	-5.80	1.39	1.46
8	1	181	ALA	C-N	5.80	1.42	1.33
20	J	328	LEU	C-N	5.80	1.41	1.33
21	W	142	ILE	CA-C	-5.80	1.45	1.52
27	N	205	SER	N-CA	-5.80	1.39	1.46
27	N	590	ALA	N-CA	-5.80	1.39	1.46
3	c	72	ILE	C-O	-5.80	1.18	1.24
20	J	116	ARG	CZ-NH2	5.80	1.41	1.33
27	N	897	LYS	N-CA	-5.80	1.39	1.46
4	d	31	ALA	C-N	5.80	1.40	1.33
3	C	120	GLY	CA-C	-5.80	1.43	1.51
14	7	161	ARG	CZ-NH2	5.80	1.41	1.33
5	e	56	ILE	CA-C	-5.80	1.46	1.52
5	e	126	MET	CA-C	-5.80	1.45	1.52
7	g	221	ASN	CA-CB	5.80	1.63	1.53
14	7	215	GLU	N-CA	-5.80	1.39	1.46
10	j	27	ARG	CZ-NH2	5.79	1.41	1.33
12	l	53	GLN	CA-C	-5.79	1.45	1.52
16	I	321	ASP	N-CA	-5.79	1.38	1.46
27	N	269	LEU	N-CA	-5.79	1.39	1.46
18	L	253	ASP	CA-CB	5.79	1.64	1.53
24	X	51	ARG	NE-CZ	5.79	1.39	1.33
26	Z	529	ALA	CA-CB	-5.79	1.44	1.53
28	S	409	LEU	N-CA	5.79	1.53	1.46
32	U	67	PHE	CA-C	-5.79	1.45	1.52
7	g	78	ILE	CA-C	5.79	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	87	PHE	C-N	5.79	1.41	1.33
6	f	188	LEU	C-N	5.79	1.41	1.33
8	h	168	SER	C-N	5.79	1.41	1.33
33	O	237	PRO	C-N	5.79	1.41	1.34
2	b	69	PRO	N-CD	-5.79	1.39	1.47
19	M	157	ASP	N-CA	-5.79	1.39	1.46
9	i	65	LEU	CA-C	-5.78	1.45	1.52
6	F	201	ARG	NE-CZ	5.78	1.39	1.33
20	J	71	TYR	CA-C	-5.78	1.45	1.52
23	T	241	GLU	C-N	5.78	1.41	1.33
26	Z	32	LYS	N-CA	-5.78	1.39	1.46
26	Z	230	ILE	CA-CB	-5.78	1.47	1.54
23	T	93	ASN	CA-C	-5.78	1.45	1.52
11	k	27	VAL	C-O	-5.78	1.17	1.24
4	D	105	GLU	CA-C	-5.78	1.45	1.52
21	W	158	ILE	C-N	5.78	1.41	1.33
32	U	227	GLY	CA-C	-5.78	1.45	1.52
5	e	16	VAL	CA-CB	-5.77	1.47	1.54
6	f	89	GLN	CA-C	-5.77	1.45	1.52
3	c	49	ARG	CD-NE	5.77	1.54	1.46
5	e	168	SER	CA-CB	5.77	1.62	1.53
14	n	65	ARG	N-CA	-5.77	1.39	1.46
29	P	112	LEU	CA-C	-5.77	1.45	1.52
11	4	19	LYS	CA-C	-5.77	1.44	1.52
11	4	70	ARG	C-O	-5.77	1.17	1.24
16	I	149	LEU	CA-C	-5.77	1.45	1.52
4	D	185	THR	N-CA	-5.77	1.38	1.45
17	K	346	ARG	CD-NE	5.77	1.54	1.46
30	Q	240	PHE	N-CA	5.77	1.53	1.46
33	O	306	ARG	NE-CZ	5.77	1.39	1.33
5	e	88	ALA	N-CA	-5.77	1.39	1.46
13	6	13	LEU	CA-C	-5.77	1.45	1.52
17	K	299	LEU	C-N	5.77	1.41	1.33
27	N	9	LEU	CA-C	-5.77	1.45	1.52
3	c	93	HIS	ND1-CE1	5.76	1.38	1.32
11	k	8	ARG	N-CA	-5.76	1.39	1.46
20	J	118	ASP	C-N	5.76	1.41	1.33
33	O	392	TRP	C-N	5.76	1.41	1.33
10	j	89	LEU	C-N	5.76	1.41	1.33
27	N	587	ALA	CA-C	5.76	1.60	1.52
16	I	93	LYS	CA-C	-5.76	1.45	1.52
26	Z	536	GLY	C-N	5.76	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	O	100	ASP	C-N	5.76	1.41	1.33
11	k	159	ASP	N-CA	-5.76	1.39	1.46
5	E	24	LYS	N-CA	-5.76	1.39	1.46
9	2	167	LEU	C-N	5.76	1.42	1.33
12	l	196	LEU	CA-C	-5.76	1.45	1.52
23	T	135	ASN	CA-C	-5.76	1.46	1.53
2	B	45	ILE	N-CA	-5.76	1.39	1.46
15	H	244	LYS	CA-C	-5.76	1.45	1.52
23	T	150	ARG	CD-NE	5.76	1.54	1.46
33	O	177	GLN	CA-CB	5.75	1.62	1.53
15	H	53	GLU	C-N	5.75	1.41	1.33
22	V	238	LEU	N-CA	-5.75	1.39	1.46
27	N	717	LEU	N-CA	-5.75	1.39	1.46
5	E	13	LEU	CA-C	-5.75	1.45	1.52
24	X	74	MET	CA-C	-5.75	1.45	1.52
13	m	191	ALA	CA-C	-5.75	1.44	1.52
7	g	128	PHE	CA-C	5.75	1.60	1.52
21	W	165	GLN	CA-C	-5.75	1.45	1.52
12	l	164	ALA	N-CA	-5.75	1.39	1.46
4	D	138	PRO	N-CA	5.75	1.53	1.47
15	H	169	GLU	N-CA	-5.75	1.38	1.45
26	Z	121	ILE	N-CA	5.75	1.53	1.46
26	Z	779	ALA	C-N	5.75	1.41	1.33
5	E	23	ILE	N-CA	5.75	1.53	1.46
15	H	291	VAL	CA-C	-5.75	1.45	1.52
30	Q	219	ASP	C-N	5.75	1.41	1.33
30	Q	290	THR	CA-C	-5.75	1.45	1.52
28	S	322	LEU	CA-CB	5.74	1.62	1.53
3	c	182	ASP	CA-CB	5.74	1.63	1.53
5	e	207	ASN	N-CA	-5.74	1.38	1.46
26	Z	505	VAL	C-N	5.74	1.41	1.33
26	Z	767	TYR	N-CA	-5.74	1.39	1.46
30	Q	410	ASP	CA-C	-5.74	1.45	1.52
23	T	151	TRP	CA-C	-5.74	1.44	1.52
27	N	314	LEU	C-O	-5.74	1.17	1.24
7	g	186	ARG	CZ-NH1	5.74	1.40	1.32
8	h	91	ASP	N-CA	-5.74	1.39	1.46
14	n	176	ALA	C-N	5.74	1.41	1.33
10	j	15	THR	N-CA	-5.74	1.38	1.45
12	l	78	ALA	N-CA	-5.74	1.39	1.46
2	B	81	ASP	CA-C	-5.74	1.45	1.52
10	3	21	ALA	C-N	5.74	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	51	GLY	C-N	5.74	1.41	1.33
33	O	256	ASN	N-CA	-5.74	1.39	1.46
3	C	155	ASN	CA-C	-5.73	1.45	1.52
12	5	210	VAL	CA-CB	-5.73	1.47	1.54
16	I	300	ARG	CZ-NH1	5.73	1.40	1.32
20	J	85	LEU	CA-C	-5.73	1.45	1.52
20	J	200	ARG	CD-NE	5.73	1.54	1.46
31	R	43	ARG	CZ-NH1	5.73	1.40	1.32
4	d	197	LEU	CA-C	-5.73	1.45	1.52
6	f	15	THR	C-N	5.73	1.42	1.33
4	D	56	ARG	CD-NE	5.73	1.54	1.46
16	I	87	LYS	CA-CB	5.73	1.63	1.53
20	J	343	LEU	CA-CB	5.73	1.62	1.53
26	Z	362	LEU	N-CA	-5.73	1.39	1.46
2	b	241	GLN	CA-C	-5.73	1.45	1.52
9	i	205	PHE	CA-CB	5.73	1.62	1.52
15	H	147	ILE	CA-C	-5.73	1.46	1.52
23	T	142	LEU	CB-CG	5.73	1.65	1.53
29	P	40	LEU	CA-C	-5.73	1.45	1.52
27	N	566	SER	CA-C	-5.72	1.45	1.52
33	O	133	ILE	CA-C	-5.72	1.45	1.52
24	X	85	ARG	CA-C	-5.72	1.45	1.53
27	N	488	CYS	C-O	5.72	1.30	1.24
27	N	780	ASP	N-CA	-5.72	1.39	1.46
3	c	96	ASN	C-O	5.72	1.30	1.24
6	f	208	ASP	C-N	5.72	1.42	1.33
7	g	197	TYR	CA-CB	5.72	1.62	1.53
6	F	86	TYR	N-CA	-5.72	1.39	1.46
8	h	130	GLY	CA-C	-5.72	1.41	1.51
4	d	129	VAL	C-O	-5.72	1.17	1.23
5	e	149	HIS	N-CA	-5.72	1.39	1.46
12	l	103	GLY	CA-C	-5.72	1.45	1.51
2	B	214	ILE	CA-C	-5.72	1.45	1.52
7	G	117	GLN	CA-C	-5.72	1.45	1.52
21	W	158	ILE	N-CA	5.72	1.53	1.46
28	S	335	GLN	CA-C	-5.72	1.44	1.52
3	c	197	SER	CA-CB	5.71	1.62	1.53
7	G	15	GLY	CA-C	-5.71	1.43	1.51
14	7	135	VAL	CA-C	-5.71	1.46	1.52
15	H	393	SER	CA-C	-5.71	1.45	1.52
19	M	154	LEU	C-N	5.71	1.39	1.33
27	N	134	THR	CA-C	-5.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	35	THR	C-N	5.71	1.41	1.33
28	S	303	ASN	C-N	5.71	1.41	1.34
6	f	158	THR	C-N	5.71	1.41	1.33
8	h	7	THR	CA-CB	5.71	1.62	1.53
9	2	201	LYS	CA-C	-5.71	1.45	1.52
28	S	167	LEU	CA-C	-5.71	1.44	1.52
29	P	416	SER	C-N	5.71	1.41	1.33
13	6	106	TYR	CA-C	-5.71	1.45	1.52
14	7	159	VAL	CA-C	-5.71	1.46	1.52
23	T	248	GLU	CA-C	-5.71	1.45	1.52
26	Z	591	ILE	CA-C	-5.71	1.46	1.52
27	N	651	PHE	C-N	5.71	1.41	1.33
29	P	101	MET	C-N	5.71	1.41	1.33
9	i	64	GLU	CA-C	-5.71	1.45	1.52
11	k	58	GLU	C-N	5.71	1.41	1.33
7	G	87	ARG	C-N	5.71	1.41	1.33
11	4	190	ARG	CZ-NH1	5.71	1.40	1.32
5	e	200	MET	CA-C	-5.71	1.45	1.52
8	h	1	THR	N-CA	5.71	1.57	1.46
9	i	50	ALA	CA-C	-5.71	1.45	1.52
5	E	26	GLY	CA-C	-5.71	1.43	1.51
10	3	13	ALA	CA-C	-5.71	1.45	1.52
15	H	273	ARG	CZ-NH2	5.71	1.40	1.33
28	S	20	HIS	CE1-NE2	5.71	1.38	1.32
13	m	50	ILE	CA-C	-5.70	1.45	1.52
16	I	291	ARG	NE-CZ	5.70	1.39	1.33
9	i	113	ILE	CA-CB	-5.70	1.47	1.54
12	l	95	LEU	N-CA	-5.70	1.38	1.46
1	A	15	ARG	CZ-NH1	5.70	1.40	1.32
13	6	153	GLN	C-N	5.70	1.41	1.33
18	L	317	ASN	N-CA	5.70	1.52	1.45
20	J	121	MET	N-CA	-5.70	1.39	1.46
27	N	60	MET	C-N	5.70	1.41	1.33
10	j	149	CYS	CA-CB	5.70	1.62	1.53
2	B	62	SER	CA-C	-5.70	1.45	1.52
23	T	185	ILE	CA-C	-5.70	1.45	1.52
27	N	864	LYS	CA-C	-5.70	1.47	1.53
3	C	71	LYS	CA-C	-5.70	1.45	1.52
1	a	17	TYR	CA-C	-5.70	1.45	1.52
5	e	199	VAL	CA-C	-5.70	1.45	1.52
7	G	153	TYR	N-CA	-5.70	1.39	1.46
19	M	61	LYS	C-N	5.70	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	340	HIS	C-N	5.70	1.41	1.33
9	i	27	ALA	N-CA	-5.69	1.39	1.46
12	l	66	HIS	C-O	-5.69	1.17	1.24
4	D	156	SER	CA-CB	5.69	1.61	1.53
11	4	107	TYR	N-CA	-5.69	1.39	1.46
11	4	147	HIS	ND1-CE1	5.69	1.38	1.32
14	7	122	ASN	CA-CB	5.69	1.62	1.53
7	g	70	ILE	CA-CB	-5.69	1.47	1.54
12	l	67	GLU	CA-C	-5.69	1.45	1.52
14	n	104	ARG	C-N	5.69	1.41	1.34
11	4	21	VAL	N-CA	-5.69	1.39	1.46
12	5	35	ILE	N-CA	-5.69	1.39	1.46
16	I	425	LYS	C-N	5.69	1.41	1.33
30	Q	264	TYR	C-N	5.69	1.41	1.33
1	a	87	ARG	CD-NE	5.69	1.54	1.46
2	b	21	ILE	N-CA	5.69	1.53	1.46
7	g	231	LEU	CA-CB	5.69	1.62	1.53
11	k	31	SER	C-O	-5.69	1.17	1.24
20	J	330	ILE	CA-C	-5.69	1.45	1.53
13	m	67	ARG	CA-C	5.69	1.60	1.52
30	Q	417	GLY	CA-C	-5.69	1.45	1.52
7	g	129	GLY	C-N	5.68	1.41	1.33
14	n	39	VAL	CA-C	-5.68	1.46	1.52
30	Q	61	LEU	C-N	5.68	1.41	1.33
30	Q	128	GLU	CA-C	-5.68	1.47	1.52
31	R	101	GLU	N-CA	-5.68	1.39	1.46
14	n	1	THR	N-CA	5.68	1.57	1.46
15	H	43	ALA	C-O	-5.68	1.19	1.24
22	V	107	TRP	N-CA	-5.68	1.38	1.45
30	Q	228	GLU	C-O	-5.68	1.17	1.24
28	S	211	ARG	CZ-NH1	5.68	1.40	1.32
1	A	19	VAL	C-N	5.68	1.41	1.33
17	K	116	MET	N-CA	-5.68	1.38	1.46
9	2	197	GLU	CA-CB	5.68	1.61	1.53
13	m	40	GLU	CA-C	-5.68	1.45	1.52
3	C	4	ARG	CZ-NH2	5.68	1.40	1.33
2	b	131	GLY	CA-C	-5.67	1.43	1.51
14	n	193	ARG	NE-CZ	5.67	1.39	1.33
5	e	214	ILE	N-CA	-5.67	1.39	1.46
26	Z	312	TYR	CA-CB	5.67	1.62	1.53
6	f	41	THR	N-CA	-5.67	1.38	1.46
3	C	142	ARG	CD-NE	5.67	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	303	ARG	NE-CZ	5.67	1.39	1.33
28	S	324	MET	N-CA	5.67	1.53	1.46
1	A	139	GLU	CA-C	-5.67	1.45	1.52
2	B	60	THR	N-CA	-5.67	1.38	1.46
22	V	39	LYS	N-CA	5.67	1.53	1.46
27	N	554	THR	C-N	5.67	1.41	1.33
5	e	11	GLY	CA-C	-5.67	1.43	1.51
12	5	161	ILE	N-CA	-5.67	1.39	1.46
17	K	347	ARG	C-N	5.67	1.41	1.33
20	J	257	ARG	CD-NE	5.67	1.54	1.46
20	J	333	ARG	CD-NE	5.67	1.54	1.46
21	W	110	ILE	N-CA	-5.67	1.39	1.46
4	d	116	GLN	N-CA	-5.66	1.39	1.46
3	C	46	ALA	CA-C	-5.66	1.45	1.52
25	Y	87	GLU	N-CA	-5.66	1.39	1.46
33	O	181	PHE	C-N	5.66	1.42	1.33
7	G	92	ALA	CA-C	-5.66	1.45	1.52
27	N	128	ILE	C-N	5.66	1.39	1.33
1	a	96	ARG	CA-C	-5.66	1.45	1.52
5	e	108	VAL	N-CA	-5.66	1.39	1.46
9	2	160	GLN	CA-C	-5.66	1.45	1.52
11	4	189	ILE	CA-CB	-5.66	1.47	1.54
15	H	233	GLU	N-CA	-5.66	1.39	1.46
33	O	8	ASP	N-CA	-5.66	1.39	1.46
10	j	174	ALA	C-N	5.65	1.41	1.34
15	H	392	HIS	CG-ND1	-5.65	1.32	1.38
16	I	116	ASP	C-N	5.65	1.40	1.33
18	L	309	LEU	CA-C	-5.65	1.45	1.52
9	i	35	HIS	N-CA	-5.65	1.38	1.45
14	n	101	TYR	CA-C	-5.65	1.45	1.52
3	C	117	ILE	N-CA	5.65	1.53	1.46
8	1	80	SER	C-N	5.65	1.41	1.33
20	J	89	GLN	CA-C	5.65	1.59	1.52
27	N	398	ARG	CZ-NH1	5.65	1.40	1.32
27	N	208	ARG	NE-CZ	5.65	1.39	1.33
7	G	231	LEU	C-N	5.65	1.41	1.33
26	Z	342	LEU	CA-C	-5.65	1.45	1.52
9	i	99	ILE	CA-C	-5.65	1.45	1.52
10	j	87	THR	N-CA	-5.65	1.39	1.46
27	N	544	GLU	CA-C	-5.65	1.45	1.52
11	4	171	ARG	CD-NE	5.64	1.54	1.46
15	H	432	ARG	CA-C	5.64	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	184	LYS	CA-CB	5.64	1.62	1.53
28	S	273	PHE	C-N	5.64	1.41	1.33
31	R	108	SER	CA-C	-5.64	1.45	1.52
7	g	68	ARG	CD-NE	5.64	1.54	1.46
7	g	89	ARG	CA-CB	5.64	1.62	1.53
9	i	4	VAL	N-CA	-5.64	1.39	1.46
17	K	264	ASN	CA-C	5.64	1.59	1.53
26	Z	328	ASP	CA-CB	5.64	1.62	1.53
17	K	121	ARG	CD-NE	5.64	1.54	1.46
26	Z	60	ASP	CA-C	-5.64	1.45	1.52
28	S	225	HIS	CA-C	-5.64	1.46	1.53
4	D	189	CYS	CA-C	-5.64	1.45	1.52
30	Q	78	ILE	C-N	5.64	1.39	1.34
1	a	83	ASN	N-CA	5.64	1.53	1.46
14	n	122	ASN	CA-C	-5.64	1.45	1.52
3	C	128	ARG	N-CA	-5.64	1.38	1.45
19	M	71	ASN	N-CA	5.64	1.53	1.46
4	d	27	ARG	NE-CZ	5.64	1.39	1.33
11	k	85	ARG	CD-NE	5.64	1.54	1.46
20	J	300	LEU	CA-C	-5.63	1.45	1.52
3	c	243	ILE	CA-CB	-5.63	1.47	1.54
7	G	184	SER	CA-C	-5.63	1.45	1.52
32	U	280	ASN	N-CA	-5.63	1.39	1.46
5	E	123	GLU	CA-CB	5.63	1.61	1.53
13	6	221	ARG	CD-NE	5.63	1.54	1.46
15	H	55	ASP	C-N	5.63	1.41	1.33
17	K	189	GLU	CA-C	-5.63	1.45	1.52
22	V	268	THR	C-N	5.63	1.41	1.33
30	Q	34	ASP	N-CA	5.63	1.53	1.46
6	f	116	GLN	N-CA	-5.63	1.39	1.46
14	n	132	LEU	C-N	5.63	1.42	1.33
2	B	152	PRO	CA-C	-5.63	1.43	1.52
8	h	10	ASP	C-N	5.63	1.41	1.33
9	2	133	ALA	C-O	-5.63	1.17	1.24
33	O	267	ASP	C-N	5.63	1.41	1.33
2	b	30	GLN	C-N	5.62	1.41	1.33
16	I	345	ASP	CA-CB	5.62	1.63	1.52
17	K	236	ARG	CA-C	-5.62	1.46	1.52
19	M	338	LEU	CA-C	-5.62	1.45	1.52
26	Z	544	THR	CA-C	-5.62	1.45	1.52
4	D	25	VAL	CA-C	-5.62	1.46	1.52
26	Z	947	GLY	C-O	-5.62	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	U	266	THR	CA-C	-5.62	1.45	1.52
33	O	7	ILE	N-CA	-5.62	1.40	1.46
2	b	72	GLY	CA-C	-5.62	1.44	1.51
3	c	206	THR	CA-C	5.62	1.59	1.52
7	g	97	LYS	N-CA	-5.62	1.39	1.46
18	L	346	LYS	C-N	5.62	1.40	1.33
8	h	111	TYR	CA-C	-5.62	1.45	1.52
19	M	166	ARG	C-N	5.62	1.41	1.33
20	J	172	GLU	N-CA	-5.62	1.39	1.46
2	b	234	ARG	NE-CZ	5.62	1.39	1.33
29	P	164	GLN	N-CA	-5.62	1.38	1.46
2	b	59	GLU	C-O	-5.62	1.17	1.24
5	e	91	HIS	CA-C	-5.62	1.45	1.52
31	R	334	ARG	C-N	5.62	1.41	1.33
5	e	61	GLU	CA-C	-5.61	1.46	1.52
12	l	103	GLY	C-O	-5.61	1.18	1.24
7	G	135	GLY	C-N	5.61	1.38	1.33
22	V	211	LYS	C-N	5.61	1.41	1.33
23	T	188	GLU	CA-C	-5.61	1.45	1.52
32	U	138	VAL	CA-C	-5.61	1.45	1.52
3	c	230	LYS	CA-CB	5.61	1.61	1.53
22	V	194	ARG	CZ-NH1	5.61	1.40	1.32
28	S	199	GLU	C-O	-5.61	1.17	1.24
6	f	95	SER	C-N	5.61	1.41	1.33
16	I	336	PRO	N-CA	-5.61	1.40	1.47
13	m	93	ILE	CA-CB	5.61	1.61	1.54
26	Z	430	LEU	N-CA	-5.61	1.39	1.46
31	R	286	LEU	CA-C	-5.61	1.45	1.52
1	a	186	ASN	CA-CB	5.61	1.61	1.53
6	F	1	PHE	C-N	5.61	1.41	1.34
20	J	290	ILE	N-CA	-5.61	1.39	1.46
21	W	35	PHE	N-CA	-5.61	1.39	1.46
23	T	107	SER	CA-C	-5.61	1.45	1.52
9	2	75	ARG	CD-NE	5.60	1.54	1.46
7	g	53	LYS	CA-C	-5.60	1.44	1.52
15	H	382	LEU	N-CA	-5.60	1.39	1.46
23	T	196	SER	N-CA	-5.60	1.39	1.46
7	G	68	ARG	CD-NE	5.60	1.54	1.46
28	S	24	LYS	C-O	-5.60	1.17	1.24
28	S	245	GLY	CA-C	-5.60	1.43	1.51
2	b	83	ARG	C-O	-5.60	1.17	1.24
12	l	180	VAL	C-N	5.60	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	ARG	NE-CZ	5.60	1.39	1.33
8	1	74	SER	N-CA	-5.60	1.39	1.45
15	H	272	ILE	CA-C	-5.60	1.45	1.52
18	L	112	LEU	C-N	5.60	1.40	1.33
20	J	280	ASP	C-N	5.60	1.40	1.34
26	Z	779	ALA	N-CA	-5.60	1.39	1.46
16	I	237	ALA	CA-C	-5.60	1.45	1.52
1	a	87	ARG	NE-CZ	5.59	1.39	1.33
28	S	76	PHE	C-N	5.59	1.40	1.33
30	Q	337	ALA	C-N	-5.59	1.26	1.33
31	R	199	GLU	CA-CB	5.59	1.62	1.53
8	h	67	THR	CA-CB	5.59	1.62	1.53
11	k	80	VAL	CA-CB	-5.59	1.47	1.54
15	H	95	HIS	N-CA	-5.59	1.40	1.45
27	N	916	LEU	C-N	5.59	1.41	1.33
30	Q	185	TYR	N-CA	-5.59	1.38	1.46
30	Q	324	GLU	N-CA	-5.59	1.39	1.46
4	d	125	ARG	CZ-NH1	5.59	1.40	1.32
13	m	214	LYS	CA-CB	5.59	1.62	1.53
7	G	83	HIS	ND1-CE1	5.59	1.38	1.32
26	Z	136	ARG	CD-NE	5.59	1.54	1.46
27	N	889	ARG	NE-CZ	5.59	1.39	1.33
32	U	268	LYS	C-N	5.59	1.41	1.33
13	6	60	ASP	CA-C	-5.59	1.45	1.52
23	T	115	SER	CA-C	-5.59	1.44	1.52
26	Z	591	ILE	N-CA	-5.59	1.39	1.46
27	N	921	ARG	CD-NE	5.59	1.54	1.46
7	g	184	SER	C-O	-5.59	1.17	1.23
12	l	168	ASP	CA-C	-5.59	1.45	1.52
6	F	129	VAL	CA-C	-5.59	1.46	1.52
27	N	442	LEU	CA-C	-5.59	1.45	1.52
32	U	224	THR	N-CA	-5.58	1.39	1.46
26	Z	418	ALA	N-CA	-5.58	1.39	1.46
2	b	153	SER	C-N	5.58	1.41	1.33
1	A	2	GLY	N-CA	5.58	1.54	1.45
20	J	200	ARG	NE-CZ	5.58	1.39	1.33
26	Z	149	TRP	CA-CB	-5.58	1.44	1.53
28	S	299	LYS	C-N	5.58	1.42	1.33
31	R	271	ILE	CB-CG1	5.58	1.64	1.53
31	R	292	LEU	CA-CB	5.58	1.61	1.53
26	Z	760	HIS	C-N	5.57	1.41	1.33
32	U	32	ARG	CD-NE	5.57	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	329	LEU	N-CA	-5.57	1.39	1.46
22	V	259	LYS	N-CA	-5.57	1.37	1.45
30	Q	431	SER	N-CA	-5.57	1.39	1.46
32	U	253	ASP	CA-CB	5.57	1.61	1.53
20	J	183	LYS	CA-CB	5.57	1.62	1.53
4	d	95	ARG	CZ-NH2	5.57	1.40	1.33
9	i	63	ILE	CA-CB	-5.57	1.47	1.54
9	2	15	ALA	C-N	5.57	1.40	1.33
10	3	166	ILE	C-N	5.57	1.41	1.33
26	Z	748	LEU	C-O	-5.57	1.17	1.24
12	l	193	VAL	C-N	5.57	1.40	1.33
9	i	193	PRO	N-CD	-5.56	1.40	1.47
11	4	181	VAL	CA-C	-5.56	1.46	1.52
24	X	56	PRO	C-N	5.56	1.40	1.33
26	Z	773	ARG	NE-CZ	5.56	1.39	1.33
26	Z	255	LEU	CA-CB	5.56	1.62	1.53
27	N	906	ARG	NE-CZ	5.56	1.39	1.33
5	e	229	ALA	C-N	5.56	1.41	1.33
2	B	164	ILE	N-CA	-5.56	1.40	1.46
2	b	178	ARG	NE-CZ	5.56	1.39	1.33
33	O	60	ARG	CD-NE	5.56	1.54	1.46
9	i	58	LEU	CA-C	-5.56	1.45	1.52
12	l	162	LEU	N-CA	5.56	1.52	1.46
26	Z	553	ARG	CD-NE	5.56	1.54	1.46
28	S	393	ARG	C-N	5.56	1.40	1.33
9	2	66	HIS	ND1-CE1	5.55	1.38	1.32
11	4	77	PRO	C-N	5.55	1.41	1.33
15	H	82	TRP	C-O	-5.55	1.17	1.24
23	T	181	LEU	N-CA	-5.55	1.39	1.46
26	Z	149	TRP	CZ2-CH2	5.55	1.47	1.37
4	d	78	ALA	CA-C	-5.55	1.45	1.52
13	6	201	GLY	C-N	-5.55	1.26	1.33
31	R	294	ILE	CA-C	-5.55	1.45	1.52
33	O	247	ASN	N-CA	-5.55	1.39	1.46
1	a	126	ARG	CA-CB	5.55	1.62	1.54
5	E	124	ARG	NE-CZ	5.55	1.39	1.33
30	Q	48	ASP	CA-C	5.55	1.58	1.53
18	L	129	VAL	CA-C	-5.55	1.46	1.52
5	e	227	LYS	CA-C	-5.55	1.45	1.52
15	H	262	ALA	CA-CB	5.55	1.61	1.53
16	I	206	GLU	CA-C	-5.55	1.45	1.52
26	Z	766	HIS	ND1-CE1	5.55	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	440	ASP	CA-C	-5.55	1.45	1.52
27	N	771	PHE	CA-C	-5.55	1.46	1.52
31	R	34	THR	C-O	5.55	1.30	1.24
11	k	35	THR	C-N	5.55	1.41	1.33
23	T	221	ALA	N-CA	-5.55	1.39	1.46
19	M	164	ASP	CA-C	-5.54	1.45	1.53
25	Y	24	ILE	CA-CB	5.54	1.61	1.54
5	e	143	ASP	CA-C	-5.54	1.45	1.52
9	i	58	LEU	N-CA	-5.54	1.39	1.46
13	6	130	SER	CA-CB	5.54	1.62	1.53
26	Z	915	ALA	C-N	5.54	1.41	1.33
27	N	61	ALA	C-N	5.54	1.41	1.34
30	Q	12	ARG	CZ-NH1	5.54	1.40	1.32
2	b	46	ALA	CA-C	-5.54	1.45	1.52
4	D	188	GLU	C-N	5.54	1.41	1.34
13	m	109	THR	CA-C	-5.54	1.46	1.52
14	7	112	ASN	CA-C	-5.54	1.45	1.52
27	N	209	LYS	C-N	5.54	1.41	1.34
4	d	152	GLY	N-CA	-5.54	1.37	1.45
7	g	37	LYS	C-N	5.54	1.42	1.33
11	4	116	LEU	CA-C	5.54	1.59	1.52
21	W	107	HIS	CB-CG	5.54	1.57	1.50
23	T	240	LYS	C-N	5.54	1.41	1.33
27	N	908	ARG	CZ-NH1	5.54	1.40	1.32
5	e	148	PHE	N-CA	-5.53	1.38	1.45
6	F	25	LEU	N-CA	5.53	1.53	1.46
16	I	343	ARG	C-N	5.53	1.40	1.33
30	Q	51	ARG	CD-NE	5.53	1.53	1.46
10	j	99	PHE	C-N	5.53	1.41	1.33
16	I	353	PRO	CA-C	-5.53	1.46	1.52
27	N	697	PHE	CA-C	-5.53	1.45	1.52
23	T	28	PRO	CA-CB	-5.53	1.46	1.54
28	S	150	LYS	CA-CB	5.53	1.62	1.53
5	e	64	ARG	NE-CZ	5.53	1.39	1.33
19	M	361	LEU	N-CA	-5.53	1.39	1.46
10	j	200	LYS	N-CA	-5.53	1.39	1.46
12	l	21	THR	C-O	-5.53	1.17	1.23
24	X	69	ILE	N-CA	-5.53	1.42	1.46
6	f	188	LEU	N-CA	-5.53	1.39	1.46
7	g	211	GLU	CA-C	-5.53	1.46	1.52
20	J	163	VAL	C-N	5.53	1.39	1.33
21	W	41	ARG	N-CA	-5.53	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	225	LEU	CA-C	5.53	1.59	1.52
27	N	367	ALA	N-CA	-5.53	1.39	1.46
28	S	208	ILE	C-N	5.53	1.40	1.33
28	S	392	ILE	CA-C	-5.53	1.44	1.52
30	Q	179	LEU	CA-CB	5.52	1.62	1.53
3	c	210	LEU	N-CA	-5.52	1.39	1.46
6	f	121	SER	N-CA	-5.52	1.39	1.46
7	G	87	ARG	CZ-NH2	5.52	1.40	1.33
26	Z	532	HIS	CB-CG	5.52	1.57	1.50
15	H	286	GLU	CA-C	-5.52	1.45	1.52
4	d	173	LEU	N-CA	-5.52	1.39	1.46
16	I	373	GLU	N-CA	-5.52	1.39	1.46
21	W	45	PRO	N-CA	-5.52	1.40	1.47
26	Z	378	GLN	N-CA	5.52	1.53	1.46
28	S	311	GLN	N-CA	-5.52	1.39	1.46
7	g	50	ILE	CA-CB	5.52	1.60	1.53
8	h	103	ASP	CA-CB	5.52	1.61	1.53
10	j	67	ARG	NE-CZ	5.52	1.39	1.33
10	j	197	ARG	NE-CZ	5.52	1.39	1.33
17	K	121	ARG	CA-CB	5.52	1.61	1.53
19	M	174	GLU	CA-CB	5.52	1.62	1.53
26	Z	343	ALA	C-N	5.52	1.41	1.33
14	n	230	THR	C-N	5.52	1.41	1.33
9	i	196	ARG	NE-CZ	5.51	1.39	1.33
14	n	71	VAL	CA-CB	-5.51	1.48	1.54
1	A	59	THR	N-CA	-5.51	1.39	1.46
6	F	141	ALA	CA-C	-5.51	1.46	1.52
12	5	13	ILE	N-CA	-5.51	1.39	1.46
31	R	410	LEU	C-N	5.51	1.41	1.33
10	3	140	THR	C-N	5.51	1.41	1.33
16	I	291	ARG	CD-NE	5.51	1.53	1.46
26	Z	113	SER	N-CA	-5.51	1.39	1.46
3	c	166	ALA	CA-C	-5.51	1.46	1.52
10	j	192	ASP	CA-CB	5.51	1.62	1.53
12	l	76	VAL	CA-CB	-5.51	1.47	1.54
28	S	174	ARG	CD-NE	5.51	1.53	1.46
9	i	149	GLU	CA-CB	5.51	1.61	1.53
29	P	41	VAL	N-CA	5.51	1.53	1.46
6	F	125	ARG	CD-NE	5.50	1.53	1.46
1	a	84	ALA	C-O	-5.50	1.17	1.24
2	b	66	LEU	CA-C	5.50	1.60	1.52
16	I	86	GLU	N-CA	-5.50	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	177	LEU	CA-CB	5.50	1.62	1.53
9	2	165	ASN	CA-C	-5.50	1.45	1.52
17	K	183	GLU	CA-C	-5.50	1.45	1.52
26	Z	940	GLY	CA-C	-5.50	1.44	1.51
27	N	801	THR	CA-CB	5.50	1.62	1.53
30	Q	112	ASP	CA-CB	5.50	1.62	1.53
19	M	378	GLU	N-CA	-5.50	1.39	1.46
27	N	799	VAL	N-CA	-5.50	1.39	1.46
2	b	226	GLY	N-CA	-5.50	1.37	1.45
13	m	85	SER	C-O	-5.50	1.17	1.23
10	3	79	ARG	N-CA	5.50	1.52	1.45
13	6	125	PHE	CA-C	-5.50	1.46	1.52
19	M	346	LYS	CA-C	-5.50	1.46	1.52
22	V	220	GLN	CA-C	-5.50	1.45	1.52
27	N	226	ASN	N-CA	-5.50	1.39	1.46
9	2	43	CYS	N-CA	-5.50	1.39	1.45
9	2	119	THR	CA-C	-5.50	1.46	1.52
23	T	250	MET	CA-C	-5.50	1.46	1.52
28	S	270	ALA	C-N	5.50	1.41	1.33
28	S	470	GLN	N-CA	-5.50	1.39	1.46
29	P	151	GLY	C-O	-5.50	1.17	1.24
6	f	215	VAL	CA-C	-5.50	1.46	1.52
16	I	198	VAL	CA-C	-5.50	1.45	1.52
16	I	273	GLU	CA-C	-5.50	1.45	1.52
2	b	150	VAL	CA-C	-5.49	1.45	1.52
4	d	26	LYS	CA-C	-5.49	1.45	1.52
5	e	136	ILE	C-O	-5.49	1.18	1.24
7	g	73	VAL	N-CA	-5.49	1.39	1.46
19	M	128	PHE	CA-C	-5.49	1.45	1.52
28	S	426	ALA	CA-C	-5.49	1.45	1.52
29	P	394	ASN	CA-C	-5.49	1.46	1.52
14	n	185	TYR	CA-C	-5.49	1.45	1.52
8	1	18	SER	CA-C	-5.49	1.45	1.52
7	G	193	ALA	N-CA	-5.49	1.39	1.46
26	Z	49	LEU	N-CA	5.49	1.53	1.46
31	R	70	TYR	CA-C	5.49	1.64	1.52
8	h	123	PRO	N-CA	-5.49	1.40	1.47
18	L	50	GLN	CA-C	-5.49	1.45	1.52
7	g	169	LYS	CA-CB	5.49	1.61	1.53
14	n	203	ASN	C-N	5.49	1.42	1.33
28	S	287	SER	CA-C	-5.49	1.45	1.52
1	a	168	GLU	CA-CB	5.48	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	51	LEU	CA-C	-5.48	1.45	1.52
20	J	212	ARG	CZ-NH1	5.48	1.40	1.32
23	T	160	ALA	CA-C	-5.48	1.45	1.52
1	a	127	PRO	N-CA	-5.48	1.40	1.47
12	l	167	ARG	CZ-NH2	5.48	1.40	1.33
33	O	166	ARG	C-N	5.48	1.40	1.33
14	n	208	PHE	CA-C	5.48	1.59	1.52
21	W	3	LEU	CA-C	-5.48	1.45	1.52
21	W	59	PRO	CA-C	-5.48	1.45	1.52
26	Z	490	ILE	N-CA	-5.48	1.39	1.46
3	c	87	ILE	CA-CB	-5.48	1.47	1.54
7	g	16	ARG	NE-CZ	5.48	1.39	1.33
10	j	182	TRP	CA-CB	5.48	1.61	1.53
20	J	233	LEU	C-N	5.48	1.41	1.33
24	X	128	VAL	CA-CB	-5.48	1.47	1.54
10	j	63	ASN	N-CA	-5.48	1.39	1.46
15	H	164	SER	N-CA	-5.48	1.36	1.45
20	J	158	LYS	CA-C	-5.48	1.45	1.52
5	e	45	ARG	CZ-NH1	5.47	1.40	1.32
10	j	108	VAL	CA-CB	-5.47	1.47	1.54
12	l	19	ARG	CZ-NH1	5.47	1.40	1.32
27	N	408	LEU	N-CA	-5.47	1.39	1.46
29	P	34	SER	CA-CB	5.47	1.61	1.53
2	b	39	ALA	CA-CB	-5.47	1.45	1.53
14	n	95	TYR	CA-CB	5.47	1.62	1.53
3	c	95	GLN	C-O	5.47	1.30	1.24
9	i	29	LYS	CA-C	5.47	1.59	1.52
12	l	32	LYS	CA-C	-5.47	1.46	1.52
19	M	64	ASP	CA-CB	5.47	1.61	1.53
33	O	186	ASN	CA-CB	5.47	1.61	1.53
13	6	105	TYR	C-N	5.47	1.42	1.33
19	M	201	MET	C-O	-5.47	1.17	1.24
27	N	468	GLU	CA-C	-5.47	1.45	1.52
30	Q	270	ILE	CA-C	-5.47	1.45	1.52
6	f	195	ALA	N-CA	-5.47	1.39	1.46
1	A	88	ALA	C-N	5.47	1.41	1.33
16	I	372	SER	CA-CB	5.46	1.61	1.53
2	b	136	ILE	CA-C	-5.46	1.45	1.52
2	b	196	LEU	N-CA	-5.46	1.39	1.46
7	G	92	ALA	CA-CB	5.46	1.61	1.53
14	7	117	ALA	N-CA	-5.46	1.39	1.45
27	N	94	LYS	CA-C	-5.46	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	354	ALA	CA-CB	5.46	1.61	1.53
10	j	172	ASN	CA-C	-5.46	1.45	1.52
26	Z	454	GLY	N-CA	-5.46	1.39	1.45
26	Z	789	GLN	CA-CB	5.46	1.62	1.53
8	l	112	THR	CA-C	-5.46	1.46	1.52
23	T	121	LYS	N-CA	-5.46	1.39	1.46
26	Z	106	TRP	C-N	5.46	1.41	1.33
32	U	118	PRO	CA-C	-5.46	1.46	1.52
18	L	224	PRO	CA-CB	5.46	1.60	1.53
23	T	40	LEU	N-CA	-5.46	1.39	1.46
1	A	102	ASP	CA-C	-5.45	1.45	1.53
20	J	118	ASP	CA-C	-5.45	1.45	1.52
24	X	110	PRO	CA-C	-5.45	1.46	1.52
1	a	73	VAL	C-N	5.45	1.41	1.33
3	c	65	LEU	N-CA	-5.45	1.39	1.46
4	d	139	ARG	NE-CZ	5.45	1.39	1.33
6	f	139	SER	N-CA	-5.45	1.39	1.46
13	m	40	GLU	CA-CB	5.45	1.62	1.53
17	K	310	THR	N-CA	-5.45	1.39	1.46
18	L	390	ASP	C-N	5.45	1.40	1.33
33	O	119	SER	CA-C	-5.45	1.45	1.52
2	b	123	GLN	CA-C	-5.45	1.46	1.53
9	i	63	ILE	N-CA	-5.45	1.39	1.46
3	C	60	THR	C-O	-5.45	1.17	1.24
7	G	120	THR	C-N	5.45	1.40	1.33
12	l	90	TYR	CA-C	-5.45	1.44	1.52
26	Z	279	THR	C-O	-5.45	1.17	1.24
5	E	50	LEU	N-CA	-5.44	1.38	1.46
22	V	61	TYR	CA-C	-5.44	1.48	1.52
11	k	27	VAL	CA-CB	-5.44	1.47	1.54
13	6	76	HIS	C-O	-5.44	1.17	1.24
6	f	163	ARG	NE-CZ	5.44	1.39	1.33
18	L	76	GLN	C-N	5.44	1.41	1.33
20	J	284	THR	C-N	5.44	1.39	1.33
26	Z	477	TYR	CZ-OH	5.44	1.49	1.38
6	F	1	PHE	CA-CB	5.44	1.64	1.53
26	Z	481	PRO	C-N	5.44	1.40	1.33
17	K	197	LEU	CA-C	-5.44	1.46	1.52
27	N	203	ARG	CD-NE	5.44	1.53	1.46
27	N	618	ARG	CA-C	-5.44	1.45	1.52
29	P	189	LEU	CA-C	-5.44	1.45	1.52
9	i	32	ALA	CA-C	-5.44	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	434	ARG	CZ-NH2	5.44	1.40	1.33
27	N	394	ARG	CA-C	-5.44	1.46	1.52
28	S	130	VAL	CA-C	-5.43	1.45	1.52
5	E	158	ARG	NE-CZ	5.43	1.39	1.33
10	3	40	GLU	N-CA	-5.43	1.39	1.46
10	3	162	LEU	CA-CB	5.43	1.61	1.53
15	H	448	ASP	C-N	5.43	1.40	1.33
15	H	426	ALA	C-O	-5.43	1.17	1.24
7	g	40	ASP	CA-C	-5.43	1.46	1.52
3	C	136	TYR	CA-C	-5.43	1.46	1.52
24	X	25	THR	C-N	5.43	1.40	1.33
27	N	201	LYS	CA-C	5.43	1.59	1.52
10	j	22	ILE	N-CA	-5.43	1.39	1.46
17	K	73	ARG	NE-CZ	5.43	1.39	1.33
2	b	80	PRO	C-N	5.43	1.41	1.33
8	1	107	LYS	C-N	5.43	1.39	1.33
23	T	150	ARG	CZ-NH1	5.43	1.40	1.32
2	b	246	ARG	CZ-NH2	5.42	1.40	1.33
13	m	201	GLY	C-O	-5.42	1.17	1.23
14	n	172	VAL	N-CA	-5.42	1.40	1.46
23	T	198	ASP	C-N	5.42	1.40	1.33
26	Z	55	ARG	CD-NE	5.42	1.53	1.46
27	N	718	GLU	N-CA	-5.42	1.39	1.46
1	a	96	ARG	CZ-NH1	5.42	1.40	1.32
13	m	168	VAL	CA-CB	-5.42	1.46	1.54
3	C	153	SER	N-CA	-5.42	1.39	1.46
14	7	121	SER	C-N	5.42	1.41	1.34
14	7	128	ARG	CZ-NH1	5.42	1.40	1.32
1	a	137	VAL	C-O	-5.42	1.18	1.24
31	R	162	ILE	C-N	5.42	1.40	1.33
32	U	274	MET	C-N	5.42	1.40	1.33
5	E	174	GLU	CA-CB	5.42	1.61	1.53
8	1	95	ALA	CA-C	-5.42	1.45	1.52
31	R	207	ARG	NE-CZ	5.42	1.39	1.33
12	l	160	SER	C-N	5.42	1.40	1.33
18	L	89	ASP	N-CA	-5.42	1.39	1.46
23	T	118	ASN	N-CA	-5.42	1.39	1.46
27	N	380	LEU	C-N	5.42	1.40	1.33
28	S	450	ASN	CA-C	-5.42	1.46	1.53
4	d	29	THR	N-CA	-5.42	1.39	1.45
28	S	192	GLU	C-N	5.42	1.41	1.33
30	Q	237	SER	N-CA	-5.42	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	139	HIS	CE1-NE2	5.42	1.38	1.32
7	G	215	CYS	N-CA	-5.42	1.40	1.46
8	l	159	LEU	N-CA	-5.42	1.39	1.46
1	a	190	TRP	CZ2-CH2	5.41	1.47	1.37
6	f	225	ASP	C-N	5.41	1.41	1.33
10	j	134	ASP	CA-CB	5.41	1.61	1.53
26	Z	137	TYR	C-N	5.41	1.41	1.33
27	N	645	THR	N-CA	-5.41	1.39	1.46
29	P	128	ASN	C-O	-5.41	1.17	1.23
5	e	203	LYS	N-CA	-5.41	1.39	1.46
30	Q	87	GLN	C-N	5.41	1.41	1.33
26	Z	534	PHE	C-N	5.41	1.40	1.33
30	Q	128	GLU	C-N	5.41	1.41	1.33
10	3	135	PHE	CA-CB	5.41	1.62	1.53
17	K	207	ARG	CZ-NH2	5.41	1.40	1.33
1	a	64	PHE	N-CA	-5.41	1.39	1.46
9	i	205	PHE	C-N	5.41	1.40	1.33
27	N	444	HIS	ND1-CE1	5.41	1.38	1.32
30	Q	12	ARG	NE-CZ	5.41	1.39	1.33
27	N	651	PHE	N-CA	5.41	1.53	1.46
30	Q	323	LYS	CA-CB	5.41	1.62	1.53
5	e	64	ARG	CZ-NH2	5.40	1.40	1.33
7	g	72	CYS	CA-C	-5.40	1.45	1.52
19	M	42	ARG	N-CA	-5.40	1.39	1.46
26	Z	923	ILE	C-O	-5.40	1.17	1.24
10	3	67	ARG	NE-CZ	5.40	1.39	1.33
28	S	137	PHE	C-N	5.40	1.40	1.33
12	l	165	ALA	N-CA	-5.40	1.39	1.46
14	n	129	TYR	CA-CB	5.40	1.62	1.53
26	Z	559	LYS	CA-C	-5.40	1.46	1.52
27	N	138	GLU	C-N	5.40	1.41	1.34
30	Q	367	GLY	C-N	5.40	1.40	1.33
32	U	174	LEU	CA-C	5.40	1.59	1.52
7	g	215	CYS	C-O	5.40	1.30	1.24
27	N	616	HIS	N-CA	-5.40	1.39	1.46
7	g	135	GLY	C-N	5.40	1.38	1.33
10	j	59	VAL	C-O	-5.40	1.18	1.24
9	2	199	LYS	N-CA	5.40	1.52	1.45
13	6	191	ALA	CA-C	-5.40	1.45	1.52
18	L	431	THR	CA-C	-5.40	1.46	1.52
26	Z	570	LEU	CA-CB	5.40	1.61	1.53
30	Q	398	TYR	CA-C	-5.40	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	23	ARG	CZ-NH1	5.39	1.40	1.32
2	B	125	GLY	C-N	5.39	1.41	1.33
11	4	131	GLY	C-N	5.39	1.40	1.33
11	4	161	LEU	N-CA	-5.39	1.39	1.46
16	I	139	GLU	N-CA	-5.39	1.39	1.46
18	L	53	HIS	CD2-NE2	5.39	1.43	1.37
21	W	78	ASP	CA-CB	5.39	1.62	1.53
26	Z	134	SER	CA-C	-5.39	1.45	1.52
11	k	93	ARG	C-O	5.39	1.30	1.24
27	N	788	TYR	CA-CB	5.39	1.61	1.53
4	d	14	HIS	N-CA	-5.39	1.40	1.46
11	k	170	LYS	C-N	5.39	1.41	1.33
32	U	158	PRO	N-CD	-5.39	1.40	1.47
1	a	88	ALA	C-N	5.39	1.41	1.33
2	B	241	GLN	CA-CB	5.39	1.61	1.53
17	K	140	HIS	ND1-CE1	5.39	1.38	1.32
18	L	177	GLU	N-CA	-5.39	1.39	1.45
26	Z	399	LEU	C-N	5.39	1.40	1.33
26	Z	574	TYR	C-N	5.39	1.40	1.33
31	R	372	ILE	C-N	5.39	1.39	1.34
27	N	728	LYS	CA-CB	5.39	1.61	1.53
29	P	28	ALA	CA-C	-5.39	1.45	1.52
26	Z	568	LEU	C-N	5.39	1.40	1.33
1	a	225	PHE	CA-CB	5.38	1.63	1.53
3	c	39	ALA	CA-C	-5.38	1.46	1.52
4	d	7	SER	C-N	5.38	1.40	1.33
24	X	28	PRO	C-N	5.38	1.41	1.33
28	S	233	LEU	CA-C	5.38	1.59	1.52
15	H	88	ARG	CZ-NH1	5.38	1.40	1.32
26	Z	435	GLN	CA-C	-5.38	1.45	1.52
32	U	4	GLN	N-CA	-5.38	1.39	1.46
5	E	138	GLY	N-CA	-5.38	1.39	1.45
18	L	118	ILE	C-N	5.38	1.41	1.33
1	a	42	THR	CA-C	-5.38	1.46	1.52
2	b	64	VAL	C-N	5.38	1.40	1.33
4	d	97	THR	CA-C	-5.38	1.45	1.52
2	B	179	TRP	C-N	5.38	1.41	1.33
4	D	83	LEU	CA-CB	5.38	1.61	1.53
20	J	304	LEU	CA-C	-5.38	1.45	1.52
27	N	32	VAL	C-O	5.38	1.30	1.24
27	N	889	ARG	CA-C	-5.38	1.46	1.52
1	A	126	ARG	CZ-NH2	5.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	77	ARG	CZ-NH1	5.38	1.40	1.32
12	l	57	THR	C-N	5.37	1.41	1.33
29	P	73	ASP	N-CA	-5.37	1.39	1.46
32	U	79	MET	C-N	5.37	1.41	1.33
8	h	124	TYR	CA-CB	5.37	1.62	1.53
12	l	202	GLU	CA-C	-5.37	1.45	1.52
14	n	48	ASN	C-N	-5.37	1.26	1.33
1	A	6	HIS	ND1-CE1	5.37	1.38	1.32
6	F	185	PRO	CA-C	-5.37	1.44	1.52
6	f	197	SER	C-N	5.37	1.41	1.33
2	b	48	GLU	C-N	5.37	1.40	1.33
26	Z	106	TRP	CA-CB	5.37	1.60	1.53
26	Z	824	ASN	C-N	5.37	1.40	1.33
12	l	64	ARG	NE-CZ	5.37	1.39	1.33
14	n	195	PHE	C-N	5.37	1.41	1.33
31	R	23	ASN	N-CA	-5.37	1.39	1.46
31	R	152	LYS	N-CA	-5.37	1.40	1.46
5	e	205	ASP	CA-C	-5.37	1.46	1.52
12	l	62	GLN	N-CA	-5.37	1.39	1.46
6	F	187	GLU	N-CA	-5.37	1.39	1.46
16	I	202	LEU	CB-CG	5.37	1.64	1.53
21	W	146	GLU	C-N	5.37	1.39	1.34
21	W	195	GLY	CA-C	-5.37	1.44	1.51
28	S	241	PHE	CA-C	-5.37	1.45	1.52
28	S	294	ILE	CA-CB	-5.37	1.47	1.54
15	H	455	LYS	CA-CB	5.36	1.61	1.53
24	X	103	GLU	CA-C	-5.36	1.46	1.52
2	b	9	LEU	N-CA	5.36	1.52	1.46
14	n	104	ARG	N-CA	-5.36	1.39	1.46
4	d	171	GLU	C-O	-5.36	1.17	1.24
11	4	28	LEU	C-N	5.36	1.40	1.33
18	L	259	SER	CA-CB	5.36	1.61	1.53
20	J	204	HIS	N-CA	-5.36	1.40	1.46
27	N	606	VAL	C-N	5.36	1.41	1.33
8	h	28	ASN	CA-C	-5.36	1.45	1.52
10	j	147	GLY	C-N	5.36	1.40	1.33
12	l	31	VAL	CA-CB	-5.36	1.48	1.54
13	m	62	ASP	N-CA	-5.36	1.40	1.46
16	I	235	ALA	C-N	5.36	1.41	1.33
30	Q	217	GLU	N-CA	-5.36	1.40	1.46
11	k	85	ARG	NE-CZ	5.36	1.39	1.33
11	4	107	TYR	C-N	5.36	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	104	ASP	CA-CB	5.36	1.63	1.54
3	c	159	TRP	CD2-CE3	-5.36	1.31	1.40
14	n	146	PHE	N-CA	-5.36	1.39	1.46
26	Z	287	ARG	CZ-NH1	5.36	1.40	1.32
4	d	117	ARG	N-CA	-5.35	1.39	1.46
15	H	60	GLU	C-O	-5.35	1.17	1.24
4	d	46	ARG	CZ-NH2	5.35	1.40	1.33
7	g	163	LYS	CA-C	-5.35	1.45	1.52
14	n	225	ILE	C-O	-5.35	1.18	1.24
5	E	90	THR	C-N	5.35	1.41	1.33
13	6	212	VAL	N-CA	-5.35	1.39	1.46
15	H	432	ARG	CZ-NH1	5.35	1.40	1.32
17	K	309	SER	CA-CB	5.35	1.62	1.53
29	P	300	VAL	CA-C	-5.35	1.45	1.52
1	a	92	ALA	CA-C	-5.35	1.45	1.52
6	F	104	VAL	N-CA	-5.35	1.39	1.46
14	7	209	LYS	CA-CB	-5.35	1.46	1.53
19	M	224	PRO	C-N	5.35	1.39	1.33
4	d	23	GLU	N-CA	-5.35	1.39	1.46
8	h	86	CYS	C-N	5.35	1.40	1.33
11	4	190	ARG	CD-NE	5.35	1.53	1.46
19	M	264	ARG	NE-CZ	5.35	1.39	1.33
27	N	596	LEU	CB-CG	5.35	1.64	1.53
30	Q	74	LEU	C-N	5.35	1.41	1.33
4	d	47	ARG	NE-CZ	5.35	1.39	1.33
17	K	48	TYR	C-N	5.35	1.41	1.33
26	Z	708	GLY	C-N	-5.35	1.27	1.33
27	N	793	GLY	N-CA	-5.35	1.39	1.45
4	d	171	GLU	N-CA	-5.34	1.39	1.46
12	l	33	LYS	N-CA	-5.34	1.39	1.46
17	K	193	VAL	CA-C	-5.34	1.46	1.52
33	O	301	PHE	CA-CB	5.34	1.61	1.53
15	H	186	PRO	C-O	5.34	1.29	1.23
18	L	433	GLU	N-CA	-5.34	1.39	1.45
9	i	213	LEU	C-N	5.34	1.40	1.33
13	m	85	SER	CA-CB	5.34	1.62	1.53
4	D	224	SER	CA-CB	5.34	1.62	1.53
23	T	248	GLU	N-CA	-5.34	1.39	1.46
26	Z	547	MET	N-CA	-5.34	1.39	1.46
27	N	490	LEU	C-N	5.34	1.40	1.33
27	N	611	LYS	N-CA	-5.34	1.39	1.46
6	f	100	ARG	CD-NE	5.34	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	133	ILE	CA-CB	-5.34	1.48	1.54
8	h	19	ARG	NE-CZ	5.34	1.39	1.33
13	6	185	ARG	CZ-NH2	5.34	1.40	1.33
3	C	177	MET	N-CA	-5.34	1.40	1.46
31	R	149	ASN	C-N	5.34	1.41	1.33
31	R	287	GLN	CA-C	-5.34	1.46	1.52
8	h	45	ARG	NE-CZ	5.34	1.39	1.33
11	k	70	ARG	NE-CZ	5.34	1.39	1.33
4	D	95	ARG	C-N	5.34	1.41	1.33
11	4	132	ALA	N-CA	-5.34	1.40	1.46
17	K	235	ILE	CA-C	-5.34	1.45	1.52
19	M	339	ARG	CZ-NH1	5.34	1.40	1.32
31	R	54	ILE	CA-C	-5.34	1.46	1.52
13	m	38	ARG	NE-CZ	5.33	1.39	1.33
8	1	12	VAL	C-N	5.33	1.40	1.33
19	M	408	SER	N-CA	-5.33	1.39	1.46
13	m	79	HIS	CA-C	-5.33	1.44	1.52
11	4	63	ASN	CA-C	-5.33	1.46	1.52
12	5	94	GLY	C-N	5.33	1.40	1.33
7	g	36	ILE	C-N	5.33	1.41	1.33
3	C	215	ILE	C-N	5.33	1.41	1.33
28	S	383	LEU	CA-C	-5.33	1.45	1.52
20	J	139	VAL	N-CA	-5.33	1.40	1.46
27	N	111	GLN	C-N	5.33	1.40	1.33
18	L	241	ALA	N-CA	-5.33	1.39	1.46
12	l	102	CYS	CA-C	-5.33	1.46	1.52
4	D	116	GLN	CA-C	-5.33	1.45	1.52
11	4	179	VAL	N-CA	-5.33	1.40	1.46
14	7	138	SER	CA-CB	5.33	1.62	1.53
20	J	252	SER	CA-CB	5.33	1.60	1.53
33	O	119	SER	C-N	5.33	1.40	1.33
1	a	37	ARG	CZ-NH2	5.32	1.40	1.33
7	g	171	GLU	N-CA	5.32	1.53	1.46
9	i	23	GLY	CA-C	-5.32	1.44	1.51
9	i	72	ARG	CZ-NH2	5.32	1.40	1.33
15	H	190	ARG	CA-C	-5.32	1.45	1.52
26	Z	401	VAL	C-N	5.32	1.41	1.34
26	Z	856	HIS	CA-C	-5.32	1.45	1.52
27	N	40	SER	C-N	5.32	1.40	1.33
27	N	347	SER	N-CA	-5.32	1.39	1.46
28	S	450	ASN	N-CA	-5.32	1.38	1.46
29	P	90	LYS	CA-C	-5.32	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	217	ILE	CA-CB	5.32	1.60	1.54
27	N	875	LEU	CA-C	-5.32	1.47	1.53
3	c	92	ILE	CA-CB	-5.32	1.47	1.54
1	A	227	LEU	C-N	5.32	1.40	1.33
9	2	161	ALA	C-N	5.32	1.40	1.33
13	6	43	VAL	CA-C	-5.32	1.46	1.52
18	L	167	VAL	CA-C	5.32	1.59	1.52
27	N	898	GLY	C-N	5.32	1.40	1.33
6	f	95	SER	CA-CB	5.32	1.61	1.53
26	Z	333	GLY	C-N	5.32	1.40	1.33
27	N	196	THR	CA-C	5.32	1.59	1.52
5	E	12	ARG	CD-NE	5.32	1.53	1.46
2	b	178	ARG	CZ-NH1	5.31	1.40	1.32
11	4	107	TYR	CA-C	-5.31	1.46	1.52
1	a	15	ARG	CZ-NH2	5.31	1.40	1.33
10	3	106	PRO	CA-CB	5.31	1.60	1.53
27	N	45	ASP	CA-CB	5.31	1.61	1.53
27	N	363	ALA	N-CA	-5.31	1.40	1.46
27	N	392	GLY	CA-C	-5.31	1.44	1.51
28	S	317	HIS	CA-CB	5.31	1.61	1.53
29	P	234	TYR	CA-C	-5.31	1.45	1.52
13	6	47	GLY	N-CA	5.31	1.50	1.45
17	K	376	ASP	N-CA	-5.31	1.39	1.46
19	M	45	ARG	NE-CZ	5.31	1.38	1.33
28	S	456	ASP	CA-CB	5.31	1.60	1.53
8	h	178	LEU	N-CA	-5.31	1.39	1.46
2	B	207	ASP	CA-CB	5.31	1.61	1.53
25	Y	33	ASP	C-N	5.31	1.41	1.33
33	O	15	ARG	CA-C	-5.31	1.45	1.52
33	O	100	ASP	CA-C	-5.31	1.45	1.52
8	h	183	VAL	N-CA	-5.31	1.39	1.46
26	Z	907	GLY	C-N	5.31	1.41	1.33
30	Q	332	ARG	CZ-NH1	5.31	1.40	1.32
1	a	55	LEU	N-CA	-5.30	1.39	1.46
3	c	235	LYS	C-N	5.30	1.40	1.33
4	d	27	ARG	N-CA	-5.30	1.39	1.46
18	L	243	PHE	N-CA	-5.30	1.39	1.46
22	V	131	GLN	C-N	5.30	1.40	1.33
32	U	263	LYS	N-CA	-5.30	1.39	1.46
17	K	53	LYS	N-CA	-5.30	1.39	1.46
26	Z	506	LEU	N-CA	-5.30	1.39	1.46
12	l	106	ARG	CZ-NH2	5.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	396	ARG	CZ-NH1	5.30	1.40	1.32
26	Z	756	MET	C-N	5.30	1.41	1.34
7	g	37	LYS	N-CA	-5.30	1.39	1.46
9	i	46	ALA	CA-CB	5.30	1.61	1.53
11	k	148	TYR	N-CA	-5.30	1.39	1.46
6	F	148	PRO	N-CA	-5.30	1.40	1.47
16	I	434	GLY	C-N	5.30	1.41	1.33
19	M	243	PHE	CA-CB	5.30	1.59	1.52
1	a	117	GLN	N-CA	-5.30	1.40	1.46
4	D	227	ILE	CA-C	-5.30	1.46	1.52
29	P	226	LYS	N-CA	-5.30	1.40	1.46
3	c	42	GLY	CA-C	-5.30	1.46	1.51
17	K	362	LEU	N-CA	-5.30	1.39	1.46
22	V	85	ASP	C-N	5.30	1.40	1.33
26	Z	561	ASP	CA-CB	5.30	1.61	1.53
5	E	85	ARG	CD-NE	5.29	1.53	1.46
7	G	186	ARG	NE-CZ	5.29	1.38	1.33
20	J	210	PHE	C-N	5.29	1.40	1.33
25	Y	31	GLU	C-N	5.29	1.38	1.33
33	O	28	GLN	C-N	5.29	1.40	1.33
4	d	18	VAL	N-CA	-5.29	1.40	1.46
5	e	68	CYS	CA-C	-5.29	1.45	1.52
13	m	167	LYS	C-O	-5.29	1.17	1.24
5	E	136	ILE	CA-C	-5.29	1.46	1.52
9	i	157	ASP	CA-C	-5.29	1.45	1.52
13	6	43	VAL	C-O	5.29	1.30	1.24
27	N	13	LEU	CA-C	-5.29	1.46	1.52
3	c	13	SER	CA-CB	5.29	1.60	1.53
3	c	132	VAL	C-O	-5.29	1.18	1.24
7	g	176	VAL	CA-CB	-5.29	1.47	1.54
14	n	225	ILE	CA-CB	5.29	1.60	1.54
1	A	96	ARG	CD-NE	5.29	1.53	1.46
15	H	373	ARG	NE-CZ	5.29	1.38	1.33
12	l	64	ARG	CZ-NH1	5.29	1.40	1.32
29	P	138	ARG	C-N	5.29	1.39	1.34
29	P	402	PHE	C-O	-5.29	1.17	1.24
31	R	258	LEU	C-N	5.29	1.40	1.33
7	g	234	GLU	N-CA	-5.29	1.39	1.46
14	7	207	THR	CA-CB	-5.29	1.46	1.53
28	S	379	LEU	N-CA	-5.29	1.39	1.46
14	n	97	ALA	CA-CB	5.28	1.61	1.53
1	A	146	TYR	N-CA	-5.28	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	75	LYS	C-N	5.28	1.40	1.33
19	M	418	GLY	CA-C	-5.28	1.45	1.51
20	J	95	ILE	C-N	5.28	1.39	1.33
26	Z	103	TYR	C-N	5.28	1.41	1.33
27	N	677	ASP	C-N	5.28	1.40	1.33
9	i	196	ARG	CZ-NH2	5.28	1.40	1.33
13	6	131	TYR	CA-C	-5.28	1.46	1.52
15	H	398	VAL	CA-CB	-5.28	1.46	1.55
17	K	211	LEU	N-CA	-5.28	1.40	1.46
20	J	18	GLY	CA-C	-5.28	1.46	1.52
32	U	247	ILE	N-CA	-5.28	1.40	1.46
6	f	71	LEU	CA-C	5.28	1.59	1.52
19	M	402	ALA	CA-C	-5.28	1.46	1.52
27	N	152	LEU	N-CA	-5.28	1.40	1.46
27	N	290	LEU	C-O	-5.28	1.17	1.24
10	j	176	ARG	N-CA	-5.28	1.39	1.46
13	m	221	ARG	CZ-NH2	5.28	1.40	1.33
7	G	187	GLU	N-CA	-5.28	1.39	1.46
10	3	111	ILE	CA-C	-5.28	1.46	1.52
27	N	515	ARG	CZ-NH2	5.28	1.40	1.33
30	Q	176	ASP	C-N	5.28	1.40	1.33
31	R	413	LYS	CA-C	-5.28	1.46	1.52
33	O	283	HIS	CA-CB	5.28	1.60	1.53
14	7	100	MET	CA-C	-5.28	1.46	1.52
31	R	153	THR	C-O	-5.28	1.17	1.24
4	d	21	ALA	N-CA	-5.27	1.39	1.46
6	F	3	ASN	CA-C	-5.27	1.46	1.53
18	L	357	ARG	CZ-NH2	5.27	1.40	1.33
22	V	164	LEU	C-N	-5.27	1.27	1.33
5	E	223	TYR	CA-C	-5.27	1.46	1.52
16	I	71	LEU	CA-CB	5.27	1.61	1.53
19	M	50	ARG	CZ-NH1	5.27	1.40	1.32
30	Q	197	SER	C-N	5.27	1.41	1.33
32	U	49	THR	C-N	5.27	1.40	1.33
4	d	126	PRO	C-N	5.27	1.40	1.33
4	d	237	GLU	CA-C	-5.27	1.45	1.52
6	f	232	TYR	CA-C	-5.27	1.45	1.52
22	V	198	SER	C-N	5.27	1.40	1.33
26	Z	846	PHE	CA-C	-5.27	1.46	1.52
27	N	917	ILE	N-CA	-5.27	1.39	1.46
28	S	34	LEU	CA-CB	5.27	1.61	1.53
4	d	46	ARG	CZ-NH1	5.27	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	241	LYS	C-N	5.27	1.41	1.33
8	h	17	ASP	CA-CB	5.27	1.60	1.53
1	A	5	ARG	CD-NE	5.27	1.53	1.46
20	J	43	ARG	CZ-NH1	5.27	1.40	1.32
23	T	202	LEU	C-O	-5.27	1.18	1.24
28	S	469	ASN	CA-C	-5.27	1.46	1.52
7	g	108	PHE	CA-C	-5.27	1.45	1.52
15	H	281	GLN	CA-CB	5.27	1.59	1.52
18	L	192	GLU	C-N	5.27	1.40	1.33
19	M	375	ASN	N-CA	-5.27	1.40	1.46
5	e	220	PHE	CA-C	-5.26	1.46	1.52
5	E	133	ALA	CA-C	-5.26	1.46	1.52
18	L	143	GLY	CA-C	-5.26	1.44	1.51
26	Z	79	THR	CA-C	-5.26	1.46	1.52
29	P	113	ASN	N-CA	-5.26	1.40	1.46
3	c	50	LYS	C-N	5.26	1.40	1.33
7	g	241	LYS	N-CA	-5.26	1.40	1.46
16	I	357	THR	N-CA	5.26	1.52	1.46
19	M	213	ARG	CZ-NH1	5.26	1.40	1.32
31	R	277	LEU	C-N	5.26	1.41	1.33
5	e	135	LEU	CA-CB	5.26	1.60	1.53
9	2	72	ARG	CZ-NH2	5.26	1.40	1.33
19	M	203	ARG	NE-CZ	5.26	1.38	1.33
27	N	159	GLU	CA-C	-5.26	1.46	1.52
13	m	151	ASP	CA-CB	-5.26	1.45	1.53
13	m	151	ASP	C-O	-5.26	1.18	1.24
2	B	4	ARG	CZ-NH2	5.26	1.40	1.33
4	D	70	VAL	C-N	5.26	1.40	1.33
27	N	470	LEU	CA-C	-5.26	1.46	1.52
27	N	771	PHE	C-N	5.26	1.41	1.33
29	P	110	LEU	CA-C	-5.26	1.45	1.52
3	c	132	VAL	N-CA	5.26	1.52	1.46
28	S	80	VAL	N-CA	-5.26	1.39	1.46
3	c	175	LEU	N-CA	-5.26	1.40	1.46
1	A	124	TYR	N-CA	-5.26	1.40	1.46
2	B	192	ALA	CA-CB	5.26	1.61	1.53
30	Q	158	ILE	CA-C	-5.26	1.46	1.52
6	F	74	ALA	C-O	5.25	1.29	1.24
19	M	171	GLU	C-N	5.25	1.40	1.33
7	g	144	LEU	C-N	5.25	1.41	1.33
11	4	4	ILE	C-N	5.25	1.41	1.33
17	K	349	ARG	C-N	5.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	320	SER	N-CA	-5.25	1.39	1.46
2	b	55	LEU	C-N	5.25	1.40	1.33
7	g	160	ALA	C-N	5.25	1.40	1.33
4	D	190	VAL	CA-CB	5.25	1.61	1.54
10	3	202	ARG	NE-CZ	5.25	1.38	1.33
17	K	101	GLU	CA-CB	5.25	1.60	1.53
26	Z	412	GLY	CA-C	5.25	1.58	1.52
29	P	171	MET	CA-C	-5.25	1.46	1.52
11	k	92	ILE	CA-CB	-5.25	1.48	1.54
1	A	72	MET	CA-C	-5.25	1.46	1.52
13	6	213	ARG	CD-NE	5.25	1.53	1.46
23	T	187	ASP	CA-C	-5.25	1.46	1.52
26	Z	399	LEU	CA-CB	5.25	1.61	1.53
32	U	113	TYR	N-CA	5.25	1.52	1.46
4	d	4	ARG	CD-NE	5.25	1.53	1.46
4	d	180	LYS	CA-CB	5.25	1.61	1.53
26	Z	344	LYS	N-CA	-5.25	1.40	1.46
28	S	338	MET	CA-CB	5.25	1.60	1.53
16	I	59	LEU	N-CA	-5.25	1.40	1.46
17	K	214	PRO	CA-CB	5.25	1.59	1.54
18	L	73	GLN	N-CA	5.25	1.52	1.46
6	f	135	GLY	C-N	5.25	1.40	1.33
12	l	4	LEU	C-N	5.25	1.40	1.33
11	4	99	GLN	CA-CB	5.25	1.62	1.53
12	l	25	TRP	N-CA	-5.24	1.39	1.46
2	B	141	GLU	C-N	5.24	1.41	1.33
4	D	223	SER	CA-C	-5.24	1.46	1.52
15	H	89	GLN	N-CA	-5.24	1.39	1.46
18	L	398	ALA	C-N	5.24	1.40	1.34
28	S	231	ALA	C-N	5.24	1.40	1.33
8	h	115	LEU	CA-CB	5.24	1.61	1.53
2	B	17	LYS	N-CA	-5.24	1.39	1.46
22	V	258	GLU	N-CA	-5.24	1.39	1.46
12	l	86	LEU	N-CA	-5.24	1.40	1.46
3	C	128	ARG	CD-NE	5.24	1.53	1.46
20	J	393	ASN	C-O	-5.24	1.18	1.24
21	W	109	ARG	CA-C	-5.24	1.46	1.52
27	N	876	PRO	N-CA	-5.24	1.40	1.47
13	m	48	ASP	CA-C	-5.24	1.46	1.53
24	X	123	ASN	CA-C	-5.24	1.46	1.52
10	3	25	ASP	CA-CB	5.24	1.61	1.53
13	6	62	ASP	C-N	5.24	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	352	VAL	CA-CB	-5.24	1.48	1.54
7	G	167	SER	N-CA	-5.24	1.40	1.46
28	S	132	ALA	C-O	-5.24	1.17	1.24
33	O	369	ARG	CZ-NH1	5.24	1.40	1.32
13	6	63	ALA	CA-C	-5.23	1.46	1.52
15	H	94	GLU	CA-CB	5.23	1.62	1.53
20	J	298	ASP	C-N	5.23	1.38	1.33
10	j	162	LEU	C-N	5.23	1.41	1.33
1	A	149	ASP	N-CA	-5.23	1.37	1.45
5	E	114	ARG	CD-NE	5.23	1.53	1.46
26	Z	941	ARG	CA-C	5.23	1.58	1.52
14	n	8	GLY	N-CA	5.23	1.51	1.45
7	G	33	SER	C-N	5.23	1.41	1.33
8	1	180	ALA	CA-CB	5.23	1.61	1.53
26	Z	591	ILE	C-N	5.23	1.40	1.33
28	S	483	GLU	CA-C	-5.23	1.45	1.52
5	e	124	ARG	CD-NE	5.23	1.53	1.46
23	T	108	LEU	C-N	5.23	1.40	1.33
26	Z	240	ASN	CA-C	-5.23	1.46	1.52
1	a	63	ILE	CA-C	-5.23	1.46	1.52
14	n	166	PRO	CA-C	-5.23	1.44	1.52
26	Z	34	GLU	CA-C	5.23	1.59	1.52
9	i	145	ASP	CA-C	-5.22	1.47	1.53
9	i	211	ALA	C-N	5.22	1.39	1.33
5	E	136	ILE	C-O	5.22	1.29	1.24
20	J	20	LYS	CA-CB	5.22	1.60	1.53
22	V	226	LYS	C-N	5.22	1.41	1.33
33	O	228	TYR	CA-C	-5.22	1.45	1.52
11	k	36	ARG	CZ-NH1	5.22	1.40	1.32
19	M	42	ARG	CZ-NH2	5.22	1.40	1.33
27	N	562	THR	C-O	-5.22	1.17	1.24
30	Q	189	ARG	N-CA	-5.22	1.39	1.46
14	7	54	SER	N-CA	-5.22	1.39	1.45
17	K	286	THR	CA-C	-5.22	1.46	1.52
19	M	190	ILE	C-N	5.22	1.40	1.33
26	Z	487	SER	CA-C	-5.22	1.46	1.52
5	e	101	VAL	C-N	-5.22	1.27	1.33
8	h	52	THR	N-CA	-5.22	1.39	1.46
5	E	16	VAL	CA-C	-5.22	1.46	1.52
5	E	178	GLU	N-CA	-5.22	1.39	1.46
17	K	215	PRO	N-CA	-5.22	1.42	1.46
26	Z	513	ALA	N-CA	-5.22	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	375	HIS	CA-C	-5.22	1.45	1.52
29	P	223	LEU	CA-CB	5.22	1.61	1.53
30	Q	195	LYS	CA-CB	5.22	1.61	1.53
33	O	95	SER	CA-C	-5.22	1.46	1.52
2	b	210	GLU	CA-C	-5.21	1.46	1.52
9	i	77	VAL	CA-CB	-5.21	1.48	1.54
14	n	137	TYR	C-N	5.21	1.40	1.33
15	H	62	ARG	CZ-NH1	5.21	1.40	1.32
26	Z	42	ASP	C-O	-5.21	1.18	1.24
27	N	94	LYS	CA-CB	5.21	1.61	1.53
30	Q	308	ASN	N-CA	-5.21	1.40	1.46
1	A	50	VAL	C-N	5.21	1.39	1.33
2	B	197	LYS	C-N	5.21	1.41	1.33
8	1	187	ILE	C-N	5.21	1.40	1.33
5	e	190	LEU	N-CA	-5.21	1.40	1.46
5	e	206	GLU	N-CA	-5.21	1.39	1.46
5	e	241	ALA	N-CA	-5.21	1.40	1.46
4	D	124	VAL	CA-C	-5.21	1.46	1.52
14	7	95	TYR	CA-CB	5.21	1.61	1.53
7	g	66	VAL	CA-C	5.21	1.58	1.52
5	e	187	GLU	C-N	5.21	1.40	1.33
15	H	88	ARG	CA-C	-5.21	1.46	1.52
19	M	261	LYS	CA-C	-5.21	1.46	1.52
20	J	116	ARG	C-N	5.21	1.41	1.33
23	T	146	ILE	C-N	5.21	1.40	1.33
6	f	94	SER	CA-CB	5.21	1.61	1.53
4	D	6	LEU	CA-C	-5.21	1.46	1.53
16	I	61	ARG	NE-CZ	5.21	1.38	1.33
16	I	212	GLY	CA-C	-5.21	1.44	1.51
28	S	238	LEU	CA-C	-5.21	1.46	1.52
33	O	26	PHE	N-CA	-5.21	1.40	1.46
10	j	56	ALA	N-CA	-5.21	1.40	1.46
18	L	404	ARG	CD-NE	5.21	1.53	1.46
28	S	160	ARG	CA-CB	5.21	1.61	1.53
2	b	15	SER	CA-CB	5.20	1.60	1.53
7	g	174	LYS	N-CA	-5.20	1.40	1.46
18	L	90	LYS	N-CA	-5.20	1.40	1.46
26	Z	462	VAL	C-N	5.20	1.41	1.33
27	N	158	LEU	CA-C	-5.20	1.46	1.52
32	U	216	ASN	N-CA	-5.20	1.39	1.46
33	O	325	GLU	C-N	5.20	1.40	1.33
6	f	104	VAL	C-O	-5.20	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	124	ASP	CA-C	-5.20	1.46	1.52
4	D	82	ILE	N-CA	-5.20	1.40	1.46
20	J	329	ARG	NE-CZ	5.20	1.38	1.33
10	3	65	MET	CA-CB	5.20	1.61	1.53
20	J	368	TYR	C-N	5.20	1.40	1.33
32	U	145	ASP	CA-C	-5.20	1.45	1.53
33	O	172	TYR	N-CA	-5.20	1.39	1.46
33	O	277	ILE	N-CA	-5.20	1.41	1.46
6	f	201	ARG	NE-CZ	5.20	1.38	1.33
8	h	114	PRO	CA-CB	-5.20	1.46	1.53
11	k	158	LEU	CA-CB	5.20	1.61	1.53
13	6	108	HIS	N-CA	-5.20	1.40	1.46
15	H	434	ARG	CA-C	5.20	1.58	1.52
13	m	198	VAL	CA-CB	-5.20	1.47	1.54
16	I	79	SER	CA-C	5.20	1.59	1.52
23	T	46	ILE	CA-C	5.20	1.58	1.52
1	a	114	ASN	CA-C	-5.19	1.46	1.52
19	M	45	ARG	CD-NE	5.19	1.53	1.46
29	P	12	ASP	C-N	5.19	1.40	1.33
9	2	70	THR	C-N	5.19	1.40	1.33
20	J	333	ARG	CZ-NH1	5.19	1.40	1.32
21	W	153	LEU	CA-C	-5.19	1.46	1.52
33	O	50	ASP	C-N	5.19	1.41	1.33
1	a	60	VAL	C-O	-5.19	1.18	1.24
10	j	144	GLN	C-N	5.19	1.40	1.33
4	D	160	GLN	N-CA	-5.19	1.39	1.45
5	E	91	HIS	ND1-CE1	5.19	1.37	1.32
23	T	74	ASN	CA-C	-5.19	1.46	1.52
27	N	398	ARG	NE-CZ	5.19	1.38	1.33
33	O	184	ASP	C-N	5.19	1.40	1.33
2	b	159	TRP	C-O	5.19	1.29	1.23
21	W	127	ARG	CA-CB	5.19	1.61	1.53
28	S	194	LEU	CA-CB	5.19	1.61	1.53
4	d	125	ARG	CZ-NH2	5.19	1.40	1.33
9	i	48	THR	C-N	5.19	1.40	1.33
10	j	33	LEU	CA-C	-5.19	1.46	1.52
3	C	186	ASP	C-N	5.19	1.41	1.33
9	2	144	GLN	C-N	5.19	1.40	1.33
10	3	45	TYR	CA-C	-5.19	1.46	1.53
20	J	125	VAL	N-CA	5.19	1.52	1.46
20	J	391	ASN	N-CA	-5.19	1.40	1.46
27	N	394	ARG	NE-CZ	5.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	296	SER	N-CA	-5.19	1.40	1.46
5	e	114	ARG	NE-CZ	5.18	1.38	1.33
8	h	135	TYR	CA-CB	5.18	1.61	1.53
1	A	160	THR	C-N	5.18	1.40	1.33
9	i	212	VAL	C-N	5.18	1.40	1.33
23	T	41	ILE	N-CA	-5.18	1.41	1.47
26	Z	102	ILE	N-CA	-5.18	1.39	1.46
26	Z	474	LEU	CA-C	5.18	1.59	1.52
26	Z	880	SER	C-N	5.18	1.40	1.33
27	N	261	LEU	C-N	5.18	1.40	1.33
10	3	78	GLU	C-N	5.18	1.40	1.33
26	Z	929	VAL	CA-C	-5.18	1.46	1.52
2	b	106	PRO	C-N	5.18	1.41	1.33
16	I	242	ALA	N-CA	-5.18	1.39	1.45
27	N	160	GLY	C-O	-5.18	1.18	1.24
31	R	206	ARG	NE-CZ	5.18	1.38	1.33
33	O	108	GLU	N-CA	-5.18	1.40	1.46
2	b	32	VAL	CA-CB	-5.18	1.48	1.54
3	c	62	THR	CA-CB	5.18	1.62	1.53
7	g	178	HIS	CG-CD2	5.18	1.41	1.35
13	m	202	LEU	C-N	5.18	1.40	1.33
3	C	82	ASP	CA-C	-5.18	1.46	1.52
5	E	45	ARG	NE-CZ	5.18	1.38	1.33
8	1	172	VAL	CA-CB	-5.18	1.48	1.54
11	4	159	ASP	C-N	5.18	1.41	1.33
18	L	354	GLU	C-O	5.18	1.30	1.24
28	S	425	ARG	N-CA	-5.18	1.40	1.46
32	U	173	HIS	CG-ND1	-5.18	1.32	1.38
6	f	193	VAL	C-O	-5.17	1.18	1.24
4	D	205	ALA	N-CA	-5.17	1.39	1.46
20	J	165	GLU	N-CA	-5.17	1.40	1.46
26	Z	732	ILE	N-CA	-5.17	1.40	1.46
18	L	428	LEU	CA-C	5.17	1.59	1.52
28	S	307	LEU	C-N	5.17	1.40	1.33
32	U	224	THR	C-N	5.17	1.40	1.33
9	i	19	ARG	NE-CZ	5.17	1.38	1.33
6	F	145	GLU	N-CA	-5.17	1.40	1.46
31	R	259	PHE	C-N	5.17	1.41	1.33
17	K	259	ARG	CD-NE	5.17	1.53	1.46
10	j	84	GLU	CA-CB	5.17	1.61	1.53
16	I	372	SER	CA-C	-5.17	1.46	1.52
18	L	319	GLY	CA-C	-5.17	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	289	LYS	CA-C	-5.17	1.46	1.52
26	Z	21	GLU	N-CA	-5.17	1.40	1.46
27	N	914	VAL	C-N	5.17	1.40	1.33
4	d	64	LYS	CA-CB	5.17	1.60	1.53
7	g	196	ILE	CA-CB	-5.17	1.48	1.54
11	k	12	SER	CA-C	-5.17	1.46	1.52
9	i	145	ASP	N-CA	-5.17	1.39	1.46
15	H	261	ARG	NE-CZ	5.17	1.38	1.33
26	Z	235	GLN	C-N	5.17	1.39	1.33
16	I	315	GLY	CA-C	-5.16	1.45	1.52
28	S	184	TRP	C-O	5.16	1.30	1.24
31	R	301	TYR	CA-C	-5.16	1.46	1.52
31	R	323	ASN	N-CA	-5.16	1.40	1.46
11	4	81	SER	CA-C	-5.16	1.46	1.52
15	H	165	PRO	CA-C	-5.16	1.45	1.52
18	L	119	VAL	CA-C	-5.16	1.46	1.52
30	Q	306	TYR	C-N	5.16	1.41	1.33
7	g	134	PHE	C-N	5.16	1.38	1.32
5	E	74	THR	C-N	5.16	1.41	1.33
30	Q	268	SER	CA-CB	5.16	1.61	1.53
4	D	113	GLY	CA-C	-5.16	1.45	1.51
13	6	28	ARG	NE-CZ	5.16	1.38	1.33
29	P	366	ASN	C-N	5.16	1.41	1.33
32	U	14	VAL	CA-C	-5.16	1.46	1.52
32	U	23	GLU	N-CA	-5.16	1.39	1.46
27	N	652	VAL	CA-CB	-5.16	1.47	1.54
28	S	81	LEU	CA-C	5.16	1.59	1.52
3	c	205	LEU	C-N	5.16	1.40	1.33
6	f	106	ARG	NE-CZ	5.16	1.38	1.33
9	i	157	ASP	N-CA	-5.16	1.39	1.46
12	l	24	ASN	CA-C	-5.16	1.45	1.52
12	5	49	ALA	N-CA	-5.16	1.40	1.46
23	T	163	LEU	C-O	-5.16	1.18	1.24
10	j	98	ARG	NE-CZ	5.15	1.38	1.33
11	4	126	VAL	CA-C	-5.15	1.46	1.52
3	c	22	GLU	CA-C	-5.15	1.46	1.52
6	F	14	PRO	N-CA	-5.15	1.40	1.47
8	1	33	LYS	CA-C	-5.15	1.46	1.52
27	N	226	ASN	C-O	-5.15	1.17	1.24
27	N	653	ARG	CZ-NH2	5.15	1.40	1.33
27	N	902	VAL	N-CA	-5.15	1.40	1.46
32	U	21	HIS	ND1-CE1	5.15	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	122	THR	CA-C	-5.15	1.46	1.52
2	B	182	GLU	CA-C	-5.15	1.46	1.52
16	I	151	HIS	CE1-NE2	-5.15	1.27	1.32
18	L	119	VAL	N-CA	-5.15	1.40	1.46
28	S	174	ARG	NE-CZ	5.15	1.38	1.33
29	P	226	LYS	C-O	-5.15	1.18	1.24
5	e	71	SER	C-O	-5.15	1.17	1.23
12	5	64	ARG	CA-C	-5.15	1.46	1.52
26	Z	528	LEU	N-CA	-5.15	1.40	1.46
9	2	179	GLU	C-N	5.15	1.38	1.33
27	N	61	ALA	CA-C	-5.15	1.46	1.52
13	m	219	LEU	CA-C	-5.15	1.46	1.52
27	N	183	VAL	C-N	5.15	1.40	1.33
4	d	200	VAL	CA-CB	5.14	1.60	1.54
5	e	125	LEU	N-CA	5.14	1.52	1.46
17	K	112	SER	N-CA	-5.14	1.39	1.45
26	Z	759	ARG	C-N	5.14	1.41	1.34
7	g	15	GLY	N-CA	-5.14	1.36	1.46
4	D	202	GLN	CA-CB	5.14	1.62	1.53
9	2	14	ILE	N-CA	-5.14	1.40	1.46
28	S	396	SER	CA-C	5.14	1.59	1.52
9	i	44	ALA	C-N	5.14	1.38	1.33
2	B	88	LYS	C-O	-5.14	1.18	1.24
5	e	41	GLY	CA-C	-5.14	1.44	1.51
13	m	49	ASN	CA-C	5.14	1.60	1.53
13	m	205	LEU	CA-C	-5.14	1.46	1.52
2	B	249	ALA	C-N	5.14	1.40	1.33
3	C	51	VAL	CA-C	-5.14	1.47	1.52
17	K	115	GLY	CA-C	-5.14	1.44	1.51
27	N	612	SER	C-N	5.14	1.40	1.33
4	d	139	ARG	CA-CB	5.14	1.61	1.53
10	3	40	GLU	CA-C	-5.14	1.46	1.52
18	L	392	ARG	CZ-NH2	5.14	1.40	1.33
26	Z	582	ASP	N-CA	-5.14	1.40	1.46
27	N	809	ARG	CZ-NH2	5.14	1.40	1.33
2	b	190	HIS	ND1-CE1	5.14	1.37	1.32
9	i	131	SER	C-O	-5.14	1.18	1.24
10	j	195	VAL	CA-CB	-5.14	1.48	1.54
13	m	71	SER	CA-C	-5.14	1.46	1.52
22	V	136	ALA	C-O	-5.14	1.17	1.23
26	Z	138	ARG	NE-CZ	5.14	1.38	1.33
28	S	184	TRP	C-N	5.14	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	401	ASN	N-CA	-5.14	1.39	1.46
30	Q	291	TYR	C-N	5.14	1.40	1.33
2	b	65	SER	C-N	5.13	1.40	1.33
3	c	118	LYS	CA-CB	5.13	1.61	1.53
10	j	149	CYS	C-O	-5.13	1.18	1.24
19	M	78	LEU	N-CA	-5.13	1.39	1.46
26	Z	928	ARG	CD-NE	5.13	1.53	1.46
27	N	786	ARG	NE-CZ	5.13	1.38	1.33
30	Q	277	ASP	N-CA	-5.13	1.39	1.46
2	b	64	VAL	N-CA	-5.13	1.40	1.46
13	m	28	ARG	CZ-NH1	5.13	1.40	1.32
30	Q	106	GLN	CA-C	-5.13	1.46	1.52
11	k	63	ASN	N-CA	-5.13	1.40	1.46
11	k	92	ILE	N-CA	-5.13	1.40	1.46
13	m	24	ALA	N-CA	-5.13	1.39	1.45
15	H	252	PRO	C-N	5.13	1.40	1.33
26	Z	903	MET	CA-C	-5.13	1.46	1.52
31	R	347	THR	CA-C	-5.13	1.46	1.52
32	U	137	TYR	N-CA	-5.13	1.39	1.46
1	a	216	VAL	N-CA	-5.13	1.39	1.46
12	l	4	LEU	C-O	-5.13	1.17	1.23
1	a	6	HIS	ND1-CE1	5.13	1.37	1.32
2	b	209	ILE	CA-CB	5.13	1.61	1.54
5	e	86	THR	C-N	5.13	1.41	1.34
6	f	101	LYS	CA-C	5.13	1.59	1.52
4	D	164	ARG	NE-CZ	5.13	1.38	1.33
5	E	98	ASP	CA-C	-5.13	1.46	1.52
10	3	98	ARG	CD-NE	5.13	1.53	1.46
27	N	234	ASP	N-CA	-5.13	1.40	1.46
27	N	889	ARG	CZ-NH2	5.13	1.40	1.33
33	O	179	PHE	C-N	5.13	1.41	1.33
10	3	143	ASP	N-CA	-5.13	1.40	1.46
26	Z	634	ASP	CA-C	-5.13	1.46	1.52
30	Q	392	GLN	C-N	5.13	1.41	1.33
3	c	237	ILE	CB-CG1	5.12	1.63	1.53
14	n	221	PHE	N-CA	-5.12	1.39	1.46
30	Q	135	HIS	CB-CG	5.12	1.57	1.50
30	Q	150	GLN	C-N	5.12	1.41	1.33
6	f	68	HIS	CA-CB	5.12	1.61	1.53
1	A	122	ARG	CZ-NH1	5.12	1.40	1.32
2	B	50	LYS	CA-C	-5.12	1.46	1.52
19	M	190	ILE	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	463	TYR	CA-C	-5.12	1.46	1.52
27	N	642	ASP	CA-C	5.12	1.58	1.52
27	N	650	ASP	N-CA	-5.12	1.40	1.46
31	R	302	ALA	N-CA	-5.12	1.40	1.46
2	b	90	ARG	CD-NE	5.12	1.53	1.46
7	g	10	VAL	C-O	5.12	1.29	1.24
1	A	57	PRO	CA-C	-5.12	1.44	1.52
15	H	299	ARG	NE-CZ	5.12	1.38	1.33
17	K	63	LEU	CA-CB	5.12	1.61	1.53
18	L	90	LYS	C-O	-5.12	1.18	1.24
31	R	390	THR	N-CA	-5.12	1.40	1.46
10	j	189	ILE	N-CA	-5.12	1.39	1.46
14	n	73	GLU	N-CA	-5.12	1.40	1.46
21	W	85	LEU	CA-C	-5.12	1.46	1.52
33	O	165	LEU	C-N	-5.12	1.27	1.33
8	h	135	TYR	CA-C	5.12	1.59	1.52
9	i	24	PRO	N-CD	-5.12	1.40	1.47
9	i	78	SER	CA-C	-5.12	1.46	1.52
9	i	93	HIS	ND1-CE1	5.12	1.37	1.32
12	l	117	SER	C-N	5.12	1.40	1.33
5	E	165	GLY	CA-C	-5.12	1.46	1.52
18	L	183	ILE	N-CA	-5.12	1.40	1.46
20	J	84	VAL	C-O	-5.12	1.18	1.24
1	a	122	ARG	CZ-NH2	5.12	1.40	1.33
8	h	18	SER	C-N	5.12	1.40	1.33
10	j	154	GLU	N-CA	-5.12	1.39	1.46
3	C	116	ASP	C-N	5.12	1.40	1.33
5	E	137	ALA	CA-C	-5.12	1.46	1.52
14	n	216	ASN	N-CA	-5.12	1.39	1.46
8	l	190	PRO	N-CA	-5.12	1.40	1.47
15	H	175	GLY	CA-C	-5.12	1.48	1.52
19	M	376	TRP	N-CA	-5.12	1.40	1.46
5	E	128	ARG	CD-NE	5.11	1.53	1.46
27	N	269	LEU	CA-CB	5.11	1.61	1.53
1	a	82	ARG	CD-NE	5.11	1.53	1.46
10	j	64	GLU	C-O	-5.11	1.18	1.24
11	4	43	LEU	N-CA	-5.11	1.39	1.46
26	Z	949	ILE	N-CA	-5.11	1.40	1.46
28	S	103	SER	C-N	5.11	1.39	1.33
30	Q	414	GLU	CA-CB	5.11	1.61	1.53
14	7	41	ARG	NE-CZ	5.11	1.38	1.33
15	H	310	GLU	C-N	5.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	257	ILE	CA-C	-5.11	1.46	1.52
2	B	47	THR	CA-C	-5.11	1.46	1.52
4	D	3	ASP	CA-CB	5.11	1.62	1.53
10	3	164	GLU	C-N	5.11	1.40	1.33
11	4	133	HIS	ND1-CE1	5.11	1.37	1.32
18	L	261	ARG	CD-NE	5.11	1.53	1.46
18	L	261	ARG	NE-CZ	5.11	1.38	1.33
6	f	118	ASN	C-N	5.11	1.40	1.33
6	f	206	THR	CA-C	-5.11	1.48	1.53
12	l	49	ALA	C-O	-5.11	1.18	1.24
3	C	214	THR	C-N	5.11	1.39	1.33
18	L	85	GLU	CA-C	-5.11	1.46	1.52
32	U	264	ALA	CA-C	-5.11	1.45	1.52
3	C	178	ASP	C-N	5.10	1.40	1.33
6	F	171	LEU	N-CA	-5.10	1.39	1.46
28	S	197	SER	CA-CB	5.10	1.61	1.53
12	l	37	ILE	CA-C	-5.10	1.46	1.52
9	2	161	ALA	CA-C	-5.10	1.45	1.52
10	3	97	ARG	NE-CZ	5.10	1.38	1.33
33	O	325	GLU	N-CA	-5.10	1.40	1.46
9	i	218	VAL	CA-C	-5.10	1.46	1.52
12	l	143	ASN	CA-C	-5.10	1.46	1.52
10	3	115	SER	CA-C	-5.10	1.45	1.52
31	R	143	GLN	CA-CB	5.10	1.61	1.53
1	a	52	ASP	C-N	5.10	1.41	1.33
7	g	71	GLY	CA-C	-5.10	1.48	1.52
19	M	33	ARG	C-N	5.10	1.40	1.33
21	W	193	GLU	CA-C	-5.10	1.46	1.52
20	J	198	LEU	N-CA	-5.10	1.39	1.46
6	f	39	SER	C-N	5.10	1.43	1.33
13	6	155	ASN	C-N	5.10	1.41	1.33
33	O	135	ARG	CZ-NH2	5.10	1.40	1.33
7	g	142	ALA	CA-C	-5.09	1.46	1.52
9	2	73	GLU	CA-C	5.09	1.59	1.53
33	O	136	THR	CA-C	-5.09	1.46	1.52
11	k	111	LYS	CA-C	-5.09	1.45	1.52
11	k	161	LEU	CA-C	-5.09	1.45	1.52
1	A	166	GLN	CA-CB	5.09	1.62	1.53
27	N	908	ARG	N-CA	-5.09	1.40	1.46
8	h	171	GLY	C-N	5.09	1.39	1.33
3	C	43	ILE	N-CA	-5.09	1.40	1.46
16	I	90	GLU	N-CA	-5.09	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	170	THR	CA-C	-5.09	1.46	1.52
17	K	215	PRO	CA-C	-5.09	1.48	1.53
19	M	209	ASP	C-N	5.09	1.41	1.34
27	N	103	SER	CA-C	-5.09	1.46	1.52
31	R	223	ASN	CA-C	-5.09	1.46	1.52
33	O	308	LEU	CA-C	-5.09	1.46	1.52
20	J	75	VAL	CA-C	-5.09	1.47	1.52
22	V	86	VAL	C-O	-5.09	1.18	1.24
26	Z	701	ILE	C-N	5.09	1.40	1.33
31	R	161	ALA	CA-C	-5.09	1.46	1.52
31	R	304	TYR	CA-CB	5.09	1.61	1.53
16	I	432	LEU	N-CA	-5.09	1.40	1.46
19	M	150	LYS	C-O	-5.09	1.17	1.24
22	V	88	GLN	CA-C	-5.09	1.46	1.52
27	N	296	CYS	CA-C	-5.09	1.46	1.52
33	O	269	LEU	CA-CB	5.09	1.61	1.53
12	5	3	THR	C-N	5.09	1.39	1.33
16	I	368	LYS	C-N	5.09	1.40	1.33
17	K	242	PHE	N-CA	-5.09	1.40	1.46
18	L	91	THR	N-CA	-5.09	1.39	1.46
31	R	186	TYR	CG-CD2	5.09	1.50	1.39
33	O	81	TYR	N-CA	-5.09	1.39	1.46
33	O	375	ASP	CA-CB	5.09	1.61	1.53
7	g	56	VAL	CA-C	-5.08	1.47	1.52
10	j	138	SER	CA-CB	5.08	1.62	1.53
1	A	5	ARG	N-CA	-5.08	1.40	1.46
13	6	16	ALA	N-CA	-5.08	1.40	1.46
15	H	50	LYS	N-CA	-5.08	1.40	1.46
27	N	281	GLY	C-N	5.08	1.40	1.33
30	Q	253	ASN	CA-C	-5.08	1.46	1.52
11	k	93	ARG	CZ-NH1	5.08	1.39	1.32
12	l	193	VAL	C-O	-5.08	1.17	1.24
15	H	48	LYS	CA-C	-5.08	1.45	1.52
22	V	271	VAL	C-N	5.08	1.40	1.33
23	T	212	ASN	C-N	5.08	1.40	1.33
33	O	201	PRO	N-CA	-5.08	1.40	1.47
11	4	120	ASP	CA-C	-5.08	1.46	1.53
15	H	373	ARG	CZ-NH1	5.08	1.39	1.32
30	Q	328	ASP	CA-CB	5.08	1.60	1.53
10	j	202	ARG	CZ-NH2	5.08	1.40	1.33
6	f	164	SER	CA-CB	5.08	1.62	1.53
9	i	127	LEU	CA-CB	5.08	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	176	ASN	CA-CB	5.08	1.61	1.53
4	D	202	GLN	C-N	5.08	1.40	1.33
15	H	228	PRO	N-CA	-5.08	1.40	1.47
2	b	109	LEU	CA-C	5.08	1.59	1.52
9	i	18	THR	CA-CB	-5.08	1.46	1.53
16	I	265	ARG	NE-CZ	5.08	1.38	1.33
6	f	32	SER	CA-C	-5.08	1.46	1.52
7	g	166	GLN	CD-NE2	5.08	1.44	1.33
10	j	67	ARG	CZ-NH2	5.08	1.40	1.33
15	H	91	LEU	CA-CB	5.08	1.62	1.53
21	W	48	THR	CA-C	-5.08	1.46	1.52
28	S	111	ARG	CA-C	-5.08	1.46	1.52
13	6	111	ILE	N-CA	-5.07	1.40	1.46
28	S	377	TYR	C-N	5.07	1.40	1.33
4	d	12	ASP	N-CA	-5.07	1.40	1.46
17	K	291	GLU	C-N	5.07	1.40	1.33
30	Q	352	GLU	CA-CB	5.07	1.59	1.53
2	B	13	SER	CA-C	5.07	1.59	1.53
32	U	128	GLN	CA-C	-5.07	1.46	1.52
14	n	172	VAL	C-N	5.07	1.40	1.33
9	2	132	LEU	CA-C	-5.07	1.45	1.52
12	5	74	ILE	CA-C	-5.07	1.47	1.52
23	T	20	TYR	CZ-OH	5.07	1.48	1.38
26	Z	499	GLY	C-N	5.07	1.40	1.33
27	N	47	GLU	CA-C	-5.07	1.46	1.52
29	P	230	HIS	ND1-CE1	5.07	1.37	1.32
30	Q	302	VAL	CA-C	-5.07	1.45	1.52
8	h	23	GLY	C-N	5.07	1.40	1.33
11	k	184	VAL	C-O	-5.07	1.18	1.24
13	m	104	PRO	CA-C	-5.07	1.46	1.52
9	2	75	ARG	N-CA	-5.07	1.39	1.45
16	I	343	ARG	NE-CZ	5.07	1.38	1.33
16	I	351	GLU	N-CA	-5.07	1.39	1.45
17	K	315	ILE	CA-C	-5.07	1.46	1.52
18	L	395	ALA	CA-C	5.07	1.59	1.52
33	O	333	SER	N-CA	5.07	1.52	1.46
13	6	1	GLN	C-N	5.06	1.40	1.33
17	K	407	LEU	C-N	5.06	1.40	1.33
6	f	85	ASN	C-N	5.06	1.40	1.33
2	B	129	PRO	CA-C	-5.06	1.46	1.52
8	1	28	ASN	CA-C	-5.06	1.45	1.52
14	7	87	LEU	CA-C	-5.06	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	273	HIS	CA-C	-5.06	1.45	1.52
26	Z	532	HIS	CG-ND1	-5.06	1.32	1.38
27	N	905	LEU	CA-CB	-5.06	1.44	1.53
5	e	154	GLY	C-O	-5.06	1.17	1.23
3	c	211	GLU	CG-CD	5.06	1.64	1.52
9	i	116	HIS	N-CA	5.06	1.52	1.46
1	A	173	LEU	CA-C	-5.06	1.46	1.52
10	3	103	PHE	N-CA	-5.06	1.40	1.46
24	X	111	LEU	N-CA	-5.06	1.39	1.46
31	R	111	LYS	C-N	5.06	1.40	1.33
32	U	233	PHE	CA-C	-5.06	1.46	1.52
5	e	99	ILE	C-N	5.06	1.40	1.33
13	m	52	MET	CA-C	-5.06	1.46	1.52
5	E	143	ASP	N-CA	-5.06	1.39	1.46
13	6	41	PRO	N-CA	-5.06	1.40	1.47
20	J	329	ARG	CZ-NH2	5.06	1.40	1.33
28	S	450	ASN	CA-CB	5.06	1.60	1.53
29	P	284	ILE	CA-CB	-5.06	1.47	1.54
3	c	71	LYS	CA-C	-5.06	1.46	1.52
8	h	106	ASN	CA-C	-5.06	1.45	1.52
13	m	28	ARG	NE-CZ	5.06	1.38	1.33
15	H	328	GLU	C-N	5.06	1.40	1.33
9	i	73	GLU	C-N	5.05	1.39	1.33
10	j	12	VAL	CA-C	-5.05	1.46	1.52
11	4	52	ASP	N-CA	-5.05	1.40	1.46
15	H	88	ARG	CD-NE	5.05	1.53	1.46
16	I	220	ILE	CA-CB	-5.05	1.47	1.54
24	X	96	ARG	CD-NE	5.05	1.53	1.46
27	N	586	ALA	CA-C	-5.05	1.46	1.52
32	U	40	ASP	CA-C	-5.05	1.46	1.53
15	H	354	ALA	C-N	5.05	1.40	1.33
17	K	165	GLU	CA-CB	5.05	1.61	1.53
27	N	768	ILE	CA-C	-5.05	1.48	1.53
11	k	181	VAL	CA-C	-5.05	1.46	1.52
12	l	67	GLU	C-N	5.05	1.40	1.33
1	A	63	ILE	C-N	5.05	1.40	1.33
1	A	216	VAL	CA-C	-5.05	1.46	1.52
15	H	151	GLN	C-N	5.05	1.40	1.33
16	I	271	ALA	C-N	5.05	1.40	1.33
18	L	68	ARG	N-CA	-5.05	1.40	1.46
24	X	41	GLU	C-N	5.05	1.41	1.33
27	N	221	ASP	C-N	5.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	189	LEU	CA-C	-5.05	1.46	1.52
29	P	364	ARG	CD-NE	5.05	1.53	1.46
26	Z	341	TYR	N-CA	-5.05	1.40	1.46
27	N	920	VAL	CA-C	-5.05	1.46	1.52
10	3	99	PHE	CA-C	-5.05	1.46	1.52
12	5	76	VAL	CA-CB	-5.05	1.48	1.54
27	N	623	PHE	C-N	5.05	1.40	1.33
32	U	278	ILE	CA-C	-5.05	1.46	1.52
1	a	97	TYR	CA-CB	5.05	1.61	1.53
5	e	78	ARG	CZ-NH2	5.05	1.40	1.33
8	h	120	HIS	CE1-NE2	-5.05	1.27	1.32
9	i	36	ARG	CA-C	5.05	1.58	1.52
10	j	2	ASP	CA-C	-5.05	1.48	1.53
13	6	133	ARG	NE-CZ	5.05	1.38	1.33
20	J	286	LYS	CA-CB	5.05	1.60	1.53
20	J	307	PRO	CA-CB	-5.05	1.48	1.54
27	N	375	HIS	N-CA	-5.05	1.40	1.46
27	N	719	ASN	CA-C	-5.05	1.46	1.52
29	P	392	LYS	N-CA	-5.05	1.39	1.46
33	O	214	ALA	CA-C	-5.05	1.46	1.52
33	O	249	ASP	CA-C	-5.05	1.48	1.53
4	D	158	SER	C-N	5.04	1.40	1.33
7	G	207	ASP	CA-C	-5.04	1.46	1.53
31	R	216	ILE	C-N	5.04	1.40	1.33
5	e	44	LYS	N-CA	-5.04	1.40	1.46
13	m	114	LEU	C-O	-5.04	1.17	1.23
1	A	11	SER	CA-CB	5.04	1.61	1.53
2	B	222	LEU	CA-C	5.04	1.59	1.52
15	H	375	VAL	C-N	5.04	1.40	1.33
16	I	199	GLU	N-CA	-5.04	1.40	1.46
23	T	130	ASP	CA-CB	5.04	1.61	1.53
27	N	660	LEU	CA-C	5.04	1.59	1.52
28	S	315	LYS	CA-C	-5.04	1.46	1.52
2	b	104	TYR	C-N	5.04	1.39	1.33
6	f	50	ARG	CZ-NH2	5.04	1.40	1.33
10	j	180	SER	C-N	5.04	1.40	1.33
8	l	126	ILE	CA-C	-5.04	1.46	1.52
19	M	367	LYS	N-CA	-5.04	1.40	1.46
20	J	205	HIS	C-N	5.04	1.40	1.33
31	R	158	LEU	CA-C	-5.04	1.46	1.52
13	m	48	ASP	N-CA	-5.04	1.39	1.46
26	Z	596	THR	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	173	ALA	C-N	5.04	1.40	1.33
14	n	41	ARG	C-N	5.04	1.40	1.33
27	N	421	ASP	CA-CB	5.04	1.61	1.53
28	S	247	VAL	N-CA	-5.04	1.40	1.46
31	R	114	ASN	CG-ND2	5.04	1.43	1.33
13	m	156	PHE	CA-CB	5.04	1.61	1.53
3	c	162	ILE	C-N	5.04	1.40	1.33
4	d	176	ASN	CA-CB	5.04	1.61	1.53
6	f	142	HIS	ND1-CE1	5.04	1.37	1.32
10	j	186	VAL	N-CA	-5.04	1.40	1.46
17	K	121	ARG	CZ-NH1	5.04	1.39	1.32
10	j	45	TYR	C-N	5.03	1.40	1.33
11	4	44	MET	C-O	-5.03	1.18	1.24
16	I	64	ARG	CD-NE	5.03	1.53	1.46
23	T	137	GLU	CA-C	-5.03	1.46	1.52
30	Q	50	ARG	N-CA	5.03	1.52	1.46
16	I	337	ALA	C-N	5.03	1.40	1.33
25	Y	28	SER	N-CA	-5.03	1.40	1.46
9	i	51	ASP	N-CA	-5.03	1.40	1.46
13	m	153	GLN	CA-C	-5.03	1.45	1.52
8	1	29	ARG	CZ-NH2	5.03	1.40	1.33
16	I	88	LYS	N-CA	-5.03	1.40	1.46
33	O	23	HIS	CD2-NE2	5.03	1.43	1.37
13	m	119	LYS	CA-C	-5.03	1.46	1.52
14	7	139	SER	CA-C	5.03	1.58	1.52
16	I	326	MET	CA-CB	5.03	1.60	1.53
26	Z	908	ILE	N-CA	-5.03	1.40	1.46
27	N	273	LEU	CA-C	-5.03	1.46	1.52
8	h	50	ALA	N-CA	-5.03	1.40	1.46
7	G	156	TYR	CA-C	-5.03	1.46	1.52
14	7	50	VAL	CA-CB	-5.03	1.47	1.54
26	Z	312	TYR	N-CA	-5.03	1.40	1.46
26	Z	847	ILE	CA-C	5.03	1.58	1.52
27	N	668	THR	CA-C	-5.03	1.46	1.52
29	P	364	ARG	C-N	5.03	1.40	1.33
4	d	212	VAL	C-O	-5.03	1.18	1.24
9	i	187	LEU	CA-C	-5.03	1.47	1.53
13	m	209	LYS	N-CA	-5.03	1.40	1.46
20	J	245	ILE	N-CA	5.03	1.52	1.46
30	Q	124	PHE	CA-CB	5.03	1.61	1.53
13	m	219	LEU	CA-CB	5.02	1.61	1.53
14	n	170	VAL	C-N	5.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	110	VAL	C-N	5.02	1.40	1.33
13	m	194	ARG	NE-CZ	5.02	1.38	1.33
9	2	94	ILE	CA-CB	-5.02	1.48	1.54
15	H	73	ASP	N-CA	-5.02	1.39	1.45
3	c	4	ARG	CZ-NH1	5.02	1.39	1.32
1	A	54	LEU	N-CA	-5.02	1.40	1.46
10	j	188	ILE	CA-C	-5.02	1.46	1.52
13	m	83	LYS	N-CA	-5.02	1.40	1.46
4	D	46	ARG	NE-CZ	5.02	1.38	1.33
8	1	103	ASP	N-CA	-5.02	1.40	1.45
32	U	38	LEU	CA-C	-5.02	1.46	1.52
33	O	166	ARG	CZ-NH2	5.02	1.40	1.33
2	b	148	TYR	C-N	5.02	1.40	1.33
14	7	35	ARG	CZ-NH2	5.02	1.40	1.33
23	T	85	LEU	CA-C	-5.02	1.46	1.52
25	Y	29	LEU	CA-C	-5.02	1.45	1.52
27	N	374	ILE	N-CA	-5.02	1.40	1.46
9	2	83	LEU	C-N	5.02	1.40	1.33
18	L	239	ILE	CA-C	-5.02	1.46	1.52
4	d	130	SER	N-CA	-5.01	1.39	1.45
5	e	176	LEU	CA-C	-5.01	1.46	1.52
7	G	179	HIS	CA-CB	5.01	1.59	1.53
18	L	205	GLU	CA-C	-5.01	1.46	1.52
19	M	374	ILE	N-CA	-5.01	1.40	1.46
30	Q	127	ARG	NE-CZ	5.01	1.38	1.33
11	k	38	LEU	N-CA	-5.01	1.40	1.46
13	6	147	MET	C-N	5.01	1.40	1.33
20	J	203	ALA	N-CA	-5.01	1.40	1.46
1	A	36	VAL	C-N	5.01	1.40	1.33
2	B	190	HIS	CA-C	-5.01	1.46	1.52
4	D	115	GLN	CA-C	-5.01	1.46	1.52
5	E	120	SER	C-N	5.01	1.40	1.33
5	E	238	LYS	CA-C	-5.01	1.45	1.52
27	N	504	TYR	CA-CB	5.01	1.61	1.53
32	U	254	ARG	CZ-NH2	5.01	1.40	1.33
1	a	135	VAL	CA-C	-5.01	1.46	1.52
8	1	83	LYS	CA-C	-5.01	1.46	1.52
20	J	270	ARG	N-CA	-5.01	1.40	1.46
20	J	391	ASN	CA-C	-5.01	1.46	1.52
28	S	318	CYS	CA-C	5.01	1.59	1.52
3	c	133	SER	CA-C	5.01	1.58	1.52
11	k	136	SER	N-CA	-5.01	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	12	ILE	C-O	-5.01	1.19	1.24
13	m	164	THR	N-CA	-5.01	1.40	1.46
21	W	141	ILE	C-N	5.01	1.40	1.33
32	U	203	LYS	C-O	-5.01	1.18	1.24
33	O	56	PRO	C-N	5.01	1.40	1.33
20	J	81	ASP	N-CA	5.00	1.52	1.45
29	P	100	VAL	CA-C	5.00	1.59	1.52
14	n	213	GLN	CA-CB	5.00	1.65	1.53
4	D	104	VAL	C-N	5.00	1.40	1.33
10	3	82	GLU	CA-C	-5.00	1.46	1.52
15	H	308	PHE	CA-CB	5.00	1.60	1.53
16	I	100	ARG	NE-CZ	5.00	1.38	1.33
31	R	311	THR	N-CA	-5.00	1.40	1.46
33	O	93	ASP	N-CA	-5.00	1.40	1.46
33	O	262	ASP	C-N	5.00	1.41	1.33
10	j	202	ARG	CD-NE	5.00	1.53	1.46
6	F	116	GLN	C-O	-5.00	1.18	1.24
14	7	63	ILE	C-N	5.00	1.40	1.33
25	Y	83	ARG	CA-C	-5.00	1.46	1.52
26	Z	327	GLN	CA-CB	5.00	1.61	1.53
26	Z	470	ALA	CA-C	-5.00	1.46	1.52
28	S	317	HIS	ND1-CE1	5.00	1.37	1.32

All (5818) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	GLU	CA-C-N	-36.37	56.24	121.70
1	A	241	GLU	C-N-CA	-36.37	56.24	121.70
22	V	187	ALA	N-CA-C	21.27	136.63	111.11
27	N	859	ASN	CB-CA-C	-20.86	80.12	110.16
22	V	186	GLN	N-CA-CB	-18.27	65.38	111.04
27	N	859	ASN	N-CA-CB	15.22	133.55	109.51
27	N	861	TYR	N-CA-CB	-15.00	85.15	110.49
1	A	241	GLU	O-C-N	14.79	142.73	122.46
22	V	187	ALA	N-CA-CB	-14.22	88.75	109.94
23	T	118	ASN	CA-CB-CG	-13.37	99.23	112.60
20	J	311	ASP	CA-CB-CG	13.16	125.76	112.60
22	V	186	GLN	CB-CA-C	12.91	131.38	116.54
6	F	4	ASN	CA-CB-CG	-12.84	99.76	112.60
1	A	242	GLN	CB-CA-C	12.74	134.30	110.10
33	O	291	ILE	CB-CA-C	-12.21	95.66	112.14
15	H	327	ASN	CA-CB-CG	11.70	124.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	53	HIS	CA-CB-CG	11.64	125.44	113.80
33	O	62	TYR	N-CA-C	11.59	123.60	110.97
26	Z	793	PHE	CA-CB-CG	-11.55	102.25	113.80
7	g	128	PHE	CA-CB-CG	-11.54	102.26	113.80
6	f	4	ASN	CA-CB-CG	11.51	124.11	112.60
27	N	877	GLN	OE1-CD-NE2	11.39	133.99	122.60
26	Z	497	PHE	CA-CB-CG	-11.38	102.42	113.80
13	6	76	HIS	CA-CB-CG	-11.36	102.44	113.80
18	L	249	SER	N-CA-C	-11.28	99.51	113.28
28	S	77	THR	CA-C-N	11.28	135.15	120.60
28	S	77	THR	C-N-CA	11.28	135.15	120.60
30	Q	67	THR	CA-C-N	11.16	141.79	121.70
30	Q	67	THR	C-N-CA	11.16	141.79	121.70
1	A	242	GLN	CA-C-O	-11.12	101.90	120.80
27	N	509	GLN	N-CA-C	-11.05	99.82	113.97
20	J	311	ASP	CA-C-N	11.04	142.64	121.54
20	J	311	ASP	C-N-CA	11.04	142.64	121.54
9	i	114	HIS	CA-CB-CG	-11.04	102.77	113.80
2	B	145	PHE	CA-CB-CG	-10.91	102.89	113.80
31	R	68	GLU	O-C-N	10.85	133.81	122.09
16	I	350	PHE	CA-CB-CG	-10.77	103.03	113.80
33	O	291	ILE	N-CA-CB	10.73	125.14	110.54
31	R	70	TYR	CB-CG-CD2	10.71	136.86	120.80
32	U	126	LYS	N-CA-C	-10.61	100.83	113.88
19	M	186	LEU	CA-C-N	10.60	134.48	120.28
19	M	186	LEU	C-N-CA	10.60	134.48	120.28
28	S	481	TYR	CA-C-O	-10.60	108.06	118.34
14	n	37	ASN	CA-CB-CG	-10.58	102.02	112.60
31	R	68	GLU	CA-C-N	10.46	138.19	120.72
31	R	68	GLU	C-N-CA	10.46	138.19	120.72
33	O	97	LYS	N-CA-C	10.39	122.19	111.07
31	R	110	ILE	N-CA-CB	10.38	128.37	111.23
15	H	250	GLY	CA-C-N	10.38	127.23	119.66
15	H	250	GLY	C-N-CA	10.38	127.23	119.66
17	K	333	ARG	N-CA-C	-10.33	100.75	113.97
8	h	133	PHE	CA-CB-CG	-10.29	103.51	113.80
27	N	890	PHE	CA-CB-CG	-10.28	103.52	113.80
10	j	204	ASP	CA-CB-CG	-10.22	102.38	112.60
17	K	194	GLN	CA-C-N	10.21	134.79	120.29
17	K	194	GLN	C-N-CA	10.21	134.79	120.29
12	l	208	ASN	CA-CB-CG	-10.19	102.41	112.60
26	Z	360	SER	CA-C-O	-10.17	109.77	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	122	THR	N-CA-CB	10.14	124.76	110.67
3	c	221	ASP	CA-CB-CG	-10.11	102.49	112.60
30	Q	92	LYS	CA-C-N	10.10	134.18	120.54
30	Q	92	LYS	C-N-CA	10.10	134.18	120.54
20	J	292	MET	N-CA-CB	10.09	127.00	110.85
15	H	78	PRO	CA-N-CD	-10.04	97.94	112.00
31	R	109	LYS	CA-C-O	-10.02	110.05	121.07
5	E	62	ILE	N-CA-C	-10.02	102.94	112.96
14	n	221	PHE	CA-CB-CG	10.02	123.81	113.80
23	T	241	GLU	CA-C-N	10.02	133.46	120.44
23	T	241	GLU	C-N-CA	10.02	133.46	120.44
31	R	377	LEU	N-CA-C	-10.01	100.82	113.43
7	G	105	ILE	CA-C-O	-9.97	110.37	118.85
31	R	327	ASP	CA-CB-CG	9.94	122.54	112.60
28	S	162	VAL	N-CA-C	9.94	119.87	110.53
29	P	337	HIS	N-CA-C	-9.94	101.66	113.88
19	M	53	HIS	CA-CB-CG	9.90	123.70	113.80
13	m	98	TYR	N-CA-C	-9.86	100.61	111.36
20	J	310	ILE	O-C-N	-9.84	110.27	122.57
16	I	124	THR	CA-C-N	9.84	133.45	120.26
16	I	124	THR	C-N-CA	9.84	133.45	120.26
9	i	37	ILE	N-CA-C	-9.82	100.80	110.72
10	j	75	LEU	CA-C-O	9.82	130.82	120.70
4	D	125	ARG	CA-C-O	-9.82	110.22	120.23
31	R	107	GLU	N-CA-C	9.81	122.88	111.11
17	K	410	ALA	CA-C-N	9.78	133.15	120.44
17	K	410	ALA	C-N-CA	9.78	133.15	120.44
14	n	184	LEU	CA-C-N	9.68	133.26	120.28
14	n	184	LEU	C-N-CA	9.68	133.26	120.28
12	l	83	LEU	N-CA-C	-9.67	100.82	111.36
29	P	152	LYS	CA-C-N	9.61	133.62	120.46
29	P	152	LYS	C-N-CA	9.61	133.62	120.46
27	N	720	ALA	N-CA-C	-9.60	101.26	113.16
4	d	78	ALA	CA-C-N	9.59	133.13	120.28
4	d	78	ALA	C-N-CA	9.59	133.13	120.28
26	Z	551	LEU	CB-CA-C	-9.59	95.83	110.88
27	N	550	GLY	CA-C-N	9.57	130.61	119.98
27	N	550	GLY	C-N-CA	9.57	130.61	119.98
22	V	161	THR	CA-C-N	9.57	130.75	120.03
22	V	161	THR	C-N-CA	9.57	130.75	120.03
1	a	166	GLN	OE1-CD-NE2	9.57	132.17	122.60
33	O	184	ASP	CA-CB-CG	-9.55	103.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	109	ARG	NE-CZ-NH2	9.55	127.79	119.20
9	i	33	LYS	N-CA-C	-9.54	100.40	112.90
33	O	236	HIS	CA-C-N	9.54	131.76	119.84
33	O	236	HIS	C-N-CA	9.54	131.76	119.84
25	Y	35	PHE	CA-CB-CG	-9.54	104.26	113.80
26	Z	773	ARG	N-CA-C	-9.53	100.54	113.30
31	R	21	VAL	N-CA-CB	9.53	117.88	110.45
14	n	152	ASN	CA-CB-CG	9.51	122.11	112.60
19	M	393	ALA	CA-C-N	9.50	132.53	120.56
19	M	393	ALA	C-N-CA	9.50	132.53	120.56
30	Q	165	PHE	CA-CB-CG	-9.49	104.31	113.80
6	f	103	ALA	CA-C-N	9.49	132.52	120.56
6	f	103	ALA	C-N-CA	9.49	132.52	120.56
33	O	284	GLU	CB-CG-CD	-9.49	96.47	112.60
29	P	93	ILE	N-CA-C	-9.48	103.44	112.83
2	b	99	ARG	N-CA-C	-9.46	102.24	113.88
32	U	33	CYS	N-CA-C	-9.45	94.37	109.59
11	k	96	ARG	CA-C-O	-9.45	112.33	119.32
33	O	264	ASP	N-CA-C	-9.44	101.07	111.36
30	Q	227	CYS	N-CA-C	-9.44	100.94	111.14
28	S	185	PHE	CA-CB-CG	-9.44	104.36	113.80
12	5	51	ASP	N-CA-C	-9.43	100.95	111.14
15	H	279	LEU	CA-C-O	9.43	131.67	120.92
23	T	8	THR	N-CA-C	-9.43	100.55	112.90
24	X	110	PRO	N-CA-CB	9.43	111.65	103.36
18	L	91	THR	CA-C-N	9.40	134.60	120.31
18	L	91	THR	C-N-CA	9.40	134.60	120.31
31	R	102	LEU	CA-C-N	9.40	133.23	120.54
31	R	102	LEU	C-N-CA	9.40	133.23	120.54
19	M	215	PRO	CA-C-N	9.38	132.63	120.44
19	M	215	PRO	C-N-CA	9.38	132.63	120.44
4	d	109	ARG	NE-CZ-NH1	-9.38	112.12	121.50
14	n	4	PRO	N-CA-CB	9.37	111.14	103.36
4	D	231	VAL	CA-C-N	9.36	132.82	120.28
4	D	231	VAL	C-N-CA	9.36	132.82	120.28
20	J	18	GLY	CA-C-O	-9.32	111.15	120.75
3	c	89	THR	N-CA-CB	9.30	123.93	110.16
23	T	224	ARG	N-CA-C	-9.30	101.49	112.92
29	P	376	THR	CA-C-N	9.29	132.52	120.44
29	P	376	THR	C-N-CA	9.29	132.52	120.44
31	R	323	ASN	CA-C-N	9.29	132.72	120.28
31	R	323	ASN	C-N-CA	9.29	132.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	331	ASP	CA-CB-CG	9.28	121.88	112.60
19	M	178	GLU	N-CA-C	-9.27	103.07	114.75
15	H	251	PRO	CA-C-O	-9.26	114.23	120.90
33	O	375	ASP	CA-CB-CG	-9.25	103.35	112.60
15	H	397	SER	N-CA-CB	9.23	123.60	109.85
6	F	8	ASP	CA-CB-CG	-9.23	103.37	112.60
28	S	469	ASN	CA-C-N	9.23	132.64	120.28
28	S	469	ASN	C-N-CA	9.23	132.64	120.28
15	H	156	VAL	N-CA-C	-9.22	94.98	108.71
28	S	159	ASN	N-CA-C	9.21	121.32	111.28
30	Q	110	SER	CA-C-N	9.21	139.13	121.54
30	Q	110	SER	C-N-CA	9.21	139.13	121.54
4	D	104	VAL	N-CA-C	-9.21	101.42	110.72
2	B	174	PHE	CA-C-N	9.19	132.60	120.28
2	B	174	PHE	C-N-CA	9.19	132.60	120.28
26	Z	857	LEU	CA-C-N	9.19	134.68	121.54
26	Z	857	LEU	C-N-CA	9.19	134.68	121.54
20	J	244	ILE	N-CA-C	-9.17	94.36	107.75
23	T	82	PHE	N-CA-C	9.13	121.23	111.28
23	T	212	ASN	CA-CB-CG	-9.11	103.49	112.60
14	n	17	ASP	CA-CB-CG	-9.08	103.52	112.60
16	I	167	MET	CA-C-N	9.08	133.31	120.42
16	I	167	MET	C-N-CA	9.08	133.31	120.42
4	d	88	ARG	CA-C-O	-9.08	110.93	120.55
21	W	119	SER	N-CA-C	-9.07	102.23	113.38
12	l	209	ASN	OD1-CG-ND2	-9.06	113.54	122.60
11	4	128	LEU	O-C-N	-9.04	115.52	121.85
14	7	11	VAL	N-CA-C	-9.04	94.32	107.78
14	n	224	ASP	CA-CB-CG	-9.03	103.57	112.60
24	X	120	GLU	N-CA-C	9.02	120.72	111.07
29	P	323	ASN	CA-CB-CG	-9.01	103.59	112.60
33	O	228	TYR	N-CA-C	-9.01	101.26	112.88
20	J	235	VAL	CB-CA-C	-9.01	99.98	112.14
2	b	138	GLY	CA-C-O	9.00	131.06	121.61
2	B	227	ILE	CA-C-O	-8.99	115.26	119.94
29	P	288	ASN	CA-C-N	8.99	132.32	120.28
29	P	288	ASN	C-N-CA	8.99	132.32	120.28
20	J	18	GLY	O-C-N	8.96	130.79	122.19
31	R	343	GLU	N-CA-CB	8.96	123.28	110.12
7	g	186	ARG	NE-CZ-NH2	8.95	127.26	119.20
27	N	96	GLN	CA-C-O	8.94	129.91	120.70
18	L	167	VAL	N-CA-C	-8.94	99.84	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	183	LEU	N-CA-C	-8.92	101.64	111.36
26	Z	201	LEU	CA-C-N	8.91	132.02	120.44
26	Z	201	LEU	C-N-CA	8.91	132.02	120.44
31	R	98	LEU	CA-C-N	8.91	132.55	120.44
31	R	98	LEU	C-N-CA	8.91	132.55	120.44
18	L	67	HIS	ND1-CE1-NE2	8.90	117.30	108.40
9	2	23	GLY	CA-C-N	8.89	128.62	119.56
9	2	23	GLY	C-N-CA	8.89	128.62	119.56
26	Z	785	VAL	N-CA-C	-8.88	103.19	111.45
27	N	639	ASP	N-CA-C	8.87	120.95	111.28
6	f	85	ASN	OD1-CG-ND2	-8.85	113.75	122.60
7	g	243	ILE	CA-CB-CG1	8.85	125.44	110.40
9	2	37	ILE	N-CA-C	-8.84	99.89	112.35
26	Z	236	PHE	CA-CB-CG	-8.83	104.97	113.80
22	V	239	ALA	CA-C-N	8.81	132.09	120.28
22	V	239	ALA	C-N-CA	8.81	132.09	120.28
9	i	34	LEU	N-CA-CB	8.81	122.98	109.85
26	Z	516	THR	CA-C-N	8.79	132.94	120.28
26	Z	516	THR	C-N-CA	8.79	132.94	120.28
7	g	99	TYR	CA-C-N	8.78	135.29	122.82
7	g	99	TYR	C-N-CA	8.78	135.29	122.82
26	Z	77	ASN	CA-CB-CG	-8.78	103.82	112.60
22	V	287	THR	N-CA-C	-8.76	101.81	111.36
13	m	128	VAL	N-CA-C	-8.76	104.61	113.10
3	C	181	ASP	CA-CB-CG	-8.74	103.86	112.60
8	h	166	ASP	CA-CB-CG	-8.74	103.86	112.60
2	B	124	SER	CA-C-N	8.73	128.40	120.10
2	B	124	SER	C-N-CA	8.73	128.40	120.10
8	h	8	PHE	CA-C-N	8.73	132.32	120.54
8	h	8	PHE	C-N-CA	8.73	132.32	120.54
28	S	462	ASP	N-CA-C	-8.73	101.73	111.07
29	P	377	GLU	N-CA-C	-8.72	101.74	111.07
1	a	55	LEU	CB-CA-C	-8.70	95.97	109.89
28	S	337	ASN	CA-CB-CG	8.69	121.29	112.60
29	P	431	HIS	N-CA-C	-8.69	101.89	111.36
27	N	912	GLU	CA-C-O	-8.68	111.59	119.75
11	k	176	PHE	N-CA-C	-8.67	103.55	114.56
13	m	101	ARG	N-CA-C	-8.65	100.42	112.45
19	M	323	VAL	N-CA-C	-8.65	95.12	107.75
11	4	120	ASP	CA-CB-CG	8.64	121.24	112.60
26	Z	104	ASP	CA-CB-CG	-8.64	103.96	112.60
26	Z	302	SER	N-CA-CB	8.64	122.59	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	278	ILE	N-CA-C	-8.63	102.00	110.72
23	T	97	SER	N-CA-CB	8.63	125.07	110.49
2	b	81	ASP	CA-CB-CG	-8.62	103.97	112.60
2	B	200	VAL	N-CA-C	-8.62	96.46	108.27
27	N	647	ASP	O-C-N	-8.61	112.43	121.30
24	X	16	GLU	N-CA-CB	8.60	122.81	109.83
4	D	21	ALA	CA-C-N	8.59	131.61	120.44
4	D	21	ALA	C-N-CA	8.59	131.61	120.44
18	L	207	PHE	CA-CB-CG	-8.59	105.21	113.80
28	S	286	TYR	N-CA-C	-8.59	102.94	113.50
2	b	90	ARG	N-CA-C	-8.58	102.00	111.36
27	N	15	GLU	CB-CA-C	-8.57	97.82	110.16
29	P	100	VAL	CA-C-N	8.56	131.75	120.28
29	P	100	VAL	C-N-CA	8.56	131.75	120.28
31	R	167	LYS	CA-C-N	8.56	131.34	120.56
31	R	167	LYS	C-N-CA	8.56	131.34	120.56
33	O	29	PHE	N-CA-CB	8.56	122.70	110.12
26	Z	795	THR	N-CA-CB	8.55	122.93	110.20
17	K	315	ILE	N-CA-C	-8.54	96.21	108.17
16	I	224	ALA	CA-C-N	8.53	128.59	119.89
16	I	224	ALA	C-N-CA	8.53	128.59	119.89
33	O	371	VAL	CA-C-N	8.53	131.71	120.28
33	O	371	VAL	C-N-CA	8.53	131.71	120.28
13	m	36	ASN	CA-CB-CG	-8.52	104.08	112.60
22	V	186	GLN	CA-C-N	-8.51	109.05	120.54
22	V	186	GLN	C-N-CA	-8.51	109.05	120.54
23	T	110	LEU	N-CA-C	-8.51	102.08	111.36
24	X	102	GLN	N-CA-C	-8.51	100.88	112.03
24	X	87	PHE	N-CA-C	-8.50	95.50	108.67
26	Z	901	PHE	CA-CB-CG	-8.48	105.32	113.80
27	N	144	CYS	O-C-N	8.47	131.10	122.12
26	Z	601	VAL	CA-C-N	8.47	132.32	120.29
26	Z	601	VAL	C-N-CA	8.47	132.32	120.29
17	K	371	LEU	CA-C-N	8.46	132.05	120.46
17	K	371	LEU	C-N-CA	8.46	132.05	120.46
23	T	84	GLN	CA-C-N	8.46	131.44	120.44
23	T	84	GLN	C-N-CA	8.46	131.44	120.44
5	e	186	LYS	N-CA-C	-8.46	102.01	111.14
19	M	39	ASN	OD1-CG-ND2	8.45	131.05	122.60
31	R	70	TYR	CA-C-O	-8.45	106.43	120.80
19	M	144	ASP	CA-CB-CG	8.45	121.05	112.60
28	S	112	ASN	N-CA-C	8.45	123.05	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	153	ASP	N-CA-C	-8.45	102.07	111.28
20	J	342	ASN	CA-CB-CG	-8.43	104.17	112.60
6	f	113	ASP	CA-CB-CG	-8.43	104.17	112.60
4	d	49	THR	N-CA-C	-8.43	102.10	111.28
6	f	106	ARG	NE-CZ-NH1	8.42	129.92	121.50
4	D	103	THR	N-CA-C	-8.42	98.63	110.50
20	J	312	ARG	N-CA-CB	8.42	124.72	110.49
29	P	10	ASP	N-CA-C	8.42	120.46	111.28
4	D	127	PHE	CB-CG-CD2	-8.40	106.41	120.70
4	D	181	GLU	CA-C-N	8.40	129.04	120.38
4	D	181	GLU	C-N-CA	8.40	129.04	120.38
2	b	3	ASP	CA-CB-CG	-8.40	104.20	112.60
28	S	71	ALA	CA-C-N	8.37	132.17	120.29
28	S	71	ALA	C-N-CA	8.37	132.17	120.29
22	V	144	ILE	N-CA-C	-8.36	102.72	111.58
8	1	78	ALA	CA-C-N	8.35	131.47	120.28
8	1	78	ALA	C-N-CA	8.35	131.47	120.28
27	N	747	HIS	ND1-CE1-NE2	8.35	116.75	108.40
29	P	394	ASN	CA-C-N	8.35	130.52	120.09
29	P	394	ASN	C-N-CA	8.35	130.52	120.09
13	6	116	GLU	O-C-N	-8.34	113.08	122.09
27	N	463	TYR	CA-C-N	8.34	131.46	120.28
27	N	463	TYR	C-N-CA	8.34	131.46	120.28
27	N	178	SER	CA-C-O	8.34	130.25	120.66
32	U	180	ASP	N-CA-C	-8.34	102.28	111.36
5	e	5	SER	N-CA-C	-8.33	102.67	113.17
9	i	205	PHE	CA-CB-CG	-8.33	105.47	113.80
2	B	190	HIS	CE1-NE2-CD2	-8.33	100.67	109.00
14	7	161	ARG	CA-C-N	8.33	132.27	120.28
14	7	161	ARG	C-N-CA	8.33	132.27	120.28
33	O	319	LEU	CA-C-N	8.33	130.25	119.84
33	O	319	LEU	C-N-CA	8.33	130.25	119.84
17	K	155	ASP	CA-C-N	8.31	133.30	120.75
17	K	155	ASP	C-N-CA	8.31	133.30	120.75
20	J	142	VAL	N-CA-CB	8.31	117.81	110.08
27	N	231	ASN	CA-C-O	8.29	129.53	120.82
28	S	160	ARG	CA-C-N	8.29	131.22	120.44
28	S	160	ARG	C-N-CA	8.29	131.22	120.44
4	D	182	PRO	N-CA-C	8.29	120.81	110.70
23	T	226	TRP	CA-C-O	-8.29	111.83	119.62
26	Z	380	ASN	CA-C-N	8.28	131.70	120.44
26	Z	380	ASN	C-N-CA	8.28	131.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	385	ARG	N-CA-C	-8.28	102.62	112.89
7	g	11	PHE	CA-CB-CG	-8.27	105.53	113.80
16	I	239	GLN	CB-CG-CD	-8.26	98.56	112.60
3	c	28	ILE	N-CA-C	-8.25	102.39	110.72
1	A	114	ASN	CA-CB-CG	-8.25	104.35	112.60
26	Z	247	GLN	N-CA-C	-8.25	102.23	111.14
26	Z	405	ASN	N-CA-CB	8.25	121.97	110.01
27	N	532	ALA	N-CA-C	-8.25	102.25	113.30
27	N	652	VAL	N-CA-C	-8.25	102.39	110.72
10	3	111	ILE	N-CA-CB	8.24	121.84	111.46
6	f	180	LYS	N-CA-C	-8.24	102.94	113.16
30	Q	167	LYS	N-CA-C	-8.24	102.30	111.28
1	A	205	LEU	N-CA-C	-8.23	102.68	112.89
1	a	152	GLY	N-CA-C	-8.23	103.15	115.00
10	3	203	GLN	N-CA-C	-8.23	102.27	112.88
17	K	122	ILE	N-CA-CB	8.22	121.03	111.66
30	Q	209	TYR	N-CA-C	-8.21	101.09	112.25
33	O	177	GLN	OE1-CD-NE2	8.20	130.80	122.60
8	1	181	ALA	CA-C-O	-8.20	112.25	120.70
26	Z	778	LEU	CA-C-N	8.19	131.09	120.44
26	Z	778	LEU	C-N-CA	8.19	131.09	120.44
14	n	225	ILE	N-CA-CB	8.18	120.32	111.00
24	X	46	TRP	N-CA-C	-8.18	97.57	109.59
27	N	231	ASN	O-C-N	-8.17	113.66	122.07
2	B	36	GLY	N-CA-C	-8.16	98.30	110.87
22	V	213	LEU	CA-C-N	8.15	131.86	120.29
22	V	213	LEU	C-N-CA	8.15	131.86	120.29
16	I	378	GLU	N-CA-CB	8.14	122.21	110.16
13	m	77	PHE	CA-CB-CG	-8.13	105.67	113.80
10	3	90	VAL	CA-C-N	8.13	131.01	120.44
10	3	90	VAL	C-N-CA	8.13	131.01	120.44
4	D	100	ASP	CA-CB-CG	-8.12	104.48	112.60
26	Z	797	THR	N-CA-C	8.12	121.05	111.71
27	N	11	ALA	N-CA-CB	-8.12	98.14	110.16
11	k	111	LYS	CA-C-N	8.12	133.68	122.07
11	k	111	LYS	C-N-CA	8.12	133.68	122.07
26	Z	436	LEU	CA-C-N	8.12	131.81	120.29
26	Z	436	LEU	C-N-CA	8.12	131.81	120.29
27	N	263	SER	CA-C-N	8.11	131.47	120.44
27	N	263	SER	C-N-CA	8.11	131.47	120.44
15	H	235	PHE	CA-CB-CG	-8.11	105.69	113.80
30	Q	8	LEU	CA-C-N	8.11	130.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	8	LEU	C-N-CA	8.11	130.98	120.44
27	N	43	LEU	CA-C-O	-8.10	110.48	118.34
15	H	306	ILE	N-CA-CB	8.09	122.46	112.10
8	h	141	ASN	N-CA-C	-8.09	101.29	112.30
27	N	178	SER	CA-C-N	8.08	131.43	120.44
27	N	178	SER	C-N-CA	8.08	131.43	120.44
3	c	80	THR	N-CA-C	-8.08	102.55	111.36
15	H	64	LYS	N-CA-C	-8.08	102.55	111.36
33	O	337	LEU	N-CA-C	-8.08	96.70	109.23
15	H	242	PRO	N-CA-CB	8.07	110.91	103.08
33	O	110	ASP	CA-CB-CG	8.07	120.67	112.60
3	c	164	VAL	N-CA-C	-8.07	98.69	108.53
20	J	70	SER	N-CA-CB	8.06	124.12	110.49
10	3	44	HIS	ND1-CE1-NE2	8.06	116.46	108.40
17	K	412	ALA	CA-C-N	8.06	135.64	120.97
17	K	412	ALA	C-N-CA	8.06	135.64	120.97
1	a	224	PHE	CA-CB-CG	-8.06	105.74	113.80
12	5	24	ASN	N-CA-C	-8.06	104.60	114.75
28	S	484	ASP	O-C-N	8.04	130.35	122.07
2	b	244	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	37	ARG	NE-CZ-NH2	8.04	126.43	119.20
22	V	37	MET	N-CA-C	-8.03	102.61	111.36
7	g	105	ILE	N-CA-CB	8.03	115.56	110.50
26	Z	465	GLY	CA-C-N	8.03	134.30	122.74
26	Z	465	GLY	C-N-CA	8.03	134.30	122.74
28	S	76	PHE	O-C-N	8.03	130.63	122.12
6	F	19	PHE	CA-CB-CG	-8.02	105.78	113.80
33	O	195	TYR	CA-C-O	-8.02	111.92	120.42
12	5	141	ASP	CA-CB-CG	8.01	120.61	112.60
5	E	142	ASP	CA-CB-CG	-8.01	104.59	112.60
19	M	53	HIS	ND1-CE1-NE2	8.01	116.41	108.40
18	L	87	LEU	CA-C-N	7.99	131.31	120.44
18	L	87	LEU	C-N-CA	7.99	131.31	120.44
13	6	116	GLU	CA-C-O	7.99	128.93	120.70
7	g	178	HIS	CA-CB-CG	-7.99	105.81	113.80
26	Z	620	LEU	N-CA-C	-7.99	105.52	114.62
19	M	362	GLN	OE1-CD-NE2	-7.98	114.62	122.60
20	J	390	MET	N-CA-C	-7.98	101.36	112.45
27	N	426	ILE	N-CA-C	-7.98	102.66	110.72
11	4	39	SER	CA-C-N	7.98	127.70	119.56
11	4	39	SER	C-N-CA	7.98	127.70	119.56
25	Y	30	GLU	N-CA-C	-7.98	102.56	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	165	ASN	CA-CB-CG	-7.98	104.62	112.60
1	A	222	ASP	N-CA-CB	7.98	124.18	112.13
27	N	598	ASP	CA-CB-CG	-7.97	104.63	112.60
22	V	259	LYS	N-CA-C	-7.97	102.83	114.39
29	P	81	LEU	CA-C-N	7.96	130.79	120.44
29	P	81	LEU	C-N-CA	7.96	130.79	120.44
15	H	232	PRO	CA-C-N	7.96	130.94	120.28
15	H	232	PRO	C-N-CA	7.96	130.94	120.28
11	k	2	ASP	CA-CB-CG	-7.95	104.65	112.60
27	N	788	TYR	N-CA-CB	7.95	121.69	109.85
7	g	106	PRO	CA-C-N	7.94	130.77	120.44
7	g	106	PRO	C-N-CA	7.94	130.77	120.44
31	R	135	ILE	CA-C-N	7.94	131.71	120.28
31	R	135	ILE	C-N-CA	7.94	131.71	120.28
29	P	113	ASN	CA-C-N	7.94	130.92	120.28
29	P	113	ASN	C-N-CA	7.94	130.92	120.28
26	Z	201	LEU	N-CA-C	-7.93	102.71	111.36
2	b	195	THR	O-C-N	7.93	130.24	122.07
33	O	232	GLU	CA-C-N	7.92	131.23	120.38
33	O	232	GLU	C-N-CA	7.92	131.23	120.38
26	Z	622	HIS	N-CA-CB	7.92	121.76	110.12
14	7	138	SER	N-CA-C	-7.92	96.84	109.59
27	N	614	ASN	CA-C-N	7.91	131.53	120.29
27	N	614	ASN	C-N-CA	7.91	131.53	120.29
15	H	146	VAL	N-CA-CB	7.91	120.47	111.21
12	l	8	PHE	CA-C-O	7.91	130.65	121.32
13	m	185	ARG	CA-C-N	7.91	131.52	120.29
13	m	185	ARG	C-N-CA	7.91	131.52	120.29
2	b	94	HIS	CE1-NE2-CD2	-7.91	101.09	109.00
10	3	146	PHE	CB-CA-C	-7.91	97.67	110.79
29	P	117	SER	CA-C-O	-7.91	112.04	120.42
29	P	407	ASN	CA-C-N	7.91	130.87	120.28
29	P	407	ASN	C-N-CA	7.91	130.87	120.28
12	l	101	ILE	CA-C-N	7.90	134.13	122.99
12	l	101	ILE	C-N-CA	7.90	134.13	122.99
24	X	106	SER	N-CA-C	-7.89	101.69	112.03
27	N	584	ARG	N-CA-C	-7.89	102.67	111.28
26	Z	551	LEU	N-CA-CB	7.89	121.45	110.01
26	Z	258	PRO	CA-C-N	7.89	127.53	119.56
26	Z	258	PRO	C-N-CA	7.89	127.53	119.56
15	H	440	GLU	CA-C-N	7.89	130.85	120.28
15	H	440	GLU	C-N-CA	7.89	130.85	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	103	THR	N-CA-CB	7.88	121.52	110.17
2	b	53	SER	CA-C-N	7.88	127.80	119.05
2	b	53	SER	C-N-CA	7.88	127.80	119.05
4	d	127	PHE	CA-CB-CG	-7.87	105.94	113.80
1	A	215	GLU	N-CA-CB	7.86	123.78	110.49
13	m	42	LYS	N-CA-C	-7.86	101.52	112.45
31	R	110	ILE	O-C-N	-7.86	112.75	122.57
7	g	67	ASP	CA-CB-CG	7.85	120.45	112.60
10	3	117	LYS	CA-C-N	7.85	127.61	119.76
10	3	117	LYS	C-N-CA	7.85	127.61	119.76
30	Q	12	ARG	O-C-N	7.85	130.15	122.07
7	g	108	PHE	CA-CB-CG	-7.84	105.96	113.80
2	B	128	ARG	CA-C-N	7.83	127.88	119.89
2	B	128	ARG	C-N-CA	7.83	127.88	119.89
26	Z	877	THR	CA-C-O	7.83	128.72	120.42
6	F	142	HIS	ND1-CE1-NE2	7.83	116.23	108.40
29	P	277	GLN	CA-C-N	7.83	131.11	120.54
29	P	277	GLN	C-N-CA	7.83	131.11	120.54
28	S	404	LEU	CA-C-N	7.83	130.77	120.28
28	S	404	LEU	C-N-CA	7.83	130.77	120.28
33	O	49	PHE	CA-CB-CG	-7.83	105.97	113.80
5	e	186	LYS	CA-C-N	7.82	130.75	120.28
5	e	186	LYS	C-N-CA	7.82	130.75	120.28
4	d	101	PRO	CA-C-N	7.81	136.03	121.97
4	d	101	PRO	C-N-CA	7.81	136.03	121.97
14	n	2	GLN	CG-CD-NE2	-7.81	104.69	116.40
7	G	203	ASN	CA-CB-CG	-7.81	104.79	112.60
29	P	313	ILE	N-CA-C	-7.80	105.10	111.81
10	j	28	LEU	CA-C-N	7.80	128.37	121.82
10	j	28	LEU	C-N-CA	7.80	128.37	121.82
14	n	201	ASP	N-CA-CB	7.80	122.86	110.85
13	6	41	PRO	N-CA-CB	7.80	111.44	103.25
18	L	59	GLN	OE1-CD-NE2	-7.80	114.80	122.60
23	T	217	THR	CA-C-N	7.80	133.94	120.68
23	T	217	THR	C-N-CA	7.80	133.94	120.68
26	Z	40	GLU	N-CA-C	-7.80	102.68	112.90
16	I	65	ILE	N-CA-C	-7.80	105.89	113.53
17	K	348	GLU	N-CA-CB	7.80	121.58	110.12
31	R	312	TYR	CA-C-N	7.80	130.73	120.28
31	R	312	TYR	C-N-CA	7.80	130.73	120.28
30	Q	208	ILE	N-CA-C	-7.79	103.67	111.77
10	j	75	LEU	O-C-N	-7.79	113.68	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	883	SER	O-C-N	-7.79	114.20	123.31
33	O	68	LYS	N-CA-C	-7.79	103.74	113.55
33	O	151	ASP	CA-C-N	7.79	130.71	120.28
33	O	151	ASP	C-N-CA	7.79	130.71	120.28
18	L	70	TYR	CA-C-N	7.79	130.71	120.28
18	L	70	TYR	C-N-CA	7.79	130.71	120.28
29	P	433	ILE	N-CA-C	-7.79	102.86	110.72
27	N	123	PHE	CA-CB-CG	7.78	121.58	113.80
4	d	226	GLU	CA-C-O	-7.78	112.30	120.55
20	J	126	LEU	CA-C-N	7.78	130.71	120.28
20	J	126	LEU	C-N-CA	7.78	130.71	120.28
30	Q	409	TYR	N-CA-CB	-7.78	98.22	110.28
1	A	29	THR	CA-C-N	7.78	135.91	123.93
1	A	29	THR	C-N-CA	7.78	135.91	123.93
8	l	177	VAL	N-CA-C	-7.78	96.33	108.23
1	a	13	GLU	CB-CA-C	-7.77	98.62	110.90
21	W	181	LEU	O-C-N	-7.77	114.06	122.07
17	K	196	ASP	CA-CB-CG	-7.77	104.83	112.60
26	Z	863	THR	N-CA-C	-7.76	104.24	112.93
1	a	85	ALA	CA-C-N	7.75	130.52	120.44
1	a	85	ALA	C-N-CA	7.75	130.52	120.44
21	W	30	ILE	N-CA-C	-7.75	102.98	110.42
6	f	175	LEU	CB-CA-C	-7.75	98.41	110.81
8	h	92	ASN	CA-CB-CG	-7.74	104.86	112.60
18	L	339	ARG	CA-C-N	7.74	129.52	119.84
18	L	339	ARG	C-N-CA	7.74	129.52	119.84
28	S	461	PHE	CB-CA-C	-7.74	95.81	110.67
26	Z	258	PRO	N-CA-C	7.73	120.14	110.70
27	N	395	ALA	N-CA-C	-7.73	102.39	113.21
32	U	157	LEU	CA-C-N	7.73	129.50	119.84
32	U	157	LEU	C-N-CA	7.73	129.50	119.84
30	Q	67	THR	N-CA-CB	7.73	123.55	110.49
16	I	360	LYS	CA-C-N	7.72	131.04	120.46
16	I	360	LYS	C-N-CA	7.72	131.04	120.46
28	S	133	GLU	CA-C-N	7.72	131.04	120.46
28	S	133	GLU	C-N-CA	7.72	131.04	120.46
18	L	286	ILE	N-CA-C	-7.72	105.49	112.90
13	m	76	HIS	CA-CB-CG	-7.71	106.09	113.80
27	N	296	CYS	CA-C-N	7.71	130.61	120.28
27	N	296	CYS	C-N-CA	7.71	130.61	120.28
31	R	255	VAL	N-CA-C	7.70	117.81	110.42
14	n	66	LEU	N-CA-CB	7.70	121.56	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	108	HIS	ND1-CE1-NE2	7.70	116.10	108.40
7	g	177	ASP	N-CA-CB	7.70	121.55	110.16
28	S	308	GLY	CA-C-O	-7.70	113.12	121.05
10	3	194	VAL	N-CA-CB	7.69	122.03	111.41
6	F	77	ALA	CA-C-O	-7.69	109.62	120.16
12	l	36	GLU	N-CA-CB	7.68	121.86	110.49
27	N	146	LYS	O-C-N	7.68	130.91	122.15
18	L	245	PHE	CA-CB-CG	-7.67	106.13	113.80
17	K	79	LEU	O-C-N	7.67	130.89	122.15
23	T	161	TRP	N-CA-C	-7.67	102.92	111.28
30	Q	4	PRO	CA-C-N	7.66	128.65	119.99
30	Q	4	PRO	C-N-CA	7.66	128.65	119.99
23	T	139	ASP	CA-CB-CG	-7.66	104.94	112.60
2	b	175	LEU	CA-C-N	7.66	130.54	120.28
2	b	175	LEU	C-N-CA	7.66	130.54	120.28
10	j	67	ARG	CA-C-O	7.66	128.53	120.42
22	V	83	VAL	N-CA-CB	7.65	119.72	110.31
18	L	150	ILE	CA-C-N	7.64	130.38	120.44
18	L	150	ILE	C-N-CA	7.64	130.38	120.44
22	V	40	HIS	CA-C-N	7.64	128.40	120.00
22	V	40	HIS	C-N-CA	7.64	128.40	120.00
11	4	78	GLN	N-CA-C	-7.64	102.90	111.07
26	Z	427	GLN	O-C-N	7.63	132.25	122.87
29	P	386	GLN	OE1-CD-NE2	7.62	130.22	122.60
2	b	90	ARG	O-C-N	-7.62	113.46	122.15
27	N	910	PRO	CA-C-N	7.62	130.50	120.28
27	N	910	PRO	C-N-CA	7.62	130.50	120.28
28	S	111	ARG	CA-C-N	7.62	133.19	122.36
28	S	111	ARG	C-N-CA	7.62	133.19	122.36
24	X	53	THR	N-CA-C	-7.62	104.13	113.50
1	A	92	ALA	O-C-N	7.62	130.32	122.09
2	B	88	LYS	CA-C-N	7.62	130.49	120.28
2	B	88	LYS	C-N-CA	7.62	130.49	120.28
3	C	152	PRO	N-CA-C	-7.62	104.66	114.03
1	a	125	MET	CG-SD-CE	-7.61	84.15	100.90
24	X	120	GLU	O-C-N	7.61	129.91	122.07
21	W	42	ASN	OD1-CG-ND2	7.61	130.21	122.60
10	j	203	GLN	N-CA-C	-7.60	102.65	112.23
18	L	350	PRO	CA-C-N	7.60	130.99	120.65
18	L	350	PRO	C-N-CA	7.60	130.99	120.65
3	c	230	LYS	O-C-N	-7.60	113.54	121.60
14	7	152	ASN	N-CA-CB	7.60	123.90	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	494	GLY	N-CA-C	7.60	121.85	112.73
33	O	13	THR	N-CA-C	-7.59	102.94	111.14
15	H	272	ILE	N-CA-C	-7.59	97.19	108.12
27	N	101	ILE	CA-C-N	7.59	130.12	120.56
27	N	101	ILE	C-N-CA	7.59	130.12	120.56
11	4	10	GLN	O-C-N	7.59	130.16	122.12
31	R	296	LEU	CA-C-N	7.59	131.84	120.31
31	R	296	LEU	C-N-CA	7.59	131.84	120.31
4	d	78	ALA	CA-C-O	7.58	128.51	120.70
18	L	80	ASN	CA-CB-CG	-7.58	105.02	112.60
29	P	74	ASP	CA-C-N	7.58	130.29	120.44
29	P	74	ASP	C-N-CA	7.58	130.29	120.44
13	6	46	CYS	N-CA-C	-7.58	104.27	113.97
8	h	122	LEU	O-C-N	-7.57	116.12	121.65
16	I	362	LEU	O-C-N	7.57	130.15	122.12
27	N	172	SER	N-CA-C	-7.57	103.50	112.89
15	H	392	HIS	CE1-NE2-CD2	-7.57	101.43	109.00
27	N	144	CYS	CA-C-O	-7.57	112.53	120.55
14	n	189	ALA	O-C-N	7.56	132.47	122.33
1	A	4	ASP	CA-CB-CG	-7.56	105.04	112.60
15	H	341	ASP	CA-CB-CG	-7.55	105.05	112.60
10	3	17	LYS	CA-C-N	7.55	132.84	122.19
10	3	17	LYS	C-N-CA	7.55	132.84	122.19
9	i	200	GLN	N-CA-CB	7.55	121.33	110.16
29	P	142	ASP	CA-CB-CG	-7.55	105.05	112.60
27	N	734	VAL	CB-CA-C	-7.54	101.96	112.14
29	P	61	LYS	N-CA-C	7.54	119.14	111.07
31	R	107	GLU	O-C-N	-7.54	114.25	122.09
20	J	310	ILE	CB-CA-C	-7.54	98.93	111.29
2	b	34	SER	CA-C-O	7.54	130.26	121.44
21	W	116	SER	O-C-N	7.54	127.43	121.55
31	R	130	GLN	CA-C-N	7.54	130.69	120.44
31	R	130	GLN	C-N-CA	7.54	130.69	120.44
18	L	162	GLU	CA-C-N	7.53	131.89	120.82
18	L	162	GLU	C-N-CA	7.53	131.89	120.82
18	L	196	VAL	N-CA-C	7.53	117.65	110.42
1	a	154	TYR	CA-C-N	-7.53	113.68	122.11
1	a	154	TYR	C-N-CA	-7.53	113.68	122.11
30	Q	240	PHE	CA-C-O	-7.53	112.57	120.55
23	T	252	GLU	CA-C-N	7.53	130.22	120.44
23	T	252	GLU	C-N-CA	7.53	130.22	120.44
16	I	344	ILE	CA-C-O	7.52	126.11	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	231	VAL	CB-CA-C	-7.52	101.98	112.14
5	E	100	ASN	OD1-CG-ND2	7.52	130.12	122.60
7	G	101	THR	N-CA-C	-7.52	101.45	108.22
30	Q	414	GLU	CA-C-N	7.52	130.22	120.44
30	Q	414	GLU	C-N-CA	7.52	130.22	120.44
26	Z	361	HIS	N-CA-C	-7.52	103.16	111.36
22	V	187	ALA	CB-CA-C	-7.52	98.78	110.81
28	S	31	VAL	CA-C-O	-7.52	113.13	120.95
2	b	22	ASP	N-CA-C	7.51	120.35	111.71
4	d	150	PRO	N-CA-C	-7.51	103.73	113.57
23	T	221	ALA	CA-C-N	7.51	130.34	120.28
23	T	221	ALA	C-N-CA	7.51	130.34	120.28
6	F	189	ILE	CA-C-N	7.51	130.20	120.44
6	F	189	ILE	C-N-CA	7.51	130.20	120.44
9	i	188	ARG	N-CA-CB	7.50	121.16	109.83
4	D	65	ILE	N-CA-C	-7.50	105.46	112.96
32	U	107	ASN	OD1-CG-ND2	-7.50	115.10	122.60
20	J	138	MET	CA-C-N	7.49	130.00	120.56
20	J	138	MET	C-N-CA	7.49	130.00	120.56
9	i	3	ILE	N-CA-C	-7.49	97.36	108.45
28	S	88	PHE	CA-CB-CG	-7.49	106.31	113.80
32	U	114	THR	O-C-N	7.49	131.45	123.06
4	d	168	THR	N-CA-CB	-7.49	99.08	110.16
16	I	77	SER	CA-C-O	-7.49	113.19	120.90
28	S	342	LEU	CA-C-N	7.48	129.06	119.78
28	S	342	LEU	C-N-CA	7.48	129.06	119.78
29	P	238	ALA	CA-C-O	7.48	128.48	120.55
33	O	150	LEU	N-CA-CB	7.48	121.23	110.16
23	T	263	ALA	CA-C-N	7.48	130.91	120.29
23	T	263	ALA	C-N-CA	7.48	130.91	120.29
10	j	3	PRO	N-CA-C	-7.47	103.80	114.18
20	J	139	VAL	CA-C-O	-7.47	113.26	121.17
22	V	20	ARG	NE-CZ-NH1	7.47	128.97	121.50
29	P	342	GLN	OE1-CD-NE2	7.47	130.07	122.60
20	J	299	ILE	CA-C-N	7.46	132.66	120.94
20	J	299	ILE	C-N-CA	7.46	132.66	120.94
2	b	190	HIS	CE1-NE2-CD2	-7.46	101.54	109.00
30	Q	241	GLU	O-C-N	-7.46	114.21	122.12
6	F	54	GLU	N-CA-C	7.46	119.05	111.07
13	6	143	ALA	N-CA-C	-7.46	103.15	111.28
27	N	267	GLN	CA-C-N	7.46	130.14	120.44
27	N	267	GLN	C-N-CA	7.46	130.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	65	LEU	CA-C-N	7.46	130.59	120.44
12	l	65	LEU	C-N-CA	7.46	130.59	120.44
7	g	63	ILE	N-CA-CB	7.46	119.30	110.95
7	g	173	GLU	CA-C-O	-7.45	112.52	120.42
27	N	283	ASP	CA-CB-CG	-7.45	105.15	112.60
32	U	284	SER	N-CA-C	-7.45	103.24	111.36
28	S	150	LYS	N-CA-CB	7.45	123.08	110.49
6	f	119	THR	N-CA-C	-7.45	104.33	113.41
10	j	64	GLU	N-CA-C	7.45	119.40	111.28
22	V	109	HIS	CE1-NE2-CD2	-7.45	101.55	109.00
32	U	94	HIS	CA-C-N	7.45	131.00	120.28
32	U	94	HIS	C-N-CA	7.45	131.00	120.28
9	i	71	SER	CA-C-N	7.44	134.28	122.59
9	i	71	SER	C-N-CA	7.44	134.28	122.59
8	l	37	VAL	N-CA-C	-7.44	104.71	113.42
22	V	126	GLN	N-CA-C	-7.44	103.19	111.82
27	N	12	LEU	CA-C-N	7.44	130.25	120.28
27	N	12	LEU	C-N-CA	7.44	130.25	120.28
23	T	205	ILE	N-CA-C	-7.44	103.28	110.42
1	a	21	TYR	CB-CG-CD2	-7.43	109.65	120.80
31	R	184	GLN	N-CA-C	-7.43	102.86	112.23
12	5	188	HIS	CA-CB-CG	-7.42	106.38	113.80
5	e	100	ASN	CA-C-O	7.42	129.34	120.81
2	B	165	GLY	O-C-N	-7.42	115.31	123.10
11	k	155	GLU	N-CA-C	-7.42	102.57	111.69
3	c	214	THR	N-CA-C	-7.41	97.79	109.50
14	7	211	ASN	OD1-CG-ND2	-7.41	115.19	122.60
26	Z	293	MET	CA-C-N	7.41	130.94	120.42
26	Z	293	MET	C-N-CA	7.41	130.94	120.42
8	h	173	ILE	N-CA-CB	7.40	119.44	111.00
7	g	203	ASN	OD1-CG-ND2	-7.40	115.20	122.60
11	k	116	LEU	N-CA-CB	7.40	122.09	110.84
26	Z	214	HIS	CA-C-N	7.40	130.80	120.29
26	Z	214	HIS	C-N-CA	7.40	130.80	120.29
27	N	650	ASP	CA-CB-CG	-7.40	105.20	112.60
29	P	234	TYR	N-CA-C	-7.40	102.91	112.23
29	P	319	GLU	O-C-N	-7.40	113.90	120.48
13	6	218	GLU	N-CA-CB	7.39	120.81	110.17
27	N	222	TYR	N-CA-C	-7.38	103.87	113.17
31	R	20	ARG	CA-C-N	7.38	126.23	120.33
31	R	20	ARG	C-N-CA	7.38	126.23	120.33
27	N	146	LYS	CA-C-O	-7.38	112.60	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	677	ASP	CA-CB-CG	7.38	119.98	112.60
11	k	108	ASP	CA-CB-CG	-7.38	105.22	112.60
33	O	167	ILE	N-CA-C	7.37	117.50	110.42
27	N	123	PHE	CA-C-N	7.37	130.46	120.44
27	N	123	PHE	C-N-CA	7.37	130.46	120.44
31	R	246	TYR	CA-C-N	7.37	130.16	120.28
31	R	246	TYR	C-N-CA	7.37	130.16	120.28
3	C	203	SER	N-CA-CB	7.37	120.75	110.07
28	S	183	LEU	CA-C-O	-7.37	112.61	120.42
15	H	335	GLU	CA-C-N	7.36	130.74	120.29
15	H	335	GLU	C-N-CA	7.36	130.74	120.29
3	c	5	TYR	N-CA-C	-7.36	102.22	112.45
12	5	126	ILE	N-CA-C	-7.36	96.88	107.77
21	W	184	ASN	O-C-N	7.36	130.54	122.15
18	L	234	ALA	CA-C-O	-7.36	113.09	120.82
4	D	220	VAL	N-CA-C	-7.36	98.64	108.35
27	N	457	SER	N-CA-C	-7.36	102.64	111.69
14	n	179	ASN	N-CA-C	-7.35	103.27	111.28
27	N	770	LYS	N-CA-CB	7.34	122.51	110.17
16	I	407	ARG	N-CA-C	-7.34	101.07	111.56
26	Z	338	HIS	N-CA-CB	7.34	122.32	110.51
30	Q	427	PHE	CA-CB-CG	-7.34	106.46	113.80
27	N	601	THR	CA-C-N	7.34	124.86	120.24
27	N	601	THR	C-N-CA	7.34	124.86	120.24
31	R	45	GLU	N-CA-C	-7.34	103.22	111.07
6	f	29	LYS	N-CA-C	7.33	120.14	111.71
13	6	140	GLY	CA-C-N	7.33	130.11	120.28
13	6	140	GLY	C-N-CA	7.33	130.11	120.28
3	C	151	ASN	CA-C-N	7.33	127.50	119.87
3	C	151	ASN	C-N-CA	7.33	127.50	119.87
4	d	238	LYS	N-CA-CB	7.33	120.89	110.12
10	j	163	PHE	CA-CB-CG	-7.33	106.47	113.80
19	M	264	ARG	CA-C-N	7.33	130.70	120.29
19	M	264	ARG	C-N-CA	7.33	130.70	120.29
29	P	78	GLN	N-CA-C	7.33	119.17	111.03
11	k	82	SER	CA-C-N	7.33	129.96	120.44
11	k	82	SER	C-N-CA	7.33	129.96	120.44
27	N	105	SER	CA-C-N	7.33	130.50	120.46
27	N	105	SER	C-N-CA	7.33	130.50	120.46
1	a	221	LYS	N-CA-CB	7.32	120.90	109.69
31	R	70	TYR	CD1-CG-CD2	-7.32	107.11	118.10
15	H	95	HIS	O-C-N	-7.32	116.31	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	357	ARG	CA-C-N	7.32	126.95	119.56
15	H	357	ARG	C-N-CA	7.32	126.95	119.56
32	U	191	THR	N-CA-C	-7.32	103.24	111.07
27	N	494	LYS	CA-C-O	-7.32	112.87	119.75
17	K	133	PRO	CA-C-O	-7.31	113.35	121.32
13	6	165	ASN	CA-CB-CG	-7.31	105.29	112.60
8	h	161	GLN	CA-C-O	-7.31	112.80	120.55
27	N	686	ILE	N-CA-C	-7.31	103.34	110.72
2	b	22	ASP	CA-CB-CG	7.31	119.91	112.60
10	3	119	PHE	CA-CB-CG	-7.31	106.49	113.80
33	O	179	PHE	CA-CB-CG	-7.30	106.50	113.80
10	3	44	HIS	CE1-NE2-CD2	-7.30	101.70	109.00
28	S	64	ARG	N-CA-CB	7.30	120.92	109.82
15	H	158	GLY	CA-C-N	7.29	131.54	120.82
15	H	158	GLY	C-N-CA	7.29	131.54	120.82
32	U	159	CYS	CA-C-N	7.29	132.17	121.31
32	U	159	CYS	C-N-CA	7.29	132.17	121.31
5	e	14	PHE	CA-CB-CG	-7.29	106.51	113.80
1	A	8	THR	CA-C-O	7.29	128.27	120.55
31	R	58	GLU	O-C-N	-7.29	112.90	122.59
10	3	149	CYS	CA-C-O	-7.29	112.83	120.55
26	Z	441	TYR	N-CA-C	-7.28	103.96	112.92
8	h	171	GLY	CA-C-N	7.28	130.47	120.35
8	h	171	GLY	C-N-CA	7.28	130.47	120.35
12	l	12	ILE	CA-C-O	-7.28	113.04	120.25
1	A	131	ILE	N-CA-C	-7.28	97.98	108.17
2	B	219	PRO	N-CA-C	-7.28	104.44	114.27
4	D	213	VAL	N-CA-CB	7.28	121.11	111.64
26	Z	181	GLY	CA-C-O	7.28	128.57	119.25
6	f	220	PRO	CB-CA-C	-7.28	101.42	110.95
28	S	209	ILE	CA-C-N	7.28	130.03	120.28
28	S	209	ILE	C-N-CA	7.28	130.03	120.28
8	l	90	LYS	CB-CA-C	-7.27	98.32	110.68
14	n	158	VAL	N-CA-C	7.27	117.36	110.53
27	N	266	SER	N-CA-CB	7.27	120.75	110.36
28	S	156	VAL	N-CA-C	7.27	117.99	110.36
5	E	45	ARG	NE-CZ-NH2	7.27	125.74	119.20
18	L	431	THR	CA-C-N	7.26	135.05	121.97
18	L	431	THR	C-N-CA	7.26	135.05	121.97
30	Q	119	GLU	N-CA-C	7.26	119.83	111.11
26	Z	484	LYS	CA-C-N	7.26	130.41	120.46
26	Z	484	LYS	C-N-CA	7.26	130.41	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	141	LEU	O-C-N	-7.26	114.42	122.12
14	7	78	ASN	CA-C-N	7.26	128.91	119.84
14	7	78	ASN	C-N-CA	7.26	128.91	119.84
26	Z	21	GLU	CA-C-N	7.26	130.00	120.28
26	Z	21	GLU	C-N-CA	7.26	130.00	120.28
13	6	181	ILE	CA-C-N	7.25	130.00	120.28
13	6	181	ILE	C-N-CA	7.25	130.00	120.28
26	Z	532	HIS	ND1-CE1-NE2	7.25	115.65	108.40
29	P	405	PRO	CA-C-O	-7.25	113.01	121.86
32	U	100	ARG	NE-CZ-NH2	-7.25	112.67	119.20
2	b	20	GLN	CB-CG-CD	-7.25	100.28	112.60
6	f	9	THR	CA-CB-OG1	7.25	120.47	109.60
15	H	438	ALA	N-CA-CB	7.25	120.87	109.71
26	Z	956	LEU	N-CA-C	-7.25	95.33	108.02
9	2	28	ASP	CA-CB-CG	7.25	119.85	112.60
10	3	2	ASP	CA-C-N	7.25	126.75	118.85
10	3	2	ASP	C-N-CA	7.25	126.75	118.85
27	N	191	THR	N-CA-C	-7.25	103.38	111.28
33	O	183	ASN	CA-CB-CG	-7.25	105.36	112.60
17	K	311	ASN	CA-CB-CG	-7.24	105.36	112.60
31	R	36	SER	N-CA-C	-7.24	102.75	113.61
9	i	190	TYR	N-CA-C	-7.24	103.32	111.14
18	L	67	HIS	CE1-NE2-CD2	-7.24	101.76	109.00
1	A	118	ILE	CA-C-N	7.24	130.70	120.28
1	A	118	ILE	C-N-CA	7.24	130.70	120.28
23	T	60	ARG	CA-C-N	7.24	129.68	120.56
23	T	60	ARG	C-N-CA	7.24	129.68	120.56
29	P	23	LYS	N-CA-C	-7.23	103.47	111.36
29	P	176	LYS	N-CA-C	-7.23	103.48	111.36
33	O	377	VAL	O-C-N	7.23	128.88	121.87
12	l	147	ASP	CA-CB-CG	-7.23	105.37	112.60
24	X	10	PHE	CA-CB-CG	-7.22	106.58	113.80
1	a	174	GLU	CB-CA-C	-7.22	98.81	110.79
12	l	179	HIS	N-CA-CB	7.22	121.91	110.65
4	d	29	THR	N-CA-CB	7.21	120.56	110.17
26	Z	532	HIS	CE1-NE2-CD2	-7.21	101.78	109.00
7	g	185	ALA	N-CA-CB	7.21	120.72	110.12
5	E	128	ARG	O-C-N	-7.21	115.15	121.71
26	Z	771	HIS	ND1-CE1-NE2	7.21	115.61	108.40
16	I	355	LEU	N-CA-C	7.21	118.79	111.07
10	3	117	LYS	CA-C-O	-7.21	112.96	119.59
18	L	366	ALA	CA-C-N	7.21	129.81	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	366	ALA	C-N-CA	7.21	129.81	120.44
7	G	193	ALA	CA-C-N	7.21	129.81	120.44
7	G	193	ALA	C-N-CA	7.21	129.81	120.44
20	J	323	ALA	CA-C-N	7.21	129.94	120.28
20	J	323	ALA	C-N-CA	7.21	129.94	120.28
33	O	29	PHE	CA-CB-CG	-7.21	106.59	113.80
7	G	160	ALA	O-C-N	-7.21	115.41	123.48
31	R	23	ASN	CA-CB-CG	-7.21	105.39	112.60
16	I	60	LEU	N-CA-CB	7.20	120.45	110.01
4	D	140	ASP	CA-C-N	7.20	133.46	122.37
4	D	140	ASP	C-N-CA	7.20	133.46	122.37
11	4	115	GLU	CA-C-N	7.20	133.15	122.99
11	4	115	GLU	C-N-CA	7.20	133.15	122.99
26	Z	918	ASP	CA-C-N	7.20	130.52	120.29
26	Z	918	ASP	C-N-CA	7.20	130.52	120.29
9	i	152	ILE	N-CA-C	-7.20	103.51	110.42
2	B	123	GLN	CA-C-O	7.20	128.05	120.42
26	Z	770	GLU	N-CA-CB	7.20	120.55	110.26
3	c	201	ASP	N-CA-C	-7.20	104.37	113.72
5	E	187	GLU	O-C-N	7.20	129.75	122.12
13	6	208	THR	CA-C-N	7.19	129.92	120.28
13	6	208	THR	C-N-CA	7.19	129.92	120.28
27	N	208	ARG	CA-C-N	7.19	129.92	120.28
27	N	208	ARG	C-N-CA	7.19	129.92	120.28
12	l	179	HIS	CB-CG-ND1	7.19	133.49	122.70
2	B	32	VAL	CA-C-N	7.19	131.08	120.87
2	B	32	VAL	C-N-CA	7.19	131.08	120.87
7	g	4	TYR	N-CA-C	-7.19	104.54	113.38
27	N	743	PHE	CA-CB-CG	-7.19	106.61	113.80
16	I	137	ASP	CA-CB-CG	-7.18	105.42	112.60
5	e	233	LYS	N-CA-C	-7.18	103.49	111.82
27	N	284	PRO	N-CA-C	-7.18	104.58	114.27
20	J	69	GLY	CA-C-N	7.18	135.25	121.54
20	J	69	GLY	C-N-CA	7.18	135.25	121.54
2	b	71	ILE	N-CA-CB	7.18	122.61	111.99
10	j	148	MET	N-CA-CB	7.17	120.41	110.01
17	K	330	ARG	N-CA-CB	7.17	118.01	111.27
6	f	27	ALA	CA-C-N	7.17	129.60	120.56
6	f	27	ALA	C-N-CA	7.17	129.60	120.56
13	m	147	MET	N-CA-C	7.17	122.57	113.25
28	S	153	GLU	CA-C-N	7.17	129.76	120.44
28	S	153	GLU	C-N-CA	7.17	129.76	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	25	ASN	CA-C-N	7.17	130.20	120.38
25	Y	25	ASN	C-N-CA	7.17	130.20	120.38
13	m	119	LYS	CA-C-N	7.17	126.80	119.92
13	m	119	LYS	C-N-CA	7.17	126.80	119.92
20	J	159	GLU	CA-C-O	7.17	128.15	120.55
27	N	417	ARG	NE-CZ-NH1	-7.16	114.34	121.50
17	K	232	ALA	O-C-N	-7.15	114.95	123.03
27	N	577	SER	CA-C-O	7.15	128.23	119.79
31	R	224	PHE	CA-C-N	7.15	129.87	120.28
31	R	224	PHE	C-N-CA	7.15	129.87	120.28
7	g	135	GLY	CA-C-N	7.15	130.23	120.72
7	g	135	GLY	C-N-CA	7.15	130.23	120.72
8	h	38	HIS	CA-C-N	7.15	129.86	120.28
8	h	38	HIS	C-N-CA	7.15	129.86	120.28
26	Z	826	ARG	NE-CZ-NH2	-7.15	112.77	119.20
26	Z	508	LEU	N-CA-C	-7.15	103.42	111.14
27	N	11	ALA	N-CA-C	-7.15	103.57	111.36
26	Z	554	THR	CA-C-N	7.15	129.86	120.28
26	Z	554	THR	C-N-CA	7.15	129.86	120.28
29	P	286	ASN	CA-CB-CG	-7.15	105.45	112.60
13	m	142	ALA	CA-C-O	7.14	128.38	119.59
17	K	155	ASP	CA-CB-CG	-7.14	105.46	112.60
3	c	168	THR	N-CA-C	-7.14	103.58	111.36
1	a	94	GLU	N-CA-C	-7.14	103.50	111.28
14	n	229	GLY	CA-C-N	7.14	129.72	120.44
14	n	229	GLY	C-N-CA	7.14	129.72	120.44
16	I	78	ASN	CA-CB-CG	7.14	119.74	112.60
6	f	81	ARG	CD-NE-CZ	7.13	134.39	124.40
2	B	185	LEU	N-CA-C	-7.13	103.58	111.36
24	X	120	GLU	CA-C-O	-7.13	113.33	120.82
11	k	86	GLN	CB-CG-CD	-7.13	100.48	112.60
25	Y	66	ASP	CA-CB-CG	7.13	119.73	112.60
2	b	67	LEU	N-CA-C	-7.13	104.57	113.55
19	M	248	ALA	CA-C-N	7.12	127.12	119.28
19	M	248	ALA	C-N-CA	7.12	127.12	119.28
27	N	49	LEU	N-CA-CB	7.12	120.59	110.12
27	N	912	GLU	CA-C-N	7.12	126.88	119.76
27	N	912	GLU	C-N-CA	7.12	126.88	119.76
13	m	55	ASN	CA-C-O	7.12	128.70	120.80
13	6	108	HIS	CE1-NE2-CD2	-7.12	101.88	109.00
31	R	187	VAL	CA-C-N	7.12	129.70	120.44
31	R	187	VAL	C-N-CA	7.12	129.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	15	GLN	N-CA-C	7.12	119.04	111.28
2	b	12	PHE	CA-C-N	7.12	137.10	124.01
2	b	12	PHE	C-N-CA	7.12	137.10	124.01
13	6	50	ILE	N-CA-C	-7.12	97.87	108.12
15	H	96	PRO	N-CA-CB	7.11	110.42	102.60
8	1	192	GLU	N-CA-C	7.11	119.03	111.28
6	F	124	GLY	CA-C-N	7.10	131.48	120.68
6	F	124	GLY	C-N-CA	7.10	131.48	120.68
17	K	190	LEU	CA-C-N	7.10	126.93	119.05
17	K	190	LEU	C-N-CA	7.10	126.93	119.05
28	S	413	LEU	N-CA-C	-7.10	99.04	110.32
26	Z	295	ARG	CA-C-O	-7.09	113.37	120.82
2	B	18	LEU	CA-C-N	7.09	127.67	119.94
2	B	18	LEU	C-N-CA	7.09	127.67	119.94
26	Z	583	ASP	CA-CB-CG	-7.09	105.51	112.60
28	S	169	CYS	N-CA-C	-7.09	104.76	113.41
2	B	90	ARG	N-CA-CB	7.09	120.29	110.01
29	P	5	ALA	CA-C-N	7.09	127.08	119.28
29	P	5	ALA	C-N-CA	7.09	127.08	119.28
2	b	130	PHE	CA-CB-CG	-7.09	106.71	113.80
8	h	188	PHE	CA-CB-CG	-7.09	106.71	113.80
27	N	419	THR	CA-C-N	7.09	129.78	120.28
27	N	419	THR	C-N-CA	7.09	129.78	120.28
29	P	429	ILE	N-CA-C	-7.08	103.39	110.62
14	7	139	SER	CA-C-N	7.08	126.56	118.85
14	7	139	SER	C-N-CA	7.08	126.56	118.85
33	O	236	HIS	N-CA-C	-7.08	100.55	110.31
3	c	112	ARG	CA-C-O	7.07	128.05	120.55
7	g	235	ALA	N-CA-C	-7.07	103.61	111.82
21	W	158	ILE	CA-C-N	7.07	129.63	120.44
21	W	158	ILE	C-N-CA	7.07	129.63	120.44
17	K	294	ARG	N-CA-CB	7.07	120.62	110.16
33	O	138	LEU	N-CA-CB	7.07	120.51	110.12
5	E	198	GLN	CA-C-N	7.07	131.94	121.77
5	E	198	GLN	C-N-CA	7.07	131.94	121.77
6	F	142	HIS	CA-CB-CG	-7.06	106.74	113.80
21	W	83	GLY	N-CA-C	-7.06	104.57	112.33
2	b	196	LEU	CA-C-N	7.06	129.74	120.28
2	b	196	LEU	C-N-CA	7.06	129.74	120.28
19	M	188	LYS	N-CA-C	-7.06	103.52	111.14
9	2	65	LEU	CA-C-N	7.05	129.61	120.44
9	2	65	LEU	C-N-CA	7.05	129.61	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	190	HIS	CG-CD2-NE2	7.05	114.25	107.20
4	D	66	ASP	CA-CB-CG	7.05	119.65	112.60
28	S	106	GLY	CA-C-N	7.05	129.73	120.28
28	S	106	GLY	C-N-CA	7.05	129.73	120.28
14	7	200	ILE	N-CA-C	-7.05	96.94	107.37
12	l	202	GLU	N-CA-C	7.05	118.96	111.28
1	A	23	PHE	CA-CB-CG	-7.04	106.76	113.80
15	H	443	PHE	CA-CB-CG	-7.04	106.76	113.80
28	S	261	HIS	N-CA-C	-7.04	102.06	113.19
16	I	189	SER	CA-C-O	-7.04	113.03	120.63
10	j	96	GLU	N-CA-CB	7.03	120.42	109.94
33	O	284	GLU	N-CA-C	7.03	118.95	111.28
30	Q	70	ALA	N-CA-CB	7.03	120.62	109.51
14	n	152	ASN	CA-C-N	7.03	127.63	119.47
14	n	152	ASN	C-N-CA	7.03	127.63	119.47
4	D	36	GLY	O-C-N	-7.03	116.76	122.81
28	S	32	GLN	OE1-CD-NE2	-7.03	115.57	122.60
5	e	119	ALA	CA-C-O	7.03	128.75	121.23
5	e	5	SER	CA-C-N	7.03	131.97	120.94
5	e	5	SER	C-N-CA	7.03	131.97	120.94
8	h	89	ASN	CA-C-O	7.03	129.47	121.32
13	m	53	SER	O-C-N	-7.03	115.19	123.41
22	V	168	LEU	N-CA-C	-7.03	103.89	113.30
19	M	292	ASP	N-CA-C	-7.02	105.90	114.75
30	Q	72	ASP	CA-C-N	7.02	129.57	120.44
30	Q	72	ASP	C-N-CA	7.02	129.57	120.44
29	P	132	VAL	N-CA-C	7.02	123.94	109.34
16	I	379	THR	CA-C-N	7.02	129.69	120.28
16	I	379	THR	C-N-CA	7.02	129.69	120.28
29	P	74	ASP	N-CA-C	-7.02	103.71	111.36
6	f	6	ASP	CA-CB-CG	7.01	119.61	112.60
4	d	140	ASP	O-C-N	-7.01	115.92	123.42
27	N	272	ILE	CA-C-N	7.01	129.67	120.28
27	N	272	ILE	C-N-CA	7.01	129.67	120.28
31	R	109	LYS	CA-C-N	7.01	134.58	121.97
31	R	109	LYS	C-N-CA	7.01	134.58	121.97
19	M	228	LYS	N-CA-C	-7.00	103.58	111.07
16	I	92	GLU	CA-C-N	7.00	129.54	120.44
16	I	92	GLU	C-N-CA	7.00	129.54	120.44
32	U	77	ASN	O-C-N	-7.00	114.81	122.09
4	d	114	VAL	N-CA-CB	7.00	119.53	110.57
13	6	80	ASN	CA-C-N	7.00	132.97	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	80	ASN	C-N-CA	7.00	132.97	122.68
17	K	140	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
31	R	422	ARG	CA-C-N	7.00	130.23	120.29
31	R	422	ARG	C-N-CA	7.00	130.23	120.29
7	G	85	VAL	CA-C-N	7.00	129.65	120.28
7	G	85	VAL	C-N-CA	7.00	129.65	120.28
3	c	230	LYS	CA-C-N	6.99	127.58	119.47
3	c	230	LYS	C-N-CA	6.99	127.58	119.47
8	h	122	LEU	N-CA-C	-6.99	100.14	108.25
19	M	64	ASP	N-CA-C	6.99	118.98	111.36
23	T	83	ASN	N-CA-C	6.99	119.50	111.11
4	d	15	ILE	N-CA-C	-6.99	99.71	109.21
12	l	191	HIS	CB-CG-ND1	6.99	133.18	122.70
3	c	23	TYR	CA-C-N	6.99	129.64	120.28
3	c	23	TYR	C-N-CA	6.99	129.64	120.28
30	Q	76	GLU	N-CA-C	6.99	125.68	110.80
18	L	246	SER	CA-C-O	-6.98	112.30	119.49
29	P	263	HIS	ND1-CE1-NE2	6.98	115.38	108.40
28	S	383	LEU	CA-C-N	6.98	129.63	120.28
28	S	383	LEU	C-N-CA	6.98	129.63	120.28
7	G	242	GLU	N-CA-C	-6.97	103.76	111.36
26	Z	613	ASP	N-CA-C	-6.97	103.76	111.36
33	O	203	THR	CA-C-N	6.97	129.62	120.28
33	O	203	THR	C-N-CA	6.97	129.62	120.28
28	S	78	VAL	CA-C-N	6.97	129.62	120.28
28	S	78	VAL	C-N-CA	6.97	129.62	120.28
20	J	349	LYS	N-CA-C	6.97	118.53	111.07
6	F	142	HIS	CE1-NE2-CD2	-6.97	102.03	109.00
11	k	111	LYS	CA-C-O	6.96	127.09	119.15
12	l	190	ASN	CA-CB-CG	-6.96	105.64	112.60
17	K	143	SER	N-CA-C	-6.96	104.92	113.41
6	f	100	ARG	CA-C-N	6.96	130.75	120.87
6	f	100	ARG	C-N-CA	6.96	130.75	120.87
26	Z	329	ILE	CA-C-N	6.96	129.33	120.56
26	Z	329	ILE	C-N-CA	6.96	129.33	120.56
30	Q	90	LYS	CA-C-N	6.96	129.90	120.44
30	Q	90	LYS	C-N-CA	6.96	129.90	120.44
9	i	133	ALA	CA-C-N	6.96	129.90	120.44
9	i	133	ALA	C-N-CA	6.96	129.90	120.44
4	D	3	ASP	CA-CB-CG	6.96	119.56	112.60
16	I	107	GLY	O-C-N	-6.96	118.59	123.95
6	f	170	TYR	CA-C-N	6.95	129.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	170	TYR	C-N-CA	6.95	129.60	120.28
7	G	244	ASN	CA-C-O	-6.95	108.98	120.80
14	7	194	ASN	N-CA-CB	6.95	120.33	109.69
17	K	150	LEU	CA-C-N	6.95	127.54	120.38
17	K	150	LEU	C-N-CA	6.95	127.54	120.38
23	T	123	HIS	CE1-NE2-CD2	-6.95	102.05	109.00
28	S	173	LEU	N-CA-C	-6.95	101.16	110.55
4	D	240	GLU	CA-C-O	-6.95	108.98	120.80
7	G	141	GLY	CA-C-O	-6.95	115.40	122.56
12	5	176	ASN	N-CA-C	-6.95	97.88	109.07
26	Z	113	SER	CA-C-N	6.95	129.47	120.44
26	Z	113	SER	C-N-CA	6.95	129.47	120.44
27	N	925	ASP	CA-C-O	-6.95	108.98	120.80
30	Q	402	THR	CA-C-N	6.95	128.53	119.84
30	Q	402	THR	C-N-CA	6.95	128.53	119.84
13	6	4	PRO	N-CA-C	-6.95	104.09	113.40
24	X	133	SER	CA-C-O	-6.95	108.99	120.80
9	2	59	ILE	N-CA-C	-6.95	103.71	110.72
18	L	272	GLU	N-CA-CB	6.95	120.33	110.12
7	g	153	TYR	CA-C-N	6.94	133.47	122.36
7	g	153	TYR	C-N-CA	6.94	133.47	122.36
26	Z	257	PRO	CA-C-N	6.94	127.53	120.38
26	Z	257	PRO	C-N-CA	6.94	127.53	120.38
5	e	22	ALA	N-CA-C	6.94	118.84	111.28
3	C	244	THR	CA-C-O	-6.94	109.00	120.80
18	L	436	LYS	CA-C-O	-6.94	109.00	120.80
9	i	154	LEU	N-CA-C	-6.94	103.72	111.28
16	I	299	GLU	N-CA-C	-6.94	102.93	113.89
20	J	296	ARG	CA-C-N	6.94	133.89	120.99
20	J	296	ARG	C-N-CA	6.94	133.89	120.99
21	W	122	ARG	CA-C-N	6.94	129.57	120.28
21	W	122	ARG	C-N-CA	6.94	129.57	120.28
17	K	121	ARG	CA-C-O	6.93	128.78	120.81
27	N	869	ASP	O-C-N	-6.93	115.13	122.96
11	4	73	TYR	N-CA-C	-6.93	96.04	110.80
26	Z	91	PHE	N-CA-C	-6.93	104.39	112.92
2	B	172	LYS	CA-C-N	6.93	129.57	120.28
2	B	172	LYS	C-N-CA	6.93	129.57	120.28
26	Z	495	ILE	N-CA-C	-6.93	104.10	110.82
12	l	12	ILE	O-C-N	6.93	130.16	123.03
19	M	79	VAL	N-CA-C	-6.93	98.50	108.48
28	S	492	LYS	CA-C-O	-6.92	109.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	183	ASP	N-CA-C	-6.92	97.93	109.07
12	5	40	PHE	CA-CB-CG	-6.92	106.88	113.80
27	N	595	LEU	CA-C-N	6.92	129.55	120.28
27	N	595	LEU	C-N-CA	6.92	129.55	120.28
2	B	159	TRP	CA-C-N	6.92	130.11	120.29
2	B	159	TRP	C-N-CA	6.92	130.11	120.29
11	k	153	THR	N-CA-CB	6.91	120.93	110.42
27	N	15	GLU	CB-CG-CD	-6.91	100.85	112.60
20	J	136	LEU	N-CA-CB	6.91	120.28	110.12
26	Z	493	LEU	N-CA-C	-6.91	103.75	111.28
29	P	440	HIS	CA-C-O	-6.91	109.06	120.80
30	Q	178	HIS	ND1-CE1-NE2	6.91	115.31	108.40
29	P	230	HIS	CE1-NE2-CD2	-6.91	102.09	109.00
3	C	151	ASN	CA-C-O	-6.91	113.55	120.66
11	4	166	GLN	CA-C-N	6.91	129.53	120.28
11	4	166	GLN	C-N-CA	6.91	129.53	120.28
26	Z	133	ASP	N-CA-C	-6.91	103.75	111.28
26	Z	825	ALA	CA-C-N	6.91	130.81	120.31
26	Z	825	ALA	C-N-CA	6.91	130.81	120.31
2	b	141	GLU	CA-C-N	6.90	130.09	120.29
2	b	141	GLU	C-N-CA	6.90	130.09	120.29
9	i	63	ILE	N-CA-C	-6.90	103.75	110.72
10	j	141	ALA	CB-CA-C	-6.90	101.55	111.14
17	K	246	TYR	CA-C-O	6.90	130.38	120.51
17	K	284	ALA	CA-C-N	6.90	129.41	120.44
17	K	284	ALA	C-N-CA	6.90	129.41	120.44
20	J	316	PHE	CB-CA-C	-6.90	101.99	109.85
9	2	226	GLU	CA-C-O	-6.90	109.08	120.80
16	I	153	THR	N-CA-CB	6.90	122.73	110.80
5	e	119	ALA	O-C-N	-6.89	116.04	123.42
16	I	139	GLU	O-C-N	6.89	129.43	122.12
30	Q	77	PHE	CB-CA-C	-6.89	99.34	110.79
10	j	2	ASP	CA-CB-CG	-6.89	105.71	112.60
14	7	68	LYS	CA-C-N	6.89	130.78	120.31
14	7	68	LYS	C-N-CA	6.89	130.78	120.31
26	Z	560	THR	CA-C-N	6.89	129.51	120.28
26	Z	560	THR	C-N-CA	6.89	129.51	120.28
2	b	32	VAL	N-CA-C	-6.89	98.45	108.71
6	f	40	ASN	N-CA-C	-6.89	106.77	114.62
17	K	151	PRO	CA-C-N	6.89	126.86	119.28
17	K	151	PRO	C-N-CA	6.89	126.86	119.28
19	M	129	LEU	CA-C-N	6.89	127.30	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	129	LEU	C-N-CA	6.89	127.30	119.93
31	R	111	LYS	N-CA-C	6.89	118.44	111.07
10	j	118	PRO	CA-C-O	-6.88	113.49	121.34
26	Z	319	THR	CA-C-N	6.88	129.50	120.28
26	Z	319	THR	C-N-CA	6.88	129.50	120.28
27	N	178	SER	N-CA-C	-6.88	97.74	109.24
6	f	174	THR	CA-C-N	6.88	129.83	120.54
6	f	174	THR	C-N-CA	6.88	129.83	120.54
7	G	126	ARG	CA-C-N	6.88	128.44	119.84
7	G	126	ARG	C-N-CA	6.88	128.44	119.84
19	M	130	PRO	CA-C-O	-6.88	113.82	121.32
28	S	163	VAL	N-CA-C	6.88	119.69	111.09
5	e	110	ASP	CA-CB-CG	-6.88	105.72	112.60
10	3	51	GLY	N-CA-C	-6.88	100.84	111.64
3	c	223	GLU	N-CA-CB	6.88	120.09	109.85
16	I	389	GLY	N-CA-C	-6.88	105.84	114.16
17	K	119	VAL	N-CA-C	-6.88	97.95	107.99
19	M	151	ASP	CA-C-N	6.88	130.51	120.82
19	M	151	ASP	C-N-CA	6.88	130.51	120.82
22	V	261	LEU	CA-C-O	-6.88	114.26	121.55
31	R	100	ASN	CA-CB-CG	-6.87	105.73	112.60
3	C	42	GLY	CA-C-O	-6.87	114.88	121.41
17	K	371	LEU	O-C-N	6.87	129.40	122.12
23	T	194	GLU	N-CA-C	-6.87	103.85	111.82
32	U	133	PRO	N-CA-C	-6.87	105.76	114.35
28	S	56	SER	CA-C-N	6.87	129.37	120.44
28	S	56	SER	C-N-CA	6.87	129.37	120.44
29	P	263	HIS	O-C-N	6.87	129.40	122.12
12	l	201	LYS	N-CA-CB	6.86	119.96	110.01
4	D	83	LEU	CA-C-N	6.86	130.17	120.42
4	D	83	LEU	C-N-CA	6.86	130.17	120.42
30	Q	28	LEU	CA-C-N	6.86	129.36	120.44
30	Q	28	LEU	C-N-CA	6.86	129.36	120.44
6	F	42	HIS	CG-CD2-NE2	6.86	114.06	107.20
2	b	94	HIS	CB-CG-CD2	-6.86	122.28	131.20
5	e	235	LEU	CB-CA-C	-6.86	99.19	110.85
11	4	37	GLN	CB-CG-CD	-6.86	100.94	112.60
31	R	338	TYR	CA-C-N	6.86	129.47	120.28
31	R	338	TYR	C-N-CA	6.86	129.47	120.28
16	I	151	HIS	ND1-CE1-NE2	6.86	115.26	108.40
26	Z	216	GLY	N-CA-C	-6.86	105.86	115.32
26	Z	79	THR	CA-C-N	6.86	131.86	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	79	THR	C-N-CA	6.86	131.86	122.19
28	S	461	PHE	CA-CB-CG	6.86	120.66	113.80
4	D	127	PHE	CB-CG-CD1	6.86	132.35	120.70
5	E	162	LYS	N-CA-CB	6.86	122.09	110.71
26	Z	918	ASP	N-CA-C	-6.86	104.39	112.89
28	S	248	ASP	CA-C-N	6.86	129.47	120.28
28	S	248	ASP	C-N-CA	6.86	129.47	120.28
3	c	153	SER	N-CA-C	-6.85	104.39	112.89
11	k	85	ARG	CA-C-O	-6.85	113.29	120.55
13	6	108	HIS	N-CA-C	-6.85	95.83	108.02
20	J	16	GLU	CA-C-N	6.85	130.72	120.31
20	J	16	GLU	C-N-CA	6.85	130.72	120.31
26	Z	565	PHE	N-CA-C	-6.85	103.81	111.28
7	g	107	ALA	O-C-N	6.84	129.12	122.07
9	i	198	GLU	N-CA-CB	6.84	120.16	109.69
13	m	154	VAL	N-CA-C	-6.84	106.36	111.90
19	M	248	ALA	CA-C-O	-6.84	110.79	120.16
30	Q	94	VAL	CA-C-N	6.84	129.33	120.44
30	Q	94	VAL	C-N-CA	6.84	129.33	120.44
5	e	39	VAL	N-CA-C	-6.84	98.60	108.17
20	J	225	GLU	N-CA-C	-6.83	100.40	110.52
27	N	193	ALA	N-CA-C	6.83	119.56	111.71
33	O	96	LEU	N-CA-C	-6.83	103.91	111.36
14	7	203	ASN	CA-CB-CG	-6.83	105.77	112.60
16	I	182	SER	N-CA-CB	6.83	121.38	111.62
26	Z	132	HIS	CE1-NE2-CD2	-6.83	102.17	109.00
30	Q	238	TYR	N-CA-C	6.83	118.80	111.36
3	C	15	GLU	N-CA-C	-6.83	104.57	113.17
26	Z	160	GLU	N-CA-C	-6.83	103.77	111.07
9	i	200	GLN	CB-CA-C	-6.82	99.25	110.85
5	E	88	ALA	CA-C-N	6.82	129.80	120.46
5	E	88	ALA	C-N-CA	6.82	129.80	120.46
17	K	227	ALA	CA-C-O	6.82	127.81	119.97
15	H	394	LYS	CA-C-O	6.82	127.81	120.10
9	i	150	GLU	CA-C-O	-6.82	113.19	120.42
10	3	1	SER	CA-C-N	6.82	129.86	120.39
10	3	1	SER	C-N-CA	6.82	129.86	120.39
20	J	126	LEU	N-CA-CB	6.82	120.51	109.95
23	T	158	GLN	CA-C-N	6.82	129.41	120.28
23	T	158	GLN	C-N-CA	6.82	129.41	120.28
13	m	92	ASN	CB-CA-C	-6.81	99.27	110.85
4	D	54	ASP	CA-C-N	6.81	130.66	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	ASP	C-N-CA	6.81	130.66	120.31
16	I	65	ILE	CA-CB-CG1	6.81	121.98	110.40
16	I	183	ASP	N-CA-C	-6.81	103.78	111.14
20	J	379	GLN	CA-C-N	6.81	129.41	120.28
20	J	379	GLN	C-N-CA	6.81	129.41	120.28
32	U	72	TYR	CA-C-N	6.81	129.28	120.56
32	U	72	TYR	C-N-CA	6.81	129.28	120.56
1	a	157	TYR	O-C-N	6.81	131.17	123.27
4	D	120	GLN	N-CA-C	-6.81	103.09	111.40
18	L	189	GLN	CA-C-N	6.81	129.79	120.46
18	L	189	GLN	C-N-CA	6.81	129.79	120.46
20	J	211	ILE	N-CA-CB	6.81	119.92	111.41
27	N	248	GLU	CA-C-N	6.80	131.78	122.19
27	N	248	GLU	C-N-CA	6.80	131.78	122.19
27	N	436	ASP	N-CA-CB	6.80	120.04	110.04
19	M	187	ASP	O-C-N	6.80	129.33	122.12
17	K	182	GLN	CA-C-N	6.80	129.95	120.29
17	K	182	GLN	C-N-CA	6.80	129.95	120.29
21	W	17	ARG	O-C-N	6.80	131.76	122.37
21	W	146	GLU	N-CA-CB	6.80	120.33	110.20
30	Q	78	ILE	CA-C-N	6.80	127.67	120.12
30	Q	78	ILE	C-N-CA	6.80	127.67	120.12
5	E	80	MET	N-CA-C	-6.80	103.95	111.36
22	V	185	ILE	CA-CB-CG2	6.80	122.06	110.50
14	7	157	LYS	CA-C-N	6.80	129.37	120.60
14	7	157	LYS	C-N-CA	6.80	129.37	120.60
2	B	89	SER	N-CA-CB	6.80	120.11	110.12
27	N	340	HIS	CG-CD2-NE2	6.80	114.00	107.20
21	W	102	GLN	N-CA-C	-6.79	103.33	111.69
5	E	89	VAL	CA-C-O	-6.79	113.89	120.95
23	T	87	PRO	CA-C-N	6.79	129.62	120.65
23	T	87	PRO	C-N-CA	6.79	129.62	120.65
23	T	123	HIS	CA-CB-CG	-6.79	107.01	113.80
7	g	243	ILE	CA-CB-CG2	-6.79	98.95	110.50
7	G	18	PHE	CA-CB-CG	6.79	120.59	113.80
17	K	345	ASP	CA-C-N	6.79	129.26	120.44
17	K	345	ASP	C-N-CA	6.79	129.26	120.44
4	d	202	GLN	OE1-CD-NE2	-6.79	115.81	122.60
6	F	178	PHE	N-CA-C	6.79	118.76	111.36
7	G	160	ALA	CA-C-O	6.79	128.35	120.89
27	N	792	SER	N-CA-C	6.79	118.33	111.07
9	2	4	VAL	CA-C-O	6.78	128.27	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	334	ASP	CA-CB-CG	-6.78	105.82	112.60
2	b	20	GLN	N-CA-CB	6.78	120.79	110.28
31	R	356	ALA	O-C-N	6.78	129.88	122.15
6	f	79	ASP	CA-C-N	6.78	129.36	120.28
6	f	79	ASP	C-N-CA	6.78	129.36	120.28
28	S	409	LEU	CA-C-N	6.77	129.24	120.44
28	S	409	LEU	C-N-CA	6.77	129.24	120.44
11	4	82	SER	CA-C-N	6.77	129.24	120.44
11	4	82	SER	C-N-CA	6.77	129.24	120.44
2	b	94	HIS	ND1-CE1-NE2	6.77	115.17	108.40
2	B	4	ARG	NE-CZ-NH2	6.77	125.29	119.20
27	N	405	LEU	CA-C-N	6.77	129.24	120.44
27	N	405	LEU	C-N-CA	6.77	129.24	120.44
7	G	171	GLU	N-CA-C	6.77	118.66	111.28
13	6	29	ASN	CA-CB-CG	-6.77	105.83	112.60
33	O	392	TRP	N-CA-C	-6.77	103.93	112.93
22	V	117	TRP	CA-C-N	6.77	130.42	120.95
22	V	117	TRP	C-N-CA	6.77	130.42	120.95
9	i	86	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
27	N	795	GLU	CB-CA-C	-6.76	99.57	110.79
10	3	161	ASP	CA-CB-CG	-6.76	105.84	112.60
30	Q	311	LEU	N-CA-C	-6.76	104.51	112.89
19	M	222	GLY	CA-C-N	6.76	127.34	120.38
19	M	222	GLY	C-N-CA	6.76	127.34	120.38
5	E	47	THR	N-CA-C	-6.75	105.60	114.31
21	W	77	HIS	CA-C-O	-6.75	113.74	120.70
30	Q	91	SER	CA-C-O	-6.75	113.74	120.70
29	P	299	LEU	CA-C-O	-6.75	113.73	120.82
4	d	14	HIS	N-CA-CB	6.75	121.10	110.84
26	Z	307	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
27	N	907	ASP	CA-CB-CG	-6.75	105.85	112.60
19	M	180	TYR	CA-C-N	6.75	130.00	120.28
19	M	180	TYR	C-N-CA	6.75	130.00	120.28
2	b	170	ALA	CA-C-N	6.75	129.87	120.29
2	b	170	ALA	C-N-CA	6.75	129.87	120.29
4	D	82	ILE	N-CA-C	-6.75	103.74	110.62
27	N	300	ASN	N-CA-CB	6.75	120.74	110.28
11	k	165	VAL	N-CA-C	-6.75	104.19	110.53
5	E	195	ILE	N-CA-C	-6.75	103.65	111.00
24	X	107	GLY	CA-C-N	6.75	129.32	120.28
24	X	107	GLY	C-N-CA	6.75	129.32	120.28
14	7	34	LEU	CA-C-N	6.74	129.87	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	34	LEU	C-N-CA	6.74	129.87	120.29
15	H	95	HIS	CB-CG-CD2	-6.74	122.44	131.20
11	k	10	GLN	CB-CA-C	-6.74	99.60	110.79
3	C	195	THR	N-CA-CB	6.74	120.14	110.16
28	S	45	THR	N-CA-C	-6.74	96.22	108.02
1	a	31	ILE	N-CA-C	-6.74	98.42	108.12
19	M	73	ARG	NE-CZ-NH2	6.74	125.26	119.20
9	2	215	GLU	CB-CG-CD	-6.74	101.15	112.60
30	Q	426	LEU	N-CA-C	-6.74	104.02	111.36
26	Z	381	LEU	CA-C-N	6.73	129.30	120.28
26	Z	381	LEU	C-N-CA	6.73	129.30	120.28
29	P	417	HIS	ND1-CE1-NE2	6.73	115.13	108.40
33	O	141	ASN	CB-CA-C	6.73	120.88	111.86
5	e	101	VAL	CA-C-N	6.73	129.30	120.28
5	e	101	VAL	C-N-CA	6.73	129.30	120.28
1	A	83	ASN	CA-C-N	6.73	129.85	120.29
1	A	83	ASN	C-N-CA	6.73	129.85	120.29
16	I	316	PHE	CA-CB-CG	-6.73	107.07	113.80
3	c	100	THR	N-CA-CB	6.73	120.01	110.12
26	Z	244	ARG	CA-C-N	6.73	129.68	120.46
26	Z	244	ARG	C-N-CA	6.73	129.68	120.46
18	L	303	ARG	O-C-N	6.73	129.25	122.12
26	Z	562	TRP	N-CA-CB	6.73	119.76	110.01
29	P	80	THR	N-CA-C	6.73	119.18	111.11
1	a	18	GLN	N-CA-C	6.72	118.61	111.28
6	f	188	LEU	CA-C-N	6.72	129.67	120.46
6	f	188	LEU	C-N-CA	6.72	129.67	120.46
20	J	15	HIS	CA-CB-CG	-6.72	107.08	113.80
16	I	344	ILE	O-C-N	-6.72	115.46	122.25
9	i	95	GLY	N-CA-C	-6.72	104.51	115.46
31	R	301	TYR	CA-C-N	6.72	129.17	120.44
31	R	301	TYR	C-N-CA	6.72	129.17	120.44
10	j	26	LEU	N-CA-C	-6.71	104.22	112.88
14	n	36	PHE	CA-CB-CG	-6.71	107.08	113.80
11	4	146	HIS	CA-C-O	-6.71	113.78	120.70
11	4	69	ILE	CA-C-O	-6.71	113.60	121.05
31	R	206	ARG	CA-C-N	6.71	129.95	120.28
31	R	206	ARG	C-N-CA	6.71	129.95	120.28
11	k	159	ASP	CA-C-N	6.71	129.27	120.28
11	k	159	ASP	C-N-CA	6.71	129.27	120.28
2	B	190	HIS	ND1-CE1-NE2	6.71	115.11	108.40
29	P	47	ARG	NE-CZ-NH2	6.71	125.24	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	31	LEU	CA-C-N	6.71	129.60	120.54
30	Q	31	LEU	C-N-CA	6.71	129.60	120.54
26	Z	786	SER	O-C-N	6.71	128.98	122.07
27	N	333	SER	N-CA-CB	6.71	119.80	110.07
28	S	93	LEU	CA-C-N	6.71	129.60	120.54
28	S	93	LEU	C-N-CA	6.71	129.60	120.54
31	R	343	GLU	CB-CA-C	-6.71	99.65	110.79
22	V	121	VAL	O-C-N	6.70	128.73	121.83
12	l	143	ASN	CA-CB-CG	-6.70	105.90	112.60
8	h	163	ILE	CB-CA-C	6.70	121.47	112.22
16	I	234	LYS	CA-C-N	6.70	129.49	120.65
16	I	234	LYS	C-N-CA	6.70	129.49	120.65
26	Z	968	ASP	CA-CB-CG	-6.70	105.90	112.60
27	N	177	ASP	N-CA-C	-6.70	103.90	111.07
31	R	178	GLY	CA-C-N	6.70	129.25	120.28
31	R	178	GLY	C-N-CA	6.70	129.25	120.28
10	3	193	GLU	N-CA-C	-6.70	97.98	108.90
18	L	374	PHE	CA-CB-CG	-6.70	107.11	113.80
19	M	277	ILE	N-CA-C	-6.70	98.48	108.12
26	Z	212	LEU	O-C-N	6.69	128.96	122.07
2	b	104	TYR	O-C-N	-6.69	114.17	121.53
11	k	30	ASP	CA-CB-CG	-6.69	105.91	112.60
12	5	110	PRO	CA-C-O	-6.69	113.71	121.34
18	L	58	ASN	CA-C-N	6.69	129.79	120.29
18	L	58	ASN	C-N-CA	6.69	129.79	120.29
33	O	376	GLN	CG-CD-NE2	-6.69	106.37	116.40
16	I	194	ILE	N-CA-C	-6.69	102.73	111.09
33	O	310	PHE	N-CA-C	-6.68	104.07	111.82
2	b	94	HIS	CB-CG-ND1	6.68	132.72	122.70
4	d	68	HIS	CG-CD2-NE2	6.68	113.88	107.20
33	O	187	SER	CA-C-O	6.68	127.50	120.42
11	4	59	TYR	CA-C-N	6.68	128.98	120.56
11	4	59	TYR	C-N-CA	6.68	128.98	120.56
3	c	108	GLU	N-CA-C	-6.68	103.92	111.07
17	K	428	LYS	N-CA-CB	6.68	121.85	110.50
4	d	146	TYR	CA-C-N	6.68	132.95	122.94
4	d	146	TYR	C-N-CA	6.68	132.95	122.94
26	Z	358	TYR	N-CA-C	-6.68	104.08	111.36
32	U	173	HIS	CE1-NE2-CD2	-6.68	102.32	109.00
12	l	191	HIS	CB-CG-CD2	-6.67	122.52	131.20
6	F	10	VAL	CA-C-N	6.67	130.35	120.87
6	F	10	VAL	C-N-CA	6.67	130.35	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	182	TRP	CE2-CD2-CE3	6.67	125.47	118.80
31	R	104	LYS	CA-C-N	6.67	131.80	121.19
31	R	104	LYS	C-N-CA	6.67	131.80	121.19
1	A	137	VAL	N-CA-C	-6.67	96.67	107.28
16	I	264	CYS	CA-C-N	6.67	129.22	120.28
16	I	264	CYS	C-N-CA	6.67	129.22	120.28
11	k	183	ILE	N-CA-C	-6.67	98.77	108.11
23	T	175	ASP	CA-C-N	6.67	131.85	120.72
23	T	175	ASP	C-N-CA	6.67	131.85	120.72
26	Z	56	LEU	N-CA-C	-6.67	105.68	113.88
20	J	376	HIS	CA-C-N	6.67	132.16	123.10
20	J	376	HIS	C-N-CA	6.67	132.16	123.10
2	B	136	ILE	N-CA-C	-6.66	98.14	107.80
26	Z	826	ARG	N-CA-C	-6.66	104.09	111.82
11	k	146	HIS	ND1-CE1-NE2	6.66	115.06	108.40
16	I	239	GLN	N-CA-CB	6.66	119.91	110.12
23	T	138	ASP	CA-C-N	-6.66	113.60	122.99
23	T	138	ASP	C-N-CA	-6.66	113.60	122.99
27	N	747	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
29	P	76	ASN	CA-C-N	6.66	129.75	120.29
29	P	76	ASN	C-N-CA	6.66	129.75	120.29
6	F	81	ARG	N-CA-C	-6.66	104.10	111.36
13	m	45	ASP	CA-CB-CG	-6.66	105.94	112.60
7	G	244	ASN	CA-CB-CG	-6.66	105.94	112.60
11	4	113	LYS	CA-C-N	6.66	126.62	120.03
11	4	113	LYS	C-N-CA	6.66	126.62	120.03
16	I	75	PHE	CA-C-O	6.66	127.81	120.82
17	K	213	GLY	N-CA-C	-6.66	98.76	112.34
30	Q	272	LEU	CA-C-N	6.66	131.81	122.36
30	Q	272	LEU	C-N-CA	6.66	131.81	122.36
31	R	48	GLU	CA-C-O	6.66	127.61	120.55
29	P	128	ASN	N-CA-C	-6.65	99.83	110.14
9	i	89	LYS	CA-C-O	-6.65	113.45	120.63
16	I	72	GLU	CA-C-O	-6.65	113.85	120.70
12	l	191	HIS	ND1-CE1-NE2	6.65	115.05	108.40
15	H	58	ASP	N-CA-C	-6.65	103.95	111.07
22	V	59	ASP	CB-CA-C	-6.65	107.11	115.89
23	T	124	SER	CA-C-N	6.65	129.19	120.28
23	T	124	SER	C-N-CA	6.65	129.19	120.28
30	Q	340	ASP	N-CA-C	6.65	118.61	111.36
20	J	23	PHE	CA-C-N	6.65	129.73	120.29
20	J	23	PHE	C-N-CA	6.65	129.73	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	22	PRO	CA-C-N	6.65	129.73	120.29
29	P	22	PRO	C-N-CA	6.65	129.73	120.29
12	l	72	GLU	CA-C-N	6.65	130.19	120.82
12	l	72	GLU	C-N-CA	6.65	130.19	120.82
29	P	375	GLN	N-CA-C	-6.64	104.12	111.36
1	a	13	GLU	N-CA-CB	6.64	119.70	110.07
7	g	232	LEU	N-CA-C	-6.64	103.96	111.07
13	m	1	GLN	OE1-CD-NE2	6.64	129.24	122.60
29	P	153	ILE	CA-C-N	6.64	129.07	120.44
29	P	153	ILE	C-N-CA	6.64	129.07	120.44
7	g	137	VAL	CA-C-O	6.64	127.52	120.48
27	N	93	GLU	N-CA-CB	6.64	120.57	110.28
1	A	92	ALA	CA-C-O	-6.64	113.86	120.70
6	F	190	LYS	CA-C-N	6.64	129.17	120.28
6	F	190	LYS	C-N-CA	6.64	129.17	120.28
19	M	315	PHE	N-CA-C	-6.64	103.97	111.14
28	S	255	SER	CA-C-N	6.64	129.17	120.28
28	S	255	SER	C-N-CA	6.64	129.17	120.28
31	R	343	GLU	N-CA-C	-6.63	104.05	111.28
12	l	141	ASP	N-CA-C	-6.63	103.98	111.14
18	L	151	THR	O-C-N	6.63	128.90	122.07
27	N	128	ILE	N-CA-C	-6.63	104.06	110.42
27	N	513	ILE	CA-C-N	6.63	129.71	120.29
27	N	513	ILE	C-N-CA	6.63	129.71	120.29
14	n	159	VAL	N-CA-CB	6.63	120.26	111.64
2	B	15	SER	CA-C-N	6.63	130.07	121.85
2	B	15	SER	C-N-CA	6.63	130.07	121.85
1	A	186	ASN	CA-CB-CG	-6.63	105.97	112.60
31	R	341	LEU	CA-C-N	6.62	130.38	120.31
31	R	341	LEU	C-N-CA	6.62	130.38	120.31
15	H	189	PRO	N-CA-C	-6.62	100.22	110.95
20	J	248	ASP	N-CA-C	-6.62	98.83	109.96
3	c	82	ASP	N-CA-CB	6.62	119.86	110.12
5	E	59	ILE	O-C-N	-6.62	116.23	123.18
29	P	227	ILE	CA-C-O	-6.62	114.15	121.17
2	b	198	GLU	CB-CG-CD	-6.62	101.35	112.60
28	S	360	PHE	CB-CA-C	-6.62	100.49	110.88
18	L	271	LYS	CA-C-N	6.62	129.15	120.28
18	L	271	LYS	C-N-CA	6.62	129.15	120.28
28	S	225	HIS	CE1-NE2-CD2	-6.62	102.39	109.00
30	Q	345	SER	N-CA-C	-6.62	104.15	111.36
1	a	84	ALA	N-CA-C	-6.61	104.15	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	19	SER	N-CA-CB	6.61	120.41	110.22
12	l	18	SER	N-CA-C	-6.61	103.61	112.94
14	7	132	LEU	N-CA-CB	-6.61	100.03	110.22
19	M	138	ASP	CA-CB-CG	-6.61	105.99	112.60
31	R	99	TYR	N-CA-CB	6.61	119.66	110.07
19	M	363	ILE	N-CA-C	-6.61	104.04	110.72
29	P	87	GLY	N-CA-C	-6.61	106.67	115.40
5	e	55	SER	N-CA-CB	6.61	119.65	110.07
3	C	182	ASP	CA-C-O	-6.61	110.65	119.11
26	Z	631	GLY	CA-C-N	6.61	129.67	120.29
26	Z	631	GLY	C-N-CA	6.61	129.67	120.29
12	l	179	HIS	CB-CG-CD2	-6.61	122.61	131.20
14	n	99	VAL	CA-C-N	6.61	129.13	120.28
14	n	99	VAL	C-N-CA	6.61	129.13	120.28
8	h	82	PHE	CA-CB-CG	-6.60	107.20	113.80
2	B	190	HIS	CG-CD2-NE2	6.60	113.80	107.20
15	H	362	ASP	N-CA-C	6.60	117.69	109.57
23	T	41	ILE	CA-C-N	6.60	127.17	120.04
23	T	41	ILE	C-N-CA	6.60	127.17	120.04
31	R	160	LYS	N-CA-C	-6.60	101.19	110.50
17	K	57	GLU	CB-CG-CD	-6.60	101.38	112.60
11	4	96	ARG	CA-C-N	6.60	126.56	119.76
11	4	96	ARG	C-N-CA	6.60	126.56	119.76
27	N	406	TYR	O-C-N	6.60	128.87	122.07
1	a	162	THR	CA-C-O	-6.60	113.72	121.44
7	G	214	TRP	CB-CG-CD1	6.59	136.79	126.90
2	B	175	LEU	CA-C-N	6.59	129.12	120.28
2	B	175	LEU	C-N-CA	6.59	129.12	120.28
23	T	235	PHE	CA-CB-CG	6.59	120.39	113.80
33	O	283	HIS	ND1-CE1-NE2	6.59	114.99	108.40
20	J	163	VAL	N-CA-C	-6.59	103.82	111.00
26	Z	303	ASP	CA-C-N	6.59	128.08	119.84
26	Z	303	ASP	C-N-CA	6.59	128.08	119.84
14	n	93	PHE	CA-CB-CG	-6.59	107.21	113.80
26	Z	451	ALA	CA-C-N	6.59	129.11	120.28
26	Z	451	ALA	C-N-CA	6.59	129.11	120.28
30	Q	6	SER	CA-C-N	6.59	129.00	120.44
30	Q	6	SER	C-N-CA	6.59	129.00	120.44
4	d	224	SER	N-CA-CB	6.58	119.80	110.12
20	J	273	LEU	CA-C-N	6.58	129.10	120.28
20	J	273	LEU	C-N-CA	6.58	129.10	120.28
2	B	139	HIS	ND1-CE1-NE2	6.58	114.98	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	334	LEU	CA-C-N	6.58	129.64	120.29
15	H	334	LEU	C-N-CA	6.58	129.64	120.29
19	M	432	PHE	CA-CB-CG	-6.58	107.22	113.80
5	e	129	PRO	CA-C-N	6.58	130.68	120.75
5	e	129	PRO	C-N-CA	6.58	130.68	120.75
16	I	373	GLU	CA-C-N	6.58	129.09	120.28
16	I	373	GLU	C-N-CA	6.58	129.09	120.28
17	K	415	VAL	CB-CA-C	-6.58	100.50	111.29
11	k	23	ARG	NE-CZ-NH2	6.58	125.12	119.20
6	F	49	LYS	CA-C-O	-6.58	114.39	121.56
17	K	393	ARG	N-CA-C	-6.58	104.19	111.82
9	i	161	ALA	N-CA-CB	6.58	119.79	110.12
5	E	173	ALA	CA-C-N	6.58	129.63	120.29
5	E	173	ALA	C-N-CA	6.58	129.63	120.29
4	D	14	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
26	Z	569	ALA	N-CA-C	-6.57	104.04	111.07
2	B	157	PHE	O-C-N	-6.57	117.25	121.85
9	2	57	GLN	N-CA-C	6.57	118.44	111.28
26	Z	768	GLY	CA-C-N	-6.57	113.01	122.93
26	Z	768	GLY	C-N-CA	-6.57	113.01	122.93
7	G	55	LEU	CA-C-N	6.57	129.85	123.02
7	G	55	LEU	C-N-CA	6.57	129.85	123.02
26	Z	900	LEU	N-CA-C	-6.57	98.98	109.76
26	Z	968	ASP	N-CA-C	-6.57	97.81	108.52
3	c	234	ILE	N-CA-C	-6.57	104.09	110.72
7	g	199	ALA	O-C-N	-6.57	113.63	122.43
6	f	80	ALA	N-CA-CB	6.57	119.77	110.12
3	C	27	SER	CA-C-O	6.57	127.52	119.97
30	Q	333	SER	N-CA-C	6.56	118.44	111.28
26	Z	355	GLU	CA-C-N	6.56	128.97	120.44
26	Z	355	GLU	C-N-CA	6.56	128.97	120.44
4	d	226	GLU	O-C-N	6.56	129.07	122.12
26	Z	19	SER	CA-C-O	-6.56	111.17	120.16
26	Z	476	ASP	CA-CB-CG	-6.56	106.04	112.60
27	N	510	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
13	m	198	VAL	N-CA-C	-6.56	100.29	109.21
2	B	68	THR	CA-C-O	-6.56	111.18	120.16
28	S	450	ASN	CA-CB-CG	-6.56	106.04	112.60
13	m	46	CYS	N-CA-C	-6.55	103.78	113.61
13	6	184	VAL	CA-C-N	6.55	128.96	120.44
13	6	184	VAL	C-N-CA	6.55	128.96	120.44
27	N	70	TYR	N-CA-CB	6.55	119.86	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	183	ASP	N-CA-CB	6.55	119.86	110.16
14	7	139	SER	N-CA-C	-6.55	97.61	108.23
20	J	318	PRO	CA-C-N	6.55	126.53	119.78
20	J	318	PRO	C-N-CA	6.55	126.53	119.78
12	l	133	GLN	CA-C-N	6.55	129.06	120.28
12	l	133	GLN	C-N-CA	6.55	129.06	120.28
16	I	82	LEU	N-CA-CB	6.55	119.57	110.07
2	B	110	LEU	CA-C-N	6.55	129.43	120.46
2	B	110	LEU	C-N-CA	6.55	129.43	120.46
32	U	121	LEU	O-C-N	-6.55	114.88	123.13
7	g	10	VAL	N-CA-CB	6.55	122.19	111.45
27	N	302	PHE	CA-CB-CG	-6.54	107.25	113.80
9	i	38	SER	CA-C-O	-6.54	115.02	120.71
9	2	69	TYR	CA-C-O	-6.54	113.95	120.82
20	J	177	LEU	N-CA-C	-6.54	104.07	111.14
26	Z	622	HIS	ND1-CE1-NE2	6.54	114.94	108.40
2	b	230	ASP	CA-C-N	6.54	129.58	120.29
2	b	230	ASP	C-N-CA	6.54	129.58	120.29
15	H	280	VAL	N-CA-C	-6.54	105.95	112.17
13	m	161	GLU	O-C-N	-6.54	114.74	121.28
4	d	164	ARG	NE-CZ-NH1	-6.54	114.96	121.50
8	l	98	ILE	O-C-N	-6.54	116.32	123.18
27	N	568	VAL	CA-C-N	6.54	129.04	120.28
27	N	568	VAL	C-N-CA	6.54	129.04	120.28
2	B	81	ASP	N-CA-C	-6.53	104.24	111.36
26	Z	632	GLU	N-CA-C	-6.53	104.24	111.36
5	e	208	ASN	OD1-CG-ND2	-6.53	116.07	122.60
8	l	120	HIS	CE1-NE2-CD2	-6.53	102.47	109.00
16	I	242	ALA	N-CA-C	-6.53	100.81	110.48
28	S	20	HIS	O-C-N	6.53	128.80	122.07
28	S	74	LEU	CA-C-N	6.53	129.33	120.38
28	S	74	LEU	C-N-CA	6.53	129.33	120.38
32	U	214	VAL	N-CA-C	-6.53	104.12	110.72
3	C	228	ILE	N-CA-CB	6.53	118.26	110.95
16	I	119	ILE	N-CA-C	-6.53	98.22	107.75
27	N	373	VAL	N-CA-C	-6.53	103.89	111.00
11	k	4	ILE	N-CA-C	-6.53	99.33	108.27
28	S	121	VAL	CB-CA-C	-6.53	103.47	112.02
3	c	136	TYR	N-CA-CB	6.52	121.06	110.43
26	Z	961	GLU	CA-C-N	6.52	130.22	120.31
26	Z	961	GLU	C-N-CA	6.52	130.22	120.31
29	P	325	ASP	CA-C-N	6.52	130.13	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	325	ASP	C-N-CA	6.52	130.13	120.87
9	i	66	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
7	G	128	PHE	CA-C-O	-6.52	113.54	121.36
15	H	445	LYS	N-CA-CB	6.52	119.81	110.16
4	D	68	HIS	CA-CB-CG	6.52	120.32	113.80
26	Z	633	GLU	O-C-N	6.52	130.70	122.23
17	K	205	PRO	CA-C-N	6.52	127.98	119.84
17	K	205	PRO	C-N-CA	6.52	127.98	119.84
20	J	144	ASP	N-CA-C	-6.51	105.06	114.12
26	Z	539	ASN	CA-CB-CG	-6.51	106.09	112.60
29	P	349	ASN	CA-C-O	-6.51	113.65	120.55
31	R	270	VAL	N-CA-C	-6.51	105.36	111.48
1	a	116	SER	CA-C-N	6.51	128.91	120.44
1	a	116	SER	C-N-CA	6.51	128.91	120.44
2	b	158	PRO	N-CA-CB	6.51	109.77	102.67
5	e	76	ASP	CA-CB-CG	-6.51	106.09	112.60
8	h	37	VAL	CA-C-O	6.51	128.92	120.78
9	i	35	HIS	CA-CB-CG	6.51	120.31	113.80
10	j	188	ILE	CB-CA-C	-6.51	101.46	110.96
2	B	244	ASN	CA-C-N	6.51	129.00	120.28
2	B	244	ASN	C-N-CA	6.51	129.00	120.28
31	R	396	LYS	CA-C-N	6.51	129.00	120.28
31	R	396	LYS	C-N-CA	6.51	129.00	120.28
29	P	170	SER	CA-C-O	-6.50	113.53	120.42
4	d	114	VAL	O-C-N	6.50	128.66	121.90
4	D	136	PHE	CA-CB-CG	-6.50	107.30	113.80
6	f	5	TYR	N-CA-C	-6.50	104.50	112.88
33	O	266	PHE	CA-CB-CG	-6.50	107.30	113.80
5	e	192	VAL	CA-C-N	6.50	129.31	120.54
5	e	192	VAL	C-N-CA	6.50	129.31	120.54
26	Z	605	SER	N-CA-C	-6.50	104.20	111.28
26	Z	899	GLN	N-CA-C	-6.50	102.42	111.52
27	N	250	ASP	CA-CB-CG	-6.50	106.10	112.60
12	l	27	ALA	O-C-N	6.50	128.76	122.07
7	G	101	THR	CA-C-O	-6.50	114.09	120.26
17	K	194	GLN	CB-CG-CD	-6.50	101.55	112.60
19	M	227	GLY	CA-C-N	6.50	128.89	120.44
19	M	227	GLY	C-N-CA	6.50	128.89	120.44
30	Q	9	GLU	O-C-N	6.50	128.76	122.07
22	V	180	LEU	CA-C-O	-6.50	113.83	120.71
10	3	140	THR	N-CA-C	-6.49	105.18	113.23
13	m	188	PHE	CA-CB-CG	-6.49	107.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	17	SER	N-CA-C	-6.49	104.29	111.82
4	D	138	PRO	CA-C-O	-6.49	114.03	121.36
1	A	110	LYS	CA-C-N	6.49	129.50	120.29
1	A	110	LYS	C-N-CA	6.49	129.50	120.29
19	M	384	ASP	CA-CB-CG	-6.49	106.11	112.60
30	Q	352	GLU	CA-C-O	-6.49	112.92	119.08
26	Z	198	GLU	CA-C-N	6.49	128.97	120.28
26	Z	198	GLU	C-N-CA	6.49	128.97	120.28
4	D	186	VAL	N-CA-C	-6.48	104.01	110.62
1	a	239	ILE	O-C-N	-6.48	115.58	121.87
3	C	230	LYS	CA-C-N	6.48	126.71	119.32
3	C	230	LYS	C-N-CA	6.48	126.71	119.32
5	E	112	ALA	CA-C-N	6.48	131.77	121.66
5	E	112	ALA	C-N-CA	6.48	131.77	121.66
11	4	39	SER	O-C-N	-6.48	116.03	121.54
13	6	3	ASN	CA-C-O	-6.48	113.37	120.69
20	J	156	GLN	OE1-CD-NE2	6.48	129.08	122.60
28	S	347	HIS	CB-CG-CD2	-6.48	122.78	131.20
11	4	146	HIS	N-CA-C	-6.48	104.14	111.14
30	Q	250	THR	CA-CB-OG1	6.48	119.32	109.60
16	I	207	LEU	N-CA-CB	6.48	119.46	110.07
13	6	8	ASN	N-CA-C	-6.48	103.55	112.03
2	b	201	GLU	N-CA-C	-6.47	105.20	113.23
10	j	124	ASP	CA-CB-CG	-6.47	106.12	112.60
33	O	185	PHE	O-C-N	6.47	129.08	122.09
6	F	13	SER	CA-C-N	6.47	127.93	119.84
6	F	13	SER	C-N-CA	6.47	127.93	119.84
7	G	178	HIS	CA-CB-CG	6.47	120.27	113.80
26	Z	87	LYS	CA-C-O	-6.47	112.93	119.08
27	N	730	VAL	CA-C-O	-6.47	114.31	121.17
29	P	15	GLN	OE1-CD-NE2	6.47	129.07	122.60
30	Q	3	LEU	CA-C-O	-6.47	112.67	118.63
26	Z	618	GLN	N-CA-CB	6.47	119.39	110.01
17	K	190	LEU	CA-C-O	-6.47	112.58	118.79
21	W	125	LEU	CA-C-O	-6.47	112.53	119.97
4	D	68	HIS	CE1-NE2-CD2	-6.46	102.54	109.00
5	E	127	SER	N-CA-C	-6.46	97.03	110.80
10	3	131	GLU	CB-CG-CD	-6.46	101.61	112.60
26	Z	617	ILE	O-C-N	6.46	128.40	121.87
5	e	65	HIS	CB-CG-CD2	-6.46	122.80	131.20
8	h	185	ARG	N-CA-CB	6.46	120.70	110.23
14	n	103	ARG	N-CA-C	6.46	118.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	165	ILE	CA-C-O	-6.46	111.29	119.95
16	I	119	ILE	O-C-N	6.46	130.05	123.20
27	N	543	ASP	CA-CB-CG	-6.46	106.14	112.60
9	2	99	ILE	N-CA-CB	6.46	119.48	111.41
1	a	155	VAL	CA-CB-CG2	6.46	121.38	110.40
1	a	174	GLU	N-CA-CB	6.46	119.61	110.12
11	k	80	VAL	N-CA-C	-6.46	104.22	110.42
14	n	25	ASP	N-CA-C	-6.46	101.39	110.50
4	D	17	GLN	O-C-N	6.46	128.97	122.12
12	5	36	GLU	N-CA-C	-6.46	98.01	108.41
23	T	16	GLU	N-CA-CB	6.46	120.02	110.33
27	N	883	SER	CA-C-N	6.46	129.93	120.82
27	N	883	SER	C-N-CA	6.46	129.93	120.82
3	c	134	PHE	N-CA-CB	6.46	121.18	110.85
17	K	154	SER	CA-C-O	-6.46	114.47	121.44
26	Z	156	HIS	CA-CB-CG	-6.46	107.34	113.80
26	Z	334	LYS	CA-C-N	6.46	128.83	120.44
26	Z	334	LYS	C-N-CA	6.46	128.83	120.44
27	N	340	HIS	CE1-NE2-CD2	-6.46	102.54	109.00
3	C	217	LYS	CA-C-O	6.46	126.86	119.18
5	e	25	LEU	O-C-N	6.45	129.50	122.15
5	e	224	ASP	N-CA-C	-6.45	100.88	110.23
1	a	212	ASN	CA-C-O	6.45	127.39	119.97
24	X	56	PRO	N-CA-C	-6.45	106.10	114.03
27	N	57	ASP	CA-CB-CG	-6.45	106.15	112.60
29	P	47	ARG	CA-C-N	6.45	128.82	120.44
29	P	47	ARG	C-N-CA	6.45	128.82	120.44
1	A	4	ASP	CA-C-N	6.44	129.44	120.29
1	A	4	ASP	C-N-CA	6.44	129.44	120.29
4	D	38	ASN	N-CA-C	-6.44	102.87	113.50
17	K	68	ILE	N-CA-C	-6.44	105.39	112.80
17	K	118	TYR	CA-C-O	6.44	127.66	120.70
27	N	396	SER	N-CA-CB	6.44	119.69	110.16
32	U	192	ASN	N-CA-C	-6.44	104.26	111.28
9	i	143	LYS	CA-C-N	6.44	129.85	120.71
9	i	143	LYS	C-N-CA	6.44	129.85	120.71
16	I	380	LEU	CA-C-N	6.44	128.67	120.56
16	I	380	LEU	C-N-CA	6.44	128.67	120.56
24	X	131	ASN	CA-CB-CG	-6.44	106.16	112.60
4	d	79	ASP	CA-CB-CG	-6.43	106.17	112.60
6	f	121	SER	N-CA-CB	6.43	119.92	109.95
13	6	7	ASP	CA-CB-CG	-6.43	106.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	317	ASP	CA-CB-CG	-6.43	106.17	112.60
26	Z	422	ILE	CA-C-N	6.43	128.18	120.14
26	Z	422	ILE	C-N-CA	6.43	128.18	120.14
4	D	207	ASN	CA-CB-CG	-6.43	106.17	112.60
32	U	70	HIS	CG-CD2-NE2	6.43	113.63	107.20
22	V	89	ALA	O-C-N	6.43	128.69	122.07
26	Z	336	SER	N-CA-C	-6.43	104.19	111.07
26	Z	634	ASP	CA-CB-CG	-6.43	106.17	112.60
26	Z	258	PRO	CB-CA-C	6.43	118.76	110.92
30	Q	297	ASP	CA-C-N	6.43	128.80	120.44
30	Q	297	ASP	C-N-CA	6.43	128.80	120.44
3	C	175	LEU	N-CA-C	-6.43	104.36	111.82
20	J	215	GLY	N-CA-C	-6.43	102.49	112.45
27	N	56	SER	N-CA-C	-6.43	105.19	114.12
5	e	149	HIS	ND1-CE1-NE2	6.42	114.82	108.40
27	N	59	GLU	CB-CA-C	-6.42	100.12	110.79
27	N	441	VAL	CA-C-N	6.42	128.79	120.44
27	N	441	VAL	C-N-CA	6.42	128.79	120.44
23	T	55	LEU	O-C-N	6.42	128.93	122.12
21	W	174	VAL	N-CA-C	-6.42	98.38	107.75
27	N	699	ALA	CA-C-O	-6.42	113.62	120.42
26	Z	768	GLY	O-C-N	6.42	129.28	122.28
17	K	164	ASN	N-CA-C	-6.42	103.80	111.69
20	J	181	GLN	CA-C-N	6.42	127.30	120.11
20	J	181	GLN	C-N-CA	6.42	127.30	120.11
26	Z	443	ASP	CA-C-N	6.42	130.41	120.60
26	Z	443	ASP	C-N-CA	6.42	130.41	120.60
3	c	182	ASP	CA-C-N	6.41	129.94	120.90
3	c	182	ASP	C-N-CA	6.41	129.94	120.90
5	E	62	ILE	O-C-N	-6.41	115.18	122.04
16	I	96	LEU	O-C-N	6.41	128.91	122.12
31	R	220	ALA	CA-C-O	6.41	127.21	120.42
10	j	117	LYS	CA-C-N	6.41	126.36	119.76
10	j	117	LYS	C-N-CA	6.41	126.36	119.76
26	Z	305	VAL	N-CA-C	-6.41	98.82	108.17
13	m	167	LYS	CB-CA-C	-6.40	99.87	110.37
22	V	43	ALA	O-C-N	6.40	129.45	122.15
2	b	120	GLU	N-CA-CB	6.40	119.63	110.16
27	N	587	ALA	CA-C-O	-6.40	113.77	120.55
10	j	44	HIS	CG-CD2-NE2	6.40	113.60	107.20
18	L	302	GLN	CA-C-O	-6.40	113.64	120.42
27	N	241	LEU	O-C-N	6.40	128.90	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	104	VAL	CA-C-N	6.39	129.17	120.54
4	D	104	VAL	C-N-CA	6.39	129.17	120.54
33	O	41	LEU	N-CA-C	-6.39	104.40	111.82
21	W	168	THR	CA-C-N	6.39	129.79	120.71
21	W	168	THR	C-N-CA	6.39	129.79	120.71
27	N	338	PHE	CA-C-N	6.39	129.13	120.38
27	N	338	PHE	C-N-CA	6.39	129.13	120.38
27	N	917	ILE	N-CA-C	-6.39	97.91	107.37
4	d	230	TYR	N-CA-C	-6.39	104.32	111.28
19	M	244	LEU	CA-C-O	6.39	127.76	120.54
27	N	98	VAL	CA-CB-CG1	-6.39	99.54	110.40
28	S	46	LEU	CA-C-N	6.39	133.74	121.54
28	S	46	LEU	C-N-CA	6.39	133.74	121.54
2	B	142	PHE	N-CA-CB	-6.39	100.67	110.44
9	i	36	ARG	CB-CA-C	-6.39	99.56	110.16
27	N	396	SER	CB-CA-C	-6.38	100.00	110.85
28	S	404	LEU	N-CA-CB	-6.38	100.38	110.28
30	Q	77	PHE	CA-CB-CG	6.38	120.18	113.80
31	R	99	TYR	CA-CB-CG	-6.38	102.41	113.90
5	e	117	GLU	N-CA-C	-6.38	101.81	110.68
10	j	148	MET	CB-CA-C	-6.38	100.86	110.88
17	K	160	VAL	CA-C-O	6.38	128.06	121.23
11	k	41	HIS	CG-CD2-NE2	6.38	113.58	107.20
1	A	76	GLY	CA-C-N	6.38	127.82	119.84
1	A	76	GLY	C-N-CA	6.38	127.82	119.84
10	3	177	ASP	CA-C-N	6.38	129.12	120.44
10	3	177	ASP	C-N-CA	6.38	129.12	120.44
15	H	198	MET	CA-C-N	6.38	128.83	120.28
15	H	198	MET	C-N-CA	6.38	128.83	120.28
14	n	112	ASN	CA-CB-CG	-6.38	106.22	112.60
3	c	195	THR	N-CA-C	-6.38	104.25	111.14
32	U	137	TYR	O-C-N	-6.38	115.95	123.41
13	m	108	HIS	CE1-NE2-CD2	-6.37	102.63	109.00
10	3	91	SER	CB-CA-C	-6.37	100.87	110.88
20	J	229	MET	N-CA-CB	6.37	120.16	110.28
23	T	21	ALA	CA-C-N	6.37	130.00	120.31
23	T	21	ALA	C-N-CA	6.37	130.00	120.31
27	N	195	THR	CA-C-O	6.37	127.78	120.00
7	g	163	LYS	N-CA-C	-6.37	103.85	111.69
10	j	100	GLY	O-C-N	-6.37	115.40	121.77
8	l	185	ARG	CD-NE-CZ	-6.37	115.48	124.40
20	J	376	HIS	CE1-NE2-CD2	-6.37	102.63	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	200	GLU	CA-C-O	6.37	127.90	120.89
14	n	125	GLN	CA-C-O	6.37	128.14	120.81
1	a	196	PHE	CA-CB-CG	6.37	120.17	113.80
1	a	217	GLY	O-C-N	-6.37	116.48	123.49
10	3	154	GLU	CA-C-N	6.37	126.73	119.92
10	3	154	GLU	C-N-CA	6.37	126.73	119.92
13	6	164	THR	CA-C-N	6.37	130.16	121.05
13	6	164	THR	C-N-CA	6.37	130.16	121.05
26	Z	560	THR	N-CA-C	-6.37	104.42	111.36
27	N	89	PHE	CA-CB-CG	-6.37	107.43	113.80
27	N	281	GLY	N-CA-C	-6.37	106.14	115.63
4	d	55	THR	CA-C-O	6.37	127.29	120.10
23	T	67	LEU	CA-C-O	-6.36	113.67	120.42
6	F	62	ILE	N-CA-C	-6.36	99.42	108.58
12	5	160	SER	N-CA-C	-6.36	104.27	111.14
16	I	180	SER	N-CA-CB	6.36	120.08	110.42
3	c	56	LEU	N-CA-C	-6.36	100.63	110.10
10	j	172	ASN	CA-CB-CG	-6.36	106.25	112.60
11	4	15	LEU	CA-C-O	6.36	127.22	120.36
19	M	362	GLN	CG-CD-NE2	6.36	125.93	116.40
31	R	211	LYS	O-C-N	6.36	128.86	122.12
27	N	340	HIS	ND1-CE1-NE2	6.35	114.75	108.40
28	S	175	SER	N-CA-C	6.35	117.87	111.07
1	a	56	ASP	CA-C-N	6.35	125.85	119.24
1	a	56	ASP	C-N-CA	6.35	125.85	119.24
17	K	133	PRO	O-C-N	6.35	130.60	122.85
24	X	48	PHE	CA-C-O	6.35	127.53	120.92
27	N	9	LEU	CA-C-N	6.35	128.79	120.28
27	N	9	LEU	C-N-CA	6.35	128.79	120.28
27	N	141	ILE	N-CA-C	-6.35	104.31	110.72
31	R	99	TYR	CB-CA-C	-6.35	100.87	110.90
2	B	58	SER	N-CA-C	-6.35	104.69	112.88
9	2	190	TYR	N-CA-C	-6.35	104.28	111.07
11	4	134	GLY	CA-C-N	6.35	128.78	120.28
11	4	134	GLY	C-N-CA	6.35	128.78	120.28
10	j	157	LEU	N-CA-C	-6.35	98.56	108.90
7	g	61	VAL	CA-CB-CG2	6.34	121.19	110.40
7	g	154	TRP	CA-C-O	6.34	128.62	121.51
7	G	69	HIS	CE1-NE2-CD2	-6.34	102.66	109.00
26	Z	833	GLN	OE1-CD-NE2	-6.34	116.26	122.60
33	O	87	LYS	N-CA-CB	6.34	119.65	110.20
27	N	758	VAL	N-CA-CB	6.34	118.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	80	HIS	CB-CG-ND1	6.34	132.21	122.70
33	O	235	HIS	CA-CB-CG	-6.34	107.46	113.80
10	j	7	ASN	N-CA-C	-6.34	105.86	113.97
12	l	186	ILE	N-CA-C	-6.34	99.24	108.11
17	K	57	GLU	N-CA-C	6.34	118.19	111.28
19	M	212	ILE	N-CA-C	-6.33	101.38	109.80
20	J	20	LYS	CA-C-N	6.33	125.96	119.56
20	J	20	LYS	C-N-CA	6.33	125.96	119.56
26	Z	887	GLY	CA-C-N	6.33	129.70	120.71
26	Z	887	GLY	C-N-CA	6.33	129.70	120.71
2	b	157	PHE	CA-CB-CG	-6.33	107.47	113.80
15	H	450	VAL	CA-C-O	6.33	127.56	120.85
10	3	192	ASP	N-CA-C	-6.33	104.02	112.94
26	Z	23	GLN	CA-C-N	6.33	128.67	120.44
26	Z	23	GLN	C-N-CA	6.33	128.67	120.44
1	A	242	GLN	N-CA-C	-6.33	93.28	111.00
6	F	86	TYR	CA-C-N	6.33	129.93	120.31
6	F	86	TYR	C-N-CA	6.33	129.93	120.31
16	I	165	ASP	N-CA-CB	6.33	121.64	110.37
19	M	375	ASN	CA-C-N	6.33	128.76	120.28
19	M	375	ASN	C-N-CA	6.33	128.76	120.28
26	Z	811	SER	N-CA-CB	6.33	119.53	110.16
9	i	189	ASN	CA-C-N	6.33	129.04	120.44
9	i	189	ASN	C-N-CA	6.33	129.04	120.44
20	J	14	THR	CA-C-O	6.33	127.12	120.42
10	j	189	ILE	N-CA-C	-6.32	98.52	107.75
12	l	146	TRP	CB-CG-CD2	-6.32	117.95	126.80
19	M	414	ASP	CA-C-N	6.32	128.75	120.28
19	M	414	ASP	C-N-CA	6.32	128.75	120.28
24	X	17	TYR	N-CA-C	-6.32	101.16	110.52
30	Q	203	THR	CA-C-O	6.32	127.12	120.42
26	Z	387	ASN	CA-CB-CG	6.32	118.92	112.60
30	Q	177	VAL	CA-C-N	6.32	129.38	120.28
30	Q	177	VAL	C-N-CA	6.32	129.38	120.28
30	Q	277	ASP	N-CA-C	-6.32	105.57	113.28
17	K	140	HIS	CG-CD2-NE2	6.32	113.52	107.20
9	2	205	PHE	CA-CB-CG	-6.32	107.48	113.80
28	S	446	THR	N-CA-C	-6.32	105.73	113.50
27	N	355	TRP	CA-C-N	6.31	128.74	120.28
27	N	355	TRP	C-N-CA	6.31	128.74	120.28
22	V	61	TYR	CB-CG-CD1	-6.31	111.33	120.80
28	S	39	ASN	OD1-CG-ND2	-6.31	116.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	91	ARG	NE-CZ-NH2	-6.31	113.52	119.20
30	Q	328	ASP	CA-C-N	6.31	129.02	120.44
30	Q	328	ASP	C-N-CA	6.31	129.02	120.44
8	h	115	LEU	CB-CA-C	-6.31	100.97	110.88
8	l	64	GLU	CA-C-N	6.31	128.74	120.28
8	l	64	GLU	C-N-CA	6.31	128.74	120.28
18	L	135	VAL	CA-C-N	6.31	131.86	121.39
18	L	135	VAL	C-N-CA	6.31	131.86	121.39
26	Z	308	LYS	CA-C-O	-6.31	114.19	120.82
26	Z	829	GLN	N-CA-C	-6.31	104.40	111.28
1	a	13	GLU	CA-C-O	-6.31	114.20	120.70
3	C	69	ASN	CA-C-N	6.31	129.02	120.38
3	C	69	ASN	C-N-CA	6.31	129.02	120.38
26	Z	754	LYS	CA-CB-CG	6.31	126.72	114.10
27	N	489	MET	CA-C-O	6.31	126.94	119.56
29	P	358	SER	N-CA-C	-6.31	104.48	111.36
31	R	147	LYS	CA-C-N	6.31	128.64	120.44
31	R	147	LYS	C-N-CA	6.31	128.64	120.44
5	e	43	GLU	O-C-N	-6.31	115.55	123.05
9	2	163	ILE	CA-C-O	6.31	127.53	120.85
24	X	131	ASN	N-CA-CB	6.31	119.24	109.97
4	d	52	LEU	N-CA-C	-6.30	104.13	113.40
9	2	161	ALA	CA-C-O	6.30	127.22	120.10
16	I	204	HIS	CG-CD2-NE2	6.30	113.50	107.20
19	M	216	LYS	N-CA-C	6.30	117.82	111.07
12	l	210	VAL	CA-C-N	6.30	129.11	120.35
12	l	210	VAL	C-N-CA	6.30	129.11	120.35
22	V	281	SER	CA-C-N	6.30	128.63	120.44
22	V	281	SER	C-N-CA	6.30	128.63	120.44
32	U	238	ASN	CA-CB-CG	-6.30	106.30	112.60
12	l	173	GLY	O-C-N	6.30	130.27	122.90
18	L	358	LEU	N-CA-C	-6.30	104.50	111.36
19	M	251	LEU	N-CA-C	-6.30	105.08	112.89
28	S	478	SER	CA-C-N	6.30	128.63	120.44
28	S	478	SER	C-N-CA	6.30	128.63	120.44
33	O	326	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
3	c	196	LEU	CA-C-N	6.30	129.35	120.28
3	c	196	LEU	C-N-CA	6.30	129.35	120.28
31	R	187	VAL	CB-CA-C	-6.29	103.64	112.14
13	m	57	PHE	CA-C-N	6.29	128.71	120.28
13	m	57	PHE	C-N-CA	6.29	128.71	120.28
15	H	95	HIS	ND1-CE1-NE2	6.29	114.69	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	161	TRP	CB-CG-CD2	-6.29	117.99	126.80
32	U	195	LYS	CA-C-N	6.29	129.23	120.29
32	U	195	LYS	C-N-CA	6.29	129.23	120.29
3	C	107	VAL	CA-C-N	6.29	128.62	120.44
3	C	107	VAL	C-N-CA	6.29	128.62	120.44
5	E	113	LEU	CA-C-N	6.29	133.56	121.54
5	E	113	LEU	C-N-CA	6.29	133.56	121.54
26	Z	358	TYR	N-CA-CB	6.29	119.47	110.16
27	N	124	TYR	N-CA-C	-6.29	104.34	111.14
30	Q	14	LEU	CA-C-N	6.29	128.49	120.56
30	Q	14	LEU	C-N-CA	6.29	128.49	120.56
7	g	149	PRO	CA-C-N	6.29	129.22	120.29
7	g	149	PRO	C-N-CA	6.29	129.22	120.29
16	I	173	MET	N-CA-C	-6.29	97.40	110.80
29	P	19	GLU	N-CA-C	-6.29	105.09	112.89
33	O	23	HIS	ND1-CE1-NE2	6.29	114.69	108.40
3	c	55	LEU	N-CA-C	-6.29	104.35	111.14
24	X	117	LYS	CA-C-N	6.29	128.62	120.44
24	X	117	LYS	C-N-CA	6.29	128.62	120.44
32	U	69	ASP	CA-C-N	6.29	128.62	120.44
32	U	69	ASP	C-N-CA	6.29	128.62	120.44
3	c	203	SER	O-C-N	6.29	128.63	122.09
13	m	95	HIS	CB-CG-CD2	6.29	139.37	131.20
9	2	79	ALA	CA-C-O	-6.28	113.76	120.42
17	K	364	PRO	CA-C-N	6.28	128.70	120.28
17	K	364	PRO	C-N-CA	6.28	128.70	120.28
33	O	317	THR	N-CA-C	-6.28	105.61	113.28
29	P	177	ILE	CA-C-N	6.28	128.70	120.28
29	P	177	ILE	C-N-CA	6.28	128.70	120.28
11	4	70	ARG	N-CA-C	6.28	118.13	111.28
20	J	167	PRO	CA-C-N	6.28	129.72	120.74
20	J	167	PRO	C-N-CA	6.28	129.72	120.74
27	N	715	ILE	CA-C-N	6.28	131.05	122.19
27	N	715	ILE	C-N-CA	6.28	131.05	122.19
30	Q	212	THR	CA-C-N	6.28	129.21	120.29
30	Q	212	THR	C-N-CA	6.28	129.21	120.29
1	A	165	LYS	N-CA-C	-6.28	103.02	111.87
3	C	9	THR	N-CA-C	-6.28	104.78	112.88
5	e	48	SER	N-CA-CB	6.28	117.69	111.10
3	C	106	PRO	CA-C-N	6.28	129.06	120.46
3	C	106	PRO	C-N-CA	6.28	129.06	120.46
23	T	65	GLY	CA-C-N	6.28	128.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	65	GLY	C-N-CA	6.28	128.60	120.44
30	Q	192	ALA	N-CA-C	-6.28	104.36	111.07
26	Z	368	VAL	CA-C-N	6.27	131.00	122.84
26	Z	368	VAL	C-N-CA	6.27	131.00	122.84
27	N	654	GLN	N-CA-C	-6.27	104.44	111.28
28	S	73	THR	O-C-N	-6.27	115.47	122.12
26	Z	237	VAL	CA-C-N	6.27	129.01	120.54
26	Z	237	VAL	C-N-CA	6.27	129.01	120.54
6	f	62	ILE	N-CA-C	-6.27	99.39	108.17
27	N	904	VAL	N-CA-C	-6.27	99.34	108.87
4	d	55	THR	N-CA-C	6.27	118.92	111.71
14	n	219	TRP	CE2-CD2-CE3	6.27	125.07	118.80
5	E	105	THR	CA-C-O	-6.27	113.91	120.55
4	D	25	VAL	CA-C-N	6.26	128.96	120.38
4	D	25	VAL	C-N-CA	6.26	128.96	120.38
28	S	41	ILE	CA-C-O	-6.26	113.70	120.47
26	Z	254	PRO	N-CA-CB	6.26	108.56	103.36
6	f	31	GLY	N-CA-C	6.26	120.64	112.25
21	W	155	ASP	N-CA-C	6.26	118.91	111.33
5	e	57	GLU	O-C-N	-6.26	114.68	122.82
9	i	165	ASN	CA-CB-CG	-6.26	106.34	112.60
15	H	85	MET	CA-C-N	6.26	127.97	120.14
15	H	85	MET	C-N-CA	6.26	127.97	120.14
17	K	120	VAL	O-C-N	6.26	130.13	123.00
18	L	190	ILE	CA-C-O	-6.26	114.44	120.95
26	Z	48	ASP	CA-C-O	-6.26	113.92	120.55
33	O	149	LEU	CA-C-N	6.26	129.18	120.29
33	O	149	LEU	C-N-CA	6.26	129.18	120.29
11	k	185	ASP	CA-C-N	6.26	130.61	120.60
11	k	185	ASP	C-N-CA	6.26	130.61	120.60
5	E	83	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
21	W	99	LYS	CA-C-O	-6.26	113.92	120.55
26	Z	272	TYR	CB-CG-CD1	6.26	130.19	120.80
27	N	674	GLN	CB-CA-C	-6.26	99.05	110.63
14	n	116	VAL	N-CA-CB	6.26	119.23	111.41
22	V	170	PRO	N-CD-CG	6.26	112.58	103.20
26	Z	617	ILE	CA-C-O	-6.26	113.88	120.57
4	d	98	LEU	N-CA-C	-6.25	105.65	113.28
23	T	51	TYR	CA-CB-CG	-6.25	102.64	113.90
5	e	143	ASP	CA-C-O	6.25	126.97	119.59
5	E	41	GLY	N-CA-C	-6.25	100.52	111.46
16	I	425	LYS	O-C-N	-6.25	115.49	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	311	ASN	CB-CA-C	-6.25	100.47	109.84
5	E	215	THR	N-CA-C	-6.25	99.98	109.85
11	4	59	TYR	CA-C-O	6.25	127.04	120.42
24	X	94	ASN	CA-CB-CG	-6.25	106.35	112.60
11	k	72	ASP	CA-CB-CG	-6.25	106.36	112.60
22	V	208	LYS	N-CA-C	-6.25	104.01	111.69
26	Z	492	GLY	N-CA-C	-6.25	105.00	113.37
20	J	370	LEU	N-CA-C	6.24	118.60	111.11
27	N	160	GLY	N-CA-C	6.24	125.77	115.34
7	g	102	PRO	CA-C-O	-6.24	114.52	121.32
17	K	89	ILE	CA-C-N	6.24	129.80	120.31
17	K	89	ILE	C-N-CA	6.24	129.80	120.31
1	a	54	LEU	CB-CA-C	-6.24	101.35	110.96
18	L	297	ALA	CA-C-N	6.24	129.80	120.31
18	L	297	ALA	C-N-CA	6.24	129.80	120.31
8	1	120	HIS	ND1-CE1-NE2	6.24	114.64	108.40
6	F	152	VAL	O-C-N	-6.24	116.49	122.98
6	f	9	THR	N-CA-C	-6.24	105.99	113.97
4	D	225	GLU	CA-C-O	-6.24	113.81	120.42
26	Z	506	LEU	N-CA-C	-6.23	104.56	111.36
4	D	5	ALA	CA-C-N	6.23	130.64	120.23
4	D	5	ALA	C-N-CA	6.23	130.64	120.23
7	G	235	ALA	CA-C-N	6.23	128.49	120.70
7	G	235	ALA	C-N-CA	6.23	128.49	120.70
23	T	123	HIS	ND1-CE1-NE2	6.23	114.63	108.40
29	P	122	ILE	CA-C-N	6.23	128.63	120.28
29	P	122	ILE	C-N-CA	6.23	128.63	120.28
1	a	9	ILE	CA-C-N	6.23	129.68	120.90
1	a	9	ILE	C-N-CA	6.23	129.68	120.90
23	T	252	GLU	CA-C-O	6.23	126.28	119.24
11	4	83	PHE	CA-C-N	6.23	128.99	120.46
11	4	83	PHE	C-N-CA	6.23	128.99	120.46
12	5	3	THR	N-CA-C	-6.23	99.58	109.23
8	h	28	ASN	O-C-N	-6.23	116.38	123.48
9	i	22	GLN	CA-C-O	-6.23	113.60	120.33
14	n	62	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
14	n	168	THR	N-CA-CB	6.23	119.14	110.17
8	1	149	GLU	N-CA-CB	6.23	119.27	110.12
18	L	74	LEU	CA-C-N	6.23	128.54	120.44
18	L	74	LEU	C-N-CA	6.23	128.54	120.44
20	J	170	HIS	CA-C-O	-6.23	113.05	121.02
21	W	102	GLN	N-CA-CB	6.23	119.48	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	326	VAL	N-CA-C	-6.23	104.43	110.72
27	N	758	VAL	N-CA-C	-6.23	98.70	108.23
28	S	159	ASN	CA-C-N	6.23	128.62	120.28
28	S	159	ASN	C-N-CA	6.23	128.62	120.28
22	V	103	MET	CA-C-N	6.23	129.86	120.77
22	V	103	MET	C-N-CA	6.23	129.86	120.77
29	P	6	PRO	N-CA-CB	6.23	110.11	103.39
12	5	209	ASN	N-CA-C	-6.22	104.03	111.69
19	M	115	LYS	N-CA-CB	6.22	121.08	110.50
27	N	439	VAL	CA-CB-CG2	-6.22	99.82	110.40
17	K	232	ALA	CA-C-O	6.22	129.25	121.66
18	L	351	LEU	CA-C-O	-6.22	113.90	119.75
26	Z	534	PHE	CA-C-O	-6.22	114.29	120.82
32	U	121	LEU	CA-C-O	6.22	127.12	120.46
7	G	241	LYS	N-CA-C	-6.22	104.50	111.28
17	K	253	MET	N-CA-C	6.22	118.86	111.71
27	N	222	TYR	CB-CG-CD1	-6.22	111.47	120.80
28	S	142	VAL	N-CA-CB	6.22	117.83	110.55
29	P	285	GLN	OE1-CD-NE2	-6.22	116.38	122.60
3	c	82	ASP	CA-C-N	6.22	128.61	120.28
3	c	82	ASP	C-N-CA	6.22	128.61	120.28
16	I	285	ASP	CA-C-N	6.22	128.61	120.28
16	I	285	ASP	C-N-CA	6.22	128.61	120.28
31	R	139	GLU	N-CA-C	-6.22	104.58	111.36
7	G	83	HIS	CE1-NE2-CD2	-6.21	102.78	109.00
28	S	118	PHE	CA-CB-CG	-6.21	107.58	113.80
20	J	40	ASN	N-CA-C	6.21	117.72	111.07
10	j	21	ALA	O-C-N	6.21	130.35	123.33
2	B	166	LYS	N-CA-C	6.21	118.85	111.33
32	U	30	ASN	OD1-CG-ND2	6.21	128.81	122.60
3	c	186	ASP	CA-CB-CG	-6.21	106.39	112.60
1	a	56	ASP	CA-CB-CG	-6.21	106.39	112.60
1	A	124	TYR	N-CA-CB	6.21	119.25	110.12
19	M	302	GLN	CA-C-O	-6.21	114.30	120.82
27	N	233	ASN	CB-CA-C	6.21	121.18	112.11
29	P	240	TYR	CA-C-O	6.21	127.00	120.42
30	Q	389	VAL	CA-C-N	6.21	131.29	122.72
30	Q	389	VAL	C-N-CA	6.21	131.29	122.72
24	X	36	LYS	CB-CA-C	-6.21	102.15	109.47
31	R	394	ASP	N-CA-C	-6.21	104.34	112.41
14	n	219	TRP	CD2-CE2-CZ2	-6.21	116.19	122.40
19	M	118	VAL	CA-C-O	-6.21	113.83	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	GLY	CA-C-N	6.20	128.59	120.28
2	B	167	GLY	C-N-CA	6.20	128.59	120.28
27	N	275	THR	CA-C-N	6.20	128.50	120.44
27	N	275	THR	C-N-CA	6.20	128.50	120.44
10	j	162	LEU	N-CA-CB	6.20	119.24	110.12
17	K	418	ASP	CA-CB-CG	-6.20	106.40	112.60
28	S	116	ALA	N-CA-C	-6.20	105.36	113.17
33	O	24	PRO	CB-CA-C	-6.20	102.54	112.21
3	c	160	LYS	CB-CA-C	-6.20	98.99	109.03
1	A	130	VAL	O-C-N	6.20	130.27	122.52
25	Y	20	LYS	N-CA-C	6.20	118.84	111.71
27	N	904	VAL	N-CA-CB	6.20	119.11	110.56
13	6	86	ILE	O-C-N	6.20	127.88	121.87
3	c	178	ASP	CA-CB-CG	-6.20	106.41	112.60
2	B	94	HIS	N-CA-C	6.20	124.00	110.80
19	M	53	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
26	Z	426	TYR	CA-CB-CG	-6.20	102.75	113.90
13	m	58	ALA	CA-C-O	-6.19	113.98	120.55
5	E	25	LEU	CA-C-O	-6.19	113.86	120.42
23	T	26	LEU	N-CA-C	-6.19	105.88	113.50
10	j	156	ASN	OD1-CG-ND2	6.19	128.79	122.60
27	N	7	ALA	CA-C-O	-6.19	112.66	118.73
30	Q	122	ILE	N-CA-CB	6.19	118.96	110.54
27	N	531	LEU	N-CA-C	-6.19	105.31	112.92
1	a	177	PHE	CA-C-N	6.19	128.86	120.44
1	a	177	PHE	C-N-CA	6.19	128.86	120.44
28	S	126	LYS	N-CA-CB	6.19	120.95	110.49
33	O	179	PHE	N-CA-CB	6.19	118.98	110.01
6	f	13	SER	CA-C-N	6.19	125.67	119.24
6	f	13	SER	C-N-CA	6.19	125.67	119.24
13	m	74	TRP	CA-C-N	6.18	128.85	120.44
13	m	74	TRP	C-N-CA	6.18	128.85	120.44
10	3	58	ASP	CA-C-O	-6.18	112.49	119.79
15	H	310	GLU	CB-CA-C	6.18	121.14	112.11
30	Q	111	LEU	CA-C-N	6.18	133.35	121.54
30	Q	111	LEU	C-N-CA	6.18	133.35	121.54
4	d	94	HIS	CG-CD2-NE2	6.18	113.38	107.20
7	G	154	TRP	CA-C-O	-6.18	113.89	121.06
21	W	139	VAL	CA-C-O	6.18	127.17	120.43
28	S	283	GLN	N-CA-C	-6.18	105.32	112.92
7	g	190	LYS	CA-C-N	6.18	128.56	120.28
7	g	190	LYS	C-N-CA	6.18	128.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	44	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
7	G	200	HIS	CA-CB-CG	6.18	119.98	113.80
6	f	184	ASN	CA-C-O	-6.18	113.13	119.49
9	2	42	TRP	CE2-CD2-CE3	6.18	124.98	118.80
9	i	191	LEU	CA-C-N	6.18	129.68	122.52
9	i	191	LEU	C-N-CA	6.18	129.68	122.52
32	U	73	ILE	N-CA-C	-6.18	104.72	110.53
14	n	112	ASN	OD1-CG-ND2	-6.17	116.43	122.60
27	N	88	ARG	N-CA-C	-6.17	102.94	111.28
7	g	31	THR	N-CA-C	6.17	118.27	110.24
1	A	200	HIS	ND1-CE1-NE2	6.17	114.57	108.40
12	5	86	LEU	CA-C-N	6.17	128.92	120.46
12	5	86	LEU	C-N-CA	6.17	128.92	120.46
28	S	33	GLU	CA-C-N	6.17	128.55	120.28
28	S	33	GLU	C-N-CA	6.17	128.55	120.28
7	g	32	THR	N-CA-CB	6.17	119.04	109.97
27	N	210	SER	N-CA-CB	6.17	119.72	110.22
12	l	146	TRP	CD2-CE2-CZ2	-6.17	116.23	122.40
14	7	74	ASN	CA-CB-CG	-6.17	106.43	112.60
17	K	368	LEU	N-CA-C	-6.17	104.64	111.36
26	Z	312	TYR	CA-C-N	6.17	128.91	120.46
26	Z	312	TYR	C-N-CA	6.17	128.91	120.46
28	S	275	TYR	CA-C-O	-6.17	114.35	120.70
4	d	152	GLY	O-C-N	-6.17	114.68	122.70
29	P	263	HIS	CE1-NE2-CD2	-6.17	102.83	109.00
29	P	425	HIS	CA-C-N	6.17	129.18	120.42
29	P	425	HIS	C-N-CA	6.17	129.18	120.42
31	R	152	LYS	N-CA-C	6.17	117.67	111.07
20	J	350	MET	N-CA-CB	6.17	121.96	111.66
10	j	191	LYS	O-C-N	-6.16	115.72	122.07
6	f	230	ALA	CA-C-O	6.16	127.06	119.97
3	C	183	MET	CA-C-O	6.16	127.97	121.19
1	a	183	ASP	CA-CB-CG	-6.16	106.44	112.60
5	e	106	GLN	N-CA-C	6.16	118.00	111.28
7	g	205	GLU	CB-CA-C	-6.16	100.56	110.79
10	j	161	ASP	CA-C-N	6.16	128.54	120.28
10	j	161	ASP	C-N-CA	6.16	128.54	120.28
16	I	136	VAL	CG1-CB-CG2	6.16	124.35	110.80
19	M	307	GLU	CA-C-N	6.16	128.53	120.28
19	M	307	GLU	C-N-CA	6.16	128.53	120.28
28	S	71	ALA	N-CA-C	-6.16	105.70	112.72
31	R	109	LYS	CG-CD-CE	6.16	125.47	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	109	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
11	k	166	GLN	CA-C-N	6.16	128.53	120.28
11	k	166	GLN	C-N-CA	6.16	128.53	120.28
3	C	58	GLN	CB-CA-C	-6.16	97.82	110.38
29	P	343	LYS	CA-C-N	6.16	128.53	120.28
29	P	343	LYS	C-N-CA	6.16	128.53	120.28
1	A	224	PHE	N-CA-C	-6.16	98.36	108.76
15	H	310	GLU	O-C-N	-6.16	115.58	122.91
19	M	117	ALA	O-C-N	-6.16	116.11	123.31
20	J	57	PHE	CA-C-N	6.16	128.31	120.56
20	J	57	PHE	C-N-CA	6.16	128.31	120.56
20	J	385	ALA	N-CA-C	-6.16	104.49	111.14
28	S	225	HIS	ND1-CE1-NE2	6.16	114.56	108.40
31	R	193	ALA	CA-C-N	6.16	128.89	120.46
31	R	193	ALA	C-N-CA	6.16	128.89	120.46
18	L	291	PHE	CB-CA-C	-6.15	109.49	116.63
4	d	201	VAL	CA-C-O	6.15	124.52	118.98
16	I	376	ASN	O-C-N	6.15	130.77	122.59
20	J	248	ASP	CA-CB-CG	-6.15	106.45	112.60
28	S	64	ARG	CA-C-N	6.15	130.05	120.82
28	S	64	ARG	C-N-CA	6.15	130.05	120.82
5	E	116	GLY	O-C-N	-6.15	114.70	122.70
26	Z	147	GLU	CA-C-N	6.15	126.94	119.99
26	Z	147	GLU	C-N-CA	6.15	126.94	119.99
19	M	159	LEU	CA-C-O	-6.15	112.66	120.04
30	Q	12	ARG	CA-C-O	-6.15	114.36	120.82
5	e	134	LEU	N-CA-C	-6.15	99.38	109.40
3	C	94	ALA	CA-C-N	6.15	128.43	120.44
3	C	94	ALA	C-N-CA	6.15	128.43	120.44
15	H	333	MET	CG-SD-CE	-6.15	87.38	100.90
27	N	642	ASP	O-C-N	-6.15	115.52	120.38
32	U	212	ASP	N-CA-CB	6.15	119.26	110.16
1	A	187	GLU	CA-C-O	6.15	127.88	120.81
13	6	81	ASP	CA-CB-CG	-6.15	106.45	112.60
27	N	518	ALA	N-CA-C	-6.15	104.50	111.14
8	h	173	ILE	N-CA-C	-6.14	98.83	108.23
18	L	213	LYS	O-C-N	-6.14	115.83	121.30
27	N	521	LEU	N-CA-C	-6.14	104.66	111.36
2	b	80	PRO	O-C-N	6.14	129.60	122.23
4	d	124	VAL	O-C-N	-6.14	116.00	123.00
6	F	183	GLY	N-CA-C	-6.14	106.77	115.43
13	6	16	ALA	CA-C-O	6.14	126.93	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	204	ALA	CB-CA-C	-6.14	101.20	110.90
5	e	10	GLU	N-CA-CB	6.14	119.09	109.94
27	N	653	ARG	N-CA-CB	6.14	119.27	110.06
4	D	168	THR	CA-C-N	6.14	130.37	120.30
4	D	168	THR	C-N-CA	6.14	130.37	120.30
26	Z	259	PRO	N-CA-C	-6.14	106.19	113.86
5	E	105	THR	N-CA-CB	6.14	119.14	110.12
9	2	69	TYR	O-C-N	6.14	128.39	122.07
26	Z	619	ASP	N-CA-C	-6.14	106.46	112.97
27	N	467	LYS	O-C-N	-6.13	115.16	122.15
29	P	199	LEU	CA-C-N	6.13	128.50	120.28
29	P	199	LEU	C-N-CA	6.13	128.50	120.28
31	R	69	GLU	CA-C-O	-6.13	111.83	119.38
6	F	142	HIS	CG-CD2-NE2	6.13	113.33	107.20
10	j	119	PHE	CA-CB-CG	-6.13	107.67	113.80
13	m	155	ASN	CA-CB-CG	-6.13	106.47	112.60
22	V	186	GLN	CA-CB-CG	6.13	126.36	114.10
8	1	86	CYS	CA-C-N	6.13	128.41	120.44
8	1	86	CYS	C-N-CA	6.13	128.41	120.44
12	5	78	ALA	CB-CA-C	-6.13	100.43	110.85
26	Z	629	VAL	N-CA-CB	6.13	118.88	110.54
27	N	306	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	a	70	ILE	CA-C-O	6.13	127.27	120.59
5	e	2	ARG	CA-C-O	-6.13	114.45	121.19
7	g	119	HIS	CE1-NE2-CD2	-6.13	102.87	109.00
9	i	141	HIS	CA-C-O	-6.13	113.92	120.42
9	i	217	ILE	N-CA-CB	6.13	117.84	110.31
26	Z	317	GLN	N-CA-C	6.13	117.96	111.28
27	N	499	HIS	CA-C-O	-6.13	114.39	120.82
27	N	623	PHE	CA-C-O	-6.13	114.06	120.55
1	a	24	LYS	CA-C-N	6.12	129.10	120.28
1	a	24	LYS	C-N-CA	6.12	129.10	120.28
27	N	226	ASN	CA-C-N	6.12	128.77	120.44
27	N	226	ASN	C-N-CA	6.12	128.77	120.44
27	N	381	GLU	CA-C-N	6.12	126.74	119.94
27	N	381	GLU	C-N-CA	6.12	126.74	119.94
28	S	176	LEU	CA-C-N	6.12	128.49	120.28
28	S	176	LEU	C-N-CA	6.12	128.49	120.28
33	O	141	ASN	CB-CG-ND2	-6.12	107.21	116.40
2	b	233	PRO	CB-CA-C	-6.12	103.93	111.64
9	i	87	LEU	CA-C-N	6.12	128.48	120.28
9	i	87	LEU	C-N-CA	6.12	128.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	24	ILE	CA-C-N	6.12	128.98	120.29
29	P	24	ILE	C-N-CA	6.12	128.98	120.29
1	a	146	TYR	CB-CG-CD2	-6.12	111.63	120.80
12	l	181	THR	CA-C-N	6.12	128.47	120.28
12	l	181	THR	C-N-CA	6.12	128.47	120.28
13	m	105	TYR	O-C-N	-6.12	116.06	123.16
7	G	80	ASP	N-CA-C	-6.12	104.73	111.82
16	I	372	SER	CA-C-N	6.12	129.09	120.28
16	I	372	SER	C-N-CA	6.12	129.09	120.28
22	V	219	GLU	N-CA-C	-6.12	105.82	113.28
10	j	199	LEU	CB-CA-C	-6.11	98.38	109.38
17	K	330	ARG	O-C-N	-6.11	115.75	122.17
23	T	14	ALA	CA-C-N	6.11	128.97	120.29
23	T	14	ALA	C-N-CA	6.11	128.97	120.29
28	S	291	GLU	N-CA-C	6.11	118.02	111.36
23	T	170	ASN	N-CA-C	-6.11	105.47	113.17
6	f	107	ALA	N-CA-C	-6.11	104.62	111.28
3	C	32	GLY	CA-C-N	6.11	130.16	121.42
3	C	32	GLY	C-N-CA	6.11	130.16	121.42
5	E	207	ASN	CA-CB-CG	-6.11	106.49	112.60
25	Y	78	LYS	N-CA-C	6.11	117.94	111.28
28	S	381	VAL	N-CA-C	-6.11	104.55	110.72
2	b	196	LEU	CA-C-O	-6.11	114.07	120.55
10	3	26	LEU	N-CA-C	-6.11	105.47	113.17
20	J	333	ARG	NE-CZ-NH1	-6.11	115.39	121.50
24	X	30	GLN	N-CA-C	-6.11	97.79	110.80
14	n	78	ASN	CA-C-N	6.11	125.81	119.64
14	n	78	ASN	C-N-CA	6.11	125.81	119.64
27	N	334	VAL	N-CA-C	6.11	116.28	110.42
30	Q	178	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
31	R	296	LEU	CA-C-O	-6.11	114.41	120.70
31	R	414	LEU	CA-C-N	6.11	128.47	120.28
31	R	414	LEU	C-N-CA	6.11	128.47	120.28
22	V	163	ALA	O-C-N	6.11	129.11	122.15
26	Z	875	LYS	CA-C-N	6.11	130.12	120.47
26	Z	875	LYS	C-N-CA	6.11	130.12	120.47
31	R	70	TYR	CA-CB-CG	6.10	124.89	113.90
26	Z	294	ILE	CB-CA-C	6.10	120.64	112.22
29	P	218	LEU	CA-C-O	-6.10	114.42	120.70
32	U	46	ILE	N-CA-C	-6.10	99.63	108.36
4	d	63	SER	N-CA-C	-6.10	98.45	108.76
7	G	12	SER	O-C-N	-6.10	115.13	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	71	GLY	N-CA-C	-6.10	103.83	112.37
3	c	22	GLU	O-C-N	6.10	128.59	122.12
6	f	12	PHE	N-CA-C	-6.10	101.25	110.28
13	m	151	ASP	N-CA-CB	6.10	119.09	110.12
17	K	172	ALA	N-CA-C	-6.10	105.42	112.92
18	L	59	GLN	N-CA-C	-6.10	104.71	111.36
21	W	175	THR	N-CA-CB	6.10	119.56	109.98
31	R	54	ILE	O-C-N	6.10	128.24	121.90
13	m	79	HIS	N-CA-C	-6.10	105.42	112.92
2	B	94	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
19	M	239	THR	CA-C-O	6.10	126.91	119.11
22	V	168	LEU	N-CA-CB	6.10	119.82	110.61
26	Z	818	CYS	N-CA-CB	6.10	119.69	110.30
5	E	228	THR	CA-C-N	6.10	128.45	120.28
5	E	228	THR	C-N-CA	6.10	128.45	120.28
2	b	166	LYS	CB-CA-C	-6.09	101.27	110.90
18	L	333	LEU	N-CA-C	-6.09	100.04	109.24
11	4	190	ARG	O-C-N	-6.09	115.96	123.33
12	5	124	GLY	CA-C-O	-6.09	115.65	121.38
33	O	29	PHE	CB-CA-C	-6.09	100.68	110.79
9	i	164	TRP	CA-C-O	6.09	126.97	119.97
14	n	30	TYR	CB-CG-CD2	-6.09	111.67	120.80
16	I	168	VAL	O-C-N	6.09	128.10	121.83
17	K	154	SER	N-CA-C	6.09	118.16	110.24
29	P	119	ILE	O-C-N	6.09	127.78	121.87
29	P	258	LYS	CA-C-N	6.09	125.81	119.05
29	P	258	LYS	C-N-CA	6.09	125.81	119.05
33	O	111	SER	N-CA-C	-6.09	104.72	111.36
29	P	18	LYS	N-CA-C	-6.09	104.92	112.90
9	i	221	CYS	N-CA-CB	6.09	118.94	110.17
7	G	48	LYS	N-CA-C	-6.08	98.60	108.52
32	U	112	LYS	CA-C-O	6.08	126.87	120.42
3	C	82	ASP	N-CA-C	-6.08	104.73	111.36
4	D	206	LYS	N-CA-C	-6.08	106.40	113.88
28	S	55	ARG	CA-C-N	6.08	129.56	120.31
28	S	55	ARG	C-N-CA	6.08	129.56	120.31
5	e	148	PHE	O-C-N	-6.08	115.76	123.24
6	f	91	CYS	CA-C-N	6.08	128.43	120.28
6	f	91	CYS	C-N-CA	6.08	128.43	120.28
12	l	139	VAL	N-CA-CB	6.08	118.81	110.54
3	c	155	ASN	CB-CG-ND2	-6.08	107.28	116.40
11	k	91	SER	CB-CA-C	-6.08	100.70	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	103	ILE	N-CA-CB	6.08	121.26	111.23
28	S	256	LYS	CA-C-N	6.08	133.15	121.54
28	S	256	LYS	C-N-CA	6.08	133.15	121.54
1	a	62	TYR	N-CA-C	-6.08	103.59	113.19
8	h	156	LYS	CA-C-N	6.08	128.34	120.44
8	h	156	LYS	C-N-CA	6.08	128.34	120.44
11	k	92	ILE	N-CA-CB	6.08	118.81	110.54
15	H	362	ASP	CA-C-N	6.08	125.97	119.28
15	H	362	ASP	C-N-CA	6.08	125.97	119.28
27	N	779	GLU	CB-CA-C	-6.08	100.70	110.79
5	e	110	ASP	CA-C-N	6.08	129.03	120.28
5	e	110	ASP	C-N-CA	6.08	129.03	120.28
29	P	123	ARG	CA-C-O	6.08	126.99	120.55
15	H	215	LYS	CA-C-N	6.07	129.03	120.28
15	H	215	LYS	C-N-CA	6.07	129.03	120.28
26	Z	143	VAL	N-CA-C	-6.07	104.93	110.82
1	a	68	ARG	NE-CZ-NH2	6.07	124.67	119.20
7	g	57	PRO	O-C-N	-6.07	115.68	123.03
5	e	75	ALA	CB-CA-C	-6.07	100.53	110.85
9	i	78	SER	N-CA-CB	6.07	119.05	110.12
13	m	184	VAL	O-C-N	6.07	127.76	121.87
2	B	20	GLN	N-CA-C	6.07	117.90	111.28
18	L	78	ARG	N-CA-C	-6.07	104.66	111.28
29	P	17	LEU	CA-C-N	6.07	132.69	121.52
29	P	17	LEU	C-N-CA	6.07	132.69	121.52
17	K	350	ARG	CA-C-N	6.07	128.41	120.28
17	K	350	ARG	C-N-CA	6.07	128.41	120.28
21	W	146	GLU	CA-C-N	6.07	130.87	121.34
21	W	146	GLU	C-N-CA	6.07	130.87	121.34
14	7	153	PRO	CA-C-N	6.07	129.22	120.79
14	7	153	PRO	C-N-CA	6.07	129.22	120.79
33	O	201	PRO	N-CA-C	-6.07	106.57	114.03
7	g	221	ASN	N-CA-CB	6.07	120.74	110.49
10	j	119	PHE	O-C-N	-6.07	115.98	123.44
7	G	101	THR	O-C-N	6.07	127.23	121.71
9	i	219	ASN	CA-CB-CG	6.06	118.66	112.60
10	3	143	ASP	O-C-N	-6.06	115.83	122.07
17	K	144	ASN	N-CA-C	-6.06	103.03	111.52
26	Z	827	LEU	CA-C-O	6.06	126.85	120.42
28	S	216	LYS	N-CA-CB	6.06	119.03	110.12
4	d	157	TRP	CB-CG-CD2	-6.06	118.31	126.80
18	L	338	LEU	CA-C-N	6.06	128.81	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	338	LEU	C-N-CA	6.06	128.81	120.39
2	b	34	SER	O-C-N	-6.06	115.27	123.15
2	b	188	ALA	CA-C-N	6.06	128.19	120.56
2	b	188	ALA	C-N-CA	6.06	128.19	120.56
1	a	59	THR	CA-C-O	-6.06	113.00	119.97
4	d	112	ALA	CB-CA-C	-6.06	100.73	110.79
1	A	163	GLY	CA-C-N	6.06	125.68	119.56
1	A	163	GLY	C-N-CA	6.06	125.68	119.56
7	g	220	THR	N-CA-C	-6.06	106.05	113.50
22	V	242	LYS	CA-C-N	6.06	128.31	120.44
22	V	242	LYS	C-N-CA	6.06	128.31	120.44
4	D	112	ALA	CA-C-N	6.05	127.91	120.22
4	D	112	ALA	C-N-CA	6.05	127.91	120.22
16	I	69	LEU	CA-C-N	6.05	128.68	120.38
16	I	69	LEU	C-N-CA	6.05	128.68	120.38
26	Z	709	LYS	N-CA-C	6.05	117.55	111.07
26	Z	439	TYR	N-CA-CB	6.05	119.02	110.12
9	i	206	PRO	N-CA-C	-6.05	102.33	111.41
5	E	129	PRO	N-CA-CB	6.05	108.58	103.25
16	I	132	ILE	N-CA-C	-6.05	99.86	108.58
5	e	180	HIS	CA-CB-CG	6.05	119.85	113.80
14	7	160	ASP	CA-CB-CG	6.05	118.65	112.60
27	N	381	GLU	N-CA-C	-6.05	105.48	112.92
28	S	139	HIS	CA-C-N	6.05	128.31	120.44
28	S	139	HIS	C-N-CA	6.05	128.31	120.44
27	N	658	ILE	N-CA-C	-6.05	104.61	110.42
6	f	177	THR	N-CA-C	-6.05	104.25	111.69
10	j	107	VAL	CA-C-O	6.05	126.24	120.25
15	H	63	ILE	O-C-N	6.05	127.73	121.87
18	L	420	ARG	CA-C-N	6.05	128.66	120.44
18	L	420	ARG	C-N-CA	6.05	128.66	120.44
1	a	109	ALA	CA-C-N	6.04	128.87	120.29
1	a	109	ALA	C-N-CA	6.04	128.87	120.29
26	Z	623	ARG	N-CA-C	-6.04	104.69	111.28
27	N	617	VAL	N-CA-C	-6.04	104.61	110.72
4	D	81	ARG	CA-C-N	6.04	128.74	120.46
4	D	81	ARG	C-N-CA	6.04	128.74	120.46
29	P	397	ALA	N-CA-CB	6.04	120.70	110.49
5	E	152	PRO	CA-C-N	6.04	128.98	120.28
5	E	152	PRO	C-N-CA	6.04	128.98	120.28
29	P	169	GLY	CA-C-N	6.04	128.87	120.29
29	P	169	GLY	C-N-CA	6.04	128.87	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	213	TYR	N-CA-C	-6.04	105.83	112.72
1	a	53	LYS	CA-C-N	6.04	128.62	120.65
1	a	53	LYS	C-N-CA	6.04	128.62	120.65
22	V	153	ILE	N-CA-C	-6.04	100.00	108.27
31	R	69	GLU	N-CA-C	-6.04	105.17	112.54
27	N	515	ARG	CA-C-N	6.04	126.79	120.03
27	N	515	ARG	C-N-CA	6.04	126.79	120.03
1	a	110	LYS	N-CA-C	-6.04	104.78	111.36
9	i	131	SER	N-CA-CB	6.04	118.99	110.12
12	5	168	ASP	CA-CB-CG	-6.04	106.56	112.60
18	L	258	GLU	CA-C-N	6.04	128.37	120.28
18	L	258	GLU	C-N-CA	6.04	128.37	120.28
26	Z	706	LYS	CB-CA-C	-6.04	100.59	110.85
27	N	765	ASP	N-CA-C	-6.04	107.74	114.62
29	P	419	VAL	N-CA-C	6.04	116.78	110.62
5	e	55	SER	CB-CA-C	-6.03	101.37	110.90
6	f	40	ASN	O-C-N	6.03	129.51	121.67
14	n	87	LEU	N-CA-CB	6.03	120.69	110.49
14	n	203	ASN	N-CA-C	-6.03	107.15	114.75
27	N	124	TYR	CA-CB-CG	-6.03	103.04	113.90
28	S	141	LEU	CA-C-N	6.03	128.16	120.56
28	S	141	LEU	C-N-CA	6.03	128.16	120.56
4	d	223	SER	N-CA-CB	6.03	118.91	110.04
13	m	115	ASP	CA-C-N	6.03	128.68	120.54
13	m	115	ASP	C-N-CA	6.03	128.68	120.54
13	6	92	ASN	N-CA-C	6.03	117.93	111.36
29	P	23	LYS	O-C-N	6.03	129.02	122.15
11	k	25	ILE	O-C-N	6.03	127.52	122.09
5	E	186	LYS	CA-C-N	6.03	128.36	120.28
5	E	186	LYS	C-N-CA	6.03	128.36	120.28
9	2	220	ILE	O-C-N	6.03	127.99	122.14
3	C	43	ILE	N-CA-C	-6.03	99.44	108.12
20	J	212	ARG	N-CA-CB	6.02	118.99	109.71
26	Z	171	LYS	N-CA-C	-6.02	105.42	112.89
27	N	65	ALA	CA-C-N	6.02	128.27	120.44
27	N	65	ALA	C-N-CA	6.02	128.27	120.44
28	S	474	GLU	CA-C-N	6.02	128.27	120.44
28	S	474	GLU	C-N-CA	6.02	128.27	120.44
16	I	375	VAL	CA-C-N	6.02	133.04	121.54
16	I	375	VAL	C-N-CA	6.02	133.04	121.54
18	L	112	LEU	N-CA-C	-6.02	106.57	114.04
13	m	96	LEU	CB-CA-C	-6.02	100.61	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	374	ILE	N-CA-C	-6.02	104.64	110.72
31	R	327	ASP	CA-C-N	6.02	128.84	120.29
31	R	327	ASP	C-N-CA	6.02	128.84	120.29
2	b	190	HIS	CA-CB-CG	-6.02	107.78	113.80
10	j	200	LYS	N-CA-CB	6.02	119.28	109.95
30	Q	41	ALA	N-CA-C	-6.02	105.84	113.43
33	O	318	HIS	CA-CB-CG	-6.02	107.78	113.80
6	F	221	PHE	CA-CB-CG	-6.02	107.78	113.80
3	c	93	HIS	CE1-NE2-CD2	-6.02	102.98	109.00
21	W	152	GLU	CA-C-N	6.02	128.83	120.29
21	W	152	GLU	C-N-CA	6.02	128.83	120.29
26	Z	809	MET	CA-C-O	-6.01	114.05	120.42
11	k	180	ILE	N-CA-C	-6.01	99.75	108.71
1	A	9	ILE	CA-CB-CG1	6.01	120.62	110.40
33	O	284	GLU	CA-C-N	6.01	128.62	120.44
33	O	284	GLU	C-N-CA	6.01	128.62	120.44
11	4	137	GLY	CA-C-N	6.01	128.34	120.28
11	4	137	GLY	C-N-CA	6.01	128.34	120.28
15	H	387	ASN	OD1-CG-ND2	6.01	128.61	122.60
16	I	83	LYS	N-CA-CB	6.01	121.07	110.37
17	K	325	ASP	CA-C-N	6.01	125.40	118.85
17	K	325	ASP	C-N-CA	6.01	125.40	118.85
30	Q	80	HIS	CB-CG-CD2	-6.01	123.38	131.20
30	Q	188	LEU	N-CA-C	-6.01	105.95	113.28
6	F	192	GLY	CA-C-N	6.01	128.13	120.56
6	F	192	GLY	C-N-CA	6.01	128.13	120.56
11	4	76	SER	CA-C-N	6.01	126.44	119.47
11	4	76	SER	C-N-CA	6.01	126.44	119.47
15	H	311	ILE	CA-C-N	6.01	128.61	120.38
15	H	311	ILE	C-N-CA	6.01	128.61	120.38
14	7	115	ILE	N-CA-C	-6.01	99.70	108.11
23	T	109	TYR	CA-C-N	6.01	128.82	120.29
23	T	109	TYR	C-N-CA	6.01	128.82	120.29
28	S	483	GLU	O-C-N	6.01	129.25	122.22
29	P	26	SER	CA-C-O	6.01	126.88	119.97
30	Q	150	GLN	CB-CA-C	-6.01	100.90	111.05
6	f	94	SER	CA-C-N	6.01	128.82	120.29
6	f	94	SER	C-N-CA	6.01	128.82	120.29
14	n	90	SER	CA-C-O	-6.01	114.05	120.42
8	1	145	ASN	CA-CB-CG	-6.01	106.59	112.60
29	P	277	GLN	OE1-CD-NE2	-6.01	116.59	122.60
30	Q	15	VAL	CB-CA-C	-6.01	104.28	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	44	SER	N-CA-CB	6.01	118.72	110.01
3	c	181	ASP	N-CA-C	-6.00	105.99	113.38
7	g	200	HIS	N-CA-C	-6.00	105.45	112.89
10	j	128	CYS	N-CA-C	-6.00	99.95	109.07
1	A	242	GLN	CA-CB-CG	6.00	126.10	114.10
21	W	36	ILE	CA-C-O	-6.00	114.71	120.95
26	Z	831	LEU	N-CA-C	-6.00	104.82	111.36
4	d	131	THR	CA-CB-OG1	6.00	118.60	109.60
6	f	181	ILE	N-CA-CB	6.00	117.84	111.00
9	i	194	ASN	CA-CB-CG	-6.00	106.60	112.60
1	A	145	ILE	N-CA-C	-6.00	99.41	108.17
15	H	358	PRO	CA-C-N	6.00	128.81	120.29
15	H	358	PRO	C-N-CA	6.00	128.81	120.29
4	d	216	ASP	CA-CB-CG	-6.00	106.60	112.60
28	S	65	ASN	CB-CA-C	-6.00	100.78	110.74
26	Z	941	ARG	O-C-N	-6.00	115.64	120.38
3	c	135	ILE	N-CA-CB	5.99	118.22	111.21
16	I	295	ASN	CA-CB-CG	-5.99	106.61	112.60
17	K	55	GLU	N-CA-C	5.99	118.60	111.71
17	K	294	ARG	CB-CA-C	-5.99	100.66	110.85
23	T	71	GLN	N-CA-CB	5.99	120.13	110.42
9	i	18	THR	CA-CB-OG1	5.99	118.59	109.60
31	R	48	GLU	O-C-N	-5.99	115.77	122.12
31	R	133	ALA	CA-C-N	5.99	129.42	120.31
31	R	133	ALA	C-N-CA	5.99	129.42	120.31
3	c	223	GLU	N-CA-C	-5.99	100.97	109.96
26	Z	217	GLU	CB-CG-CD	-5.99	102.42	112.60
14	7	190	ARG	N-CA-C	-5.99	104.50	112.94
19	M	400	MET	CA-C-N	5.99	128.66	120.46
19	M	400	MET	C-N-CA	5.99	128.66	120.46
22	V	111	HIS	N-CA-C	-5.99	99.15	109.15
23	T	75	PHE	CA-CB-CG	-5.99	107.81	113.80
1	a	10	PHE	CA-CB-CG	-5.99	107.81	113.80
13	6	38	ARG	NE-CZ-NH2	5.99	124.59	119.20
17	K	181	LYS	N-CA-C	-5.99	104.84	111.36
18	L	95	ILE	N-CA-C	-5.99	104.67	110.72
26	Z	598	ALA	CA-C-N	5.98	128.92	120.42
26	Z	598	ALA	C-N-CA	5.98	128.92	120.42
27	N	746	ALA	CA-C-N	5.98	130.18	120.60
27	N	746	ALA	C-N-CA	5.98	130.18	120.60
1	a	114	ASN	CA-C-N	5.98	128.30	120.28
1	a	114	ASN	C-N-CA	5.98	128.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	98	THR	CA-C-N	5.98	128.10	120.56
14	n	98	THR	C-N-CA	5.98	128.10	120.56
4	D	14	HIS	ND1-CE1-NE2	5.98	114.38	108.40
29	P	225	VAL	O-C-N	5.98	127.67	121.87
29	P	323	ASN	N-CA-C	-5.98	105.47	112.89
5	e	187	GLU	N-CA-CB	5.98	118.91	110.12
10	j	188	ILE	N-CA-C	-5.98	99.13	107.80
22	V	186	GLN	O-C-N	5.98	130.62	121.23
1	a	107	VAL	CA-C-N	5.98	128.21	120.44
1	a	107	VAL	C-N-CA	5.98	128.21	120.44
7	g	77	LEU	CA-C-O	-5.98	113.83	120.70
21	W	80	GLN	CA-C-O	5.98	126.58	120.24
22	V	57	PHE	CA-CB-CG	-5.98	107.82	113.80
9	i	114	HIS	CA-C-N	5.97	128.28	120.28
9	i	114	HIS	C-N-CA	5.97	128.28	120.28
13	6	108	HIS	CB-CG-CD2	-5.97	123.43	131.20
18	L	400	PHE	CA-CB-CG	-5.97	107.83	113.80
19	M	408	SER	CA-C-O	5.97	126.84	119.97
24	X	52	PRO	N-CA-CB	5.97	107.23	103.23
26	Z	299	ASP	CA-CB-CG	5.97	118.57	112.60
14	n	208	PHE	N-CA-C	-5.97	99.46	109.07
26	Z	294	ILE	CA-C-N	5.97	128.20	120.44
26	Z	294	ILE	C-N-CA	5.97	128.20	120.44
16	I	415	ASP	CB-CA-C	-5.97	101.51	110.88
18	L	173	PHE	CB-CA-C	-5.97	101.56	110.16
8	h	124	TYR	CB-CG-CD2	-5.97	111.85	120.80
8	h	163	ILE	O-C-N	-5.97	115.68	121.83
1	A	188	GLU	N-CA-C	5.97	117.58	111.14
7	G	125	VAL	O-C-N	-5.97	116.88	123.03
26	Z	296	SER	N-CA-CB	5.97	118.99	110.16
27	N	301	THR	CA-C-N	5.97	128.59	120.54
27	N	301	THR	C-N-CA	5.97	128.59	120.54
27	N	888	ASP	N-CA-C	-5.97	102.23	110.35
28	S	447	GLU	CA-C-N	5.97	132.94	121.54
28	S	447	GLU	C-N-CA	5.97	132.94	121.54
12	5	13	ILE	CA-C-N	5.96	130.87	123.12
12	5	13	ILE	C-N-CA	5.96	130.87	123.12
16	I	362	LEU	CB-CG-CD1	5.96	128.59	110.70
30	Q	182	SER	CA-C-N	5.96	128.27	120.28
30	Q	182	SER	C-N-CA	5.96	128.27	120.28
31	R	370	LYS	N-CA-C	-5.96	104.35	111.69
9	2	99	ILE	CB-CA-C	-5.96	102.96	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	26	PRO	CA-C-O	-5.96	114.39	121.67
33	O	56	PRO	CA-C-N	5.96	128.27	120.28
33	O	56	PRO	C-N-CA	5.96	128.27	120.28
29	P	77	GLU	CA-C-N	5.96	128.74	120.63
29	P	77	GLU	C-N-CA	5.96	128.74	120.63
30	Q	52	ASN	CA-C-O	-5.96	114.19	120.63
3	c	90	ALA	N-CA-C	-5.96	104.91	111.82
12	l	86	LEU	O-C-N	5.96	128.21	122.07
18	L	413	ASP	CA-C-N	5.96	128.26	120.28
18	L	413	ASP	C-N-CA	5.96	128.26	120.28
20	J	376	HIS	CG-CD2-NE2	5.96	113.16	107.20
23	T	102	LYS	N-CA-CB	5.96	118.65	110.01
14	n	76	TYR	N-CA-CB	5.96	119.16	109.69
7	G	224	HIS	CA-CB-CG	-5.96	107.84	113.80
5	e	61	GLU	N-CA-C	-5.96	99.49	108.96
31	R	70	TYR	N-CA-CB	5.96	120.62	110.50
33	O	383	LYS	CA-C-O	-5.96	114.57	120.82
4	d	225	GLU	CA-C-N	5.95	128.26	120.28
4	d	225	GLU	C-N-CA	5.95	128.26	120.28
9	i	86	HIS	CG-CD2-NE2	5.95	113.15	107.20
6	F	115	ALA	CA-C-N	5.95	128.18	120.44
6	F	115	ALA	C-N-CA	5.95	128.18	120.44
16	I	268	PHE	CA-CB-CG	-5.95	107.85	113.80
24	X	124	LYS	N-CA-C	-5.95	104.70	111.07
11	k	113	LYS	CB-CA-C	-5.95	102.24	110.16
8	l	56	ALA	CB-CA-C	-5.95	101.54	110.88
24	X	37	PRO	O-C-N	5.95	130.30	122.27
31	R	303	SER	CA-C-N	5.95	128.18	120.44
31	R	303	SER	C-N-CA	5.95	128.18	120.44
9	2	146	LEU	N-CA-CB	5.95	118.71	109.85
18	L	240	GLY	CA-C-N	5.95	129.16	120.71
18	L	240	GLY	C-N-CA	5.95	129.16	120.71
25	Y	87	GLU	CB-CG-CD	-5.95	102.49	112.60
7	G	31	THR	N-CA-CB	5.95	119.49	110.45
2	b	227	ILE	CA-C-N	5.94	125.64	119.64
2	b	227	ILE	C-N-CA	5.94	125.64	119.64
6	F	197	SER	CA-C-N	5.94	128.73	120.29
6	F	197	SER	C-N-CA	5.94	128.73	120.29
23	T	173	GLU	N-CA-CB	5.94	120.53	110.49
4	d	172	PHE	CA-C-N	5.94	128.84	120.28
4	d	172	PHE	C-N-CA	5.94	128.84	120.28
9	i	144	GLN	CA-C-O	5.94	127.73	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	170	GLY	CA-C-O	-5.94	116.43	121.66
18	L	59	GLN	CA-C-N	5.94	130.11	120.60
18	L	59	GLN	C-N-CA	5.94	130.11	120.60
27	N	551	GLY	CA-C-N	5.94	128.24	120.28
27	N	551	GLY	C-N-CA	5.94	128.24	120.28
6	f	174	THR	N-CA-C	-5.94	105.69	113.17
6	F	58	TYR	N-CA-C	5.94	118.37	110.53
1	a	93	ALA	O-C-N	5.94	128.41	122.12
9	i	93	HIS	CB-CG-CD2	-5.94	123.48	131.20
15	H	420	ARG	N-CA-CB	5.94	118.95	110.16
18	L	231	LEU	N-CA-C	-5.94	105.70	113.12
29	P	237	VAL	N-CA-CB	5.94	118.62	110.54
1	A	50	VAL	CA-C-O	5.94	124.98	119.76
18	L	76	GLN	OE1-CD-NE2	5.94	128.54	122.60
8	h	58	ILE	CB-CA-C	-5.93	104.03	112.22
14	n	131	ASN	CA-C-N	5.93	130.09	120.60
14	n	131	ASN	C-N-CA	5.93	130.09	120.60
2	B	84	VAL	CB-CA-C	-5.93	104.03	112.22
5	E	62	ILE	CA-C-O	5.93	124.28	119.29
7	G	23	ALA	CA-C-N	5.93	129.85	120.47
7	G	23	ALA	C-N-CA	5.93	129.85	120.47
20	J	23	PHE	CA-C-O	5.93	126.84	120.55
4	d	175	LYS	N-CA-C	-5.93	106.08	113.38
15	H	157	VAL	N-CA-C	-5.93	101.58	108.82
16	I	125	MET	CA-C-O	-5.93	112.92	118.73
23	T	84	GLN	N-CA-CB	5.93	118.84	110.12
7	g	166	GLN	CB-CA-C	-5.93	100.94	110.79
2	B	154	GLY	N-CA-C	-5.93	105.35	115.08
2	b	211	LEU	N-CA-C	-5.93	98.42	108.26
1	A	2	GLY	CA-C-N	5.93	128.22	120.28
1	A	2	GLY	C-N-CA	5.93	128.22	120.28
1	A	235	ARG	N-CA-CB	5.93	118.94	110.16
22	V	222	GLN	CA-C-N	5.93	128.82	120.28
22	V	222	GLN	C-N-CA	5.93	128.82	120.28
24	X	99	PHE	CA-CB-CG	-5.93	107.87	113.80
31	R	272	ASP	CA-CB-CG	-5.93	106.67	112.60
9	i	21	THR	CA-CB-OG1	5.93	118.49	109.60
11	k	111	LYS	N-CA-C	-5.93	106.09	113.38
26	Z	730	ALA	CA-C-N	5.93	131.34	120.79
26	Z	730	ALA	C-N-CA	5.93	131.34	120.79
3	c	85	ILE	N-CA-C	-5.93	104.73	110.42
6	f	67	GLU	CB-CG-CD	-5.93	102.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	81	ARG	CA-C-N	-5.93	113.09	120.56
6	F	81	ARG	C-N-CA	-5.93	113.09	120.56
6	F	139	SER	N-CA-C	-5.92	102.69	111.81
16	I	321	ASP	N-CA-C	-5.92	105.63	112.92
26	Z	791	LYS	N-CA-C	-5.92	105.54	112.89
28	S	100	HIS	CA-CB-CG	-5.92	107.88	113.80
6	f	66	ASP	CA-CB-CG	5.92	118.52	112.60
8	h	91	ASP	CA-C-N	5.92	128.14	120.44
8	h	91	ASP	C-N-CA	5.92	128.14	120.44
15	H	72	SER	N-CA-C	-5.92	104.73	113.61
22	V	124	ASN	CA-C-N	5.92	128.14	120.44
22	V	124	ASN	C-N-CA	5.92	128.14	120.44
27	N	626	GLY	CA-C-N	5.92	128.83	120.42
27	N	626	GLY	C-N-CA	5.92	128.83	120.42
8	h	120	HIS	CB-CG-CD2	5.92	138.89	131.20
9	2	72	ARG	NE-CZ-NH2	-5.92	113.87	119.20
16	I	230	THR	CA-C-O	5.92	126.82	120.55
14	n	134	GLY	N-CA-C	-5.92	107.08	115.30
5	E	123	GLU	N-CA-CB	5.91	120.07	110.43
26	Z	707	LYS	O-C-N	5.91	128.39	122.12
27	N	567	ALA	O-C-N	5.91	128.39	122.12
1	a	168	GLU	N-CA-C	5.91	117.72	111.28
13	m	6	GLY	N-CA-C	-5.91	99.17	113.18
4	D	31	ALA	N-CA-C	-5.91	100.07	109.23
6	F	222	THR	O-C-N	-5.91	116.18	123.33
30	Q	381	ILE	CB-CA-C	-5.91	104.06	112.22
10	3	187	TYR	CA-C-O	-5.91	114.45	120.71
29	P	230	HIS	ND1-CE1-NE2	5.91	114.31	108.40
2	b	156	TYR	CB-CG-CD2	-5.91	111.94	120.80
1	A	173	LEU	CA-C-N	5.91	128.12	120.44
1	A	173	LEU	C-N-CA	5.91	128.12	120.44
12	5	195	GLU	CA-C-N	5.91	128.19	120.28
12	5	195	GLU	C-N-CA	5.91	128.19	120.28
14	7	62	HIS	CA-CB-CG	-5.91	107.89	113.80
19	M	434	ALA	CB-CA-C	-5.91	101.64	110.50
26	Z	137	TYR	N-CA-C	-5.91	104.76	111.14
28	S	227	ASN	N-CA-C	-5.91	104.92	111.36
32	U	27	THR	CB-CA-C	5.91	119.65	110.67
11	k	105	GLY	N-CA-C	-5.90	101.68	110.71
10	3	83	PRO	CB-CA-C	-5.90	103.49	112.11
27	N	62	ALA	CB-CA-C	-5.90	99.33	110.67
3	c	122	THR	N-CA-C	-5.90	106.42	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	151	ASN	CA-C-O	-5.90	115.13	121.27
10	j	161	ASP	N-CA-CB	5.90	119.00	110.20
8	l	157	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
13	6	155	ASN	CA-CB-CG	-5.90	106.70	112.60
18	L	171	THR	CA-C-N	5.90	128.78	120.28
18	L	171	THR	C-N-CA	5.90	128.78	120.28
18	L	348	GLU	N-CA-CB	5.90	119.84	110.57
32	U	27	THR	CA-CB-OG1	5.90	118.45	109.60
1	a	91	GLU	O-C-N	5.90	128.37	122.12
10	j	185	VAL	N-CA-CB	5.90	121.66	111.39
12	l	145	LYS	CA-CB-CG	5.90	125.90	114.10
14	n	73	GLU	N-CA-C	-5.90	104.93	111.36
26	Z	133	ASP	N-CA-CB	5.90	118.79	110.12
26	Z	606	CYS	O-C-N	5.90	128.88	122.15
27	N	798	LYS	CB-CA-C	-5.90	100.82	110.85
31	R	175	ALA	CA-C-N	5.90	128.19	120.28
31	R	175	ALA	C-N-CA	5.90	128.19	120.28
26	Z	399	LEU	N-CA-C	5.90	117.38	111.07
29	P	139	VAL	CA-C-N	5.90	128.19	120.28
29	P	139	VAL	C-N-CA	5.90	128.19	120.28
30	Q	133	LEU	N-CA-C	-5.90	104.93	111.36
3	c	183	MET	CB-CA-C	-5.90	100.20	109.70
11	k	28	LEU	N-CA-C	-5.90	104.93	111.36
14	n	62	HIS	CA-C-N	5.90	129.97	120.30
14	n	62	HIS	C-N-CA	5.90	129.97	120.30
1	a	111	ARG	N-CA-C	-5.89	104.76	111.07
6	f	154	GLU	N-CA-CB	5.89	119.78	110.23
9	i	141	HIS	O-C-N	5.89	128.87	122.15
15	H	176	VAL	CA-C-N	5.89	129.65	120.75
15	H	176	VAL	C-N-CA	5.89	129.65	120.75
1	a	203	ASP	CA-CB-CG	-5.89	106.71	112.60
7	g	127	PRO	O-C-N	5.89	129.77	123.23
11	k	23	ARG	CB-CA-C	-5.89	97.42	109.38
9	2	84	LYS	CA-C-N	5.89	128.18	120.28
9	2	84	LYS	C-N-CA	5.89	128.18	120.28
22	V	109	HIS	CG-CD2-NE2	5.89	113.09	107.20
22	V	286	GLU	CA-C-N	5.89	128.66	120.29
22	V	286	GLU	C-N-CA	5.89	128.66	120.29
25	Y	34	GLU	CA-C-N	5.89	128.18	120.28
25	Y	34	GLU	C-N-CA	5.89	128.18	120.28
29	P	239	GLN	OE1-CD-NE2	-5.89	116.71	122.60
33	O	367	LYS	CA-C-N	5.89	128.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	367	LYS	C-N-CA	5.89	128.18	120.28
31	R	404	VAL	N-CA-CB	5.89	121.43	110.77
2	b	138	GLY	O-C-N	-5.89	116.61	123.44
13	m	40	GLU	CA-C-N	5.89	126.23	119.93
13	m	40	GLU	C-N-CA	5.89	126.23	119.93
7	G	14	ASP	CA-CB-CG	-5.89	106.71	112.60
16	I	406	GLU	CB-CG-CD	-5.89	102.59	112.60
17	K	195	ALA	CA-C-N	5.89	128.10	120.44
17	K	195	ALA	C-N-CA	5.89	128.10	120.44
18	L	94	ASP	CA-C-N	5.89	128.78	120.42
18	L	94	ASP	C-N-CA	5.89	128.78	120.42
21	W	165	GLN	CA-C-N	5.89	128.49	120.54
21	W	165	GLN	C-N-CA	5.89	128.49	120.54
27	N	59	GLU	CA-C-N	5.89	129.26	120.31
27	N	59	GLU	C-N-CA	5.89	129.26	120.31
2	b	109	LEU	N-CA-C	-5.89	104.94	111.36
3	c	119	GLN	CA-C-N	5.89	126.62	120.03
3	c	119	GLN	C-N-CA	5.89	126.62	120.03
10	j	126	ILE	N-CA-C	-5.89	104.78	110.72
27	N	786	ARG	NE-CZ-NH1	-5.89	115.61	121.50
28	S	477	VAL	N-CA-CB	5.89	119.41	110.58
29	P	117	SER	N-CA-CB	5.89	118.87	110.16
29	P	253	ASP	N-CA-CB	5.89	119.07	109.95
31	R	156	LYS	CB-CA-C	-5.89	100.84	110.85
31	R	399	GLN	CA-C-N	5.89	128.17	120.28
31	R	399	GLN	C-N-CA	5.89	128.17	120.28
11	k	141	PHE	CA-C-N	5.88	128.65	120.29
11	k	141	PHE	C-N-CA	5.88	128.65	120.29
13	m	79	HIS	CB-CG-CD2	-5.88	123.55	131.20
31	R	360	SER	N-CA-C	-5.88	102.06	110.59
2	b	91	LYS	N-CA-C	5.88	117.36	111.07
3	C	105	ILE	CA-C-O	-5.88	114.17	119.82
10	3	146	PHE	O-C-N	5.88	128.35	122.12
18	L	60	PHE	CA-CB-CG	-5.88	107.92	113.80
4	d	140	ASP	CA-C-O	5.88	127.52	121.23
5	E	132	VAL	N-CA-C	-5.88	99.28	108.81
27	N	404	SER	N-CA-C	-5.88	105.20	112.90
31	R	145	GLY	N-CA-C	-5.88	104.76	114.76
11	k	132	ALA	N-CA-C	-5.88	99.58	108.52
1	A	58	THR	CA-CB-OG1	5.88	118.42	109.60
4	D	85	GLU	CA-C-N	5.88	128.16	120.28
4	D	85	GLU	C-N-CA	5.88	128.16	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	104	PRO	CA-C-N	5.88	129.06	120.71
13	6	104	PRO	C-N-CA	5.88	129.06	120.71
15	H	225	VAL	CA-CB-CG2	-5.88	100.41	110.40
22	V	143	PRO	N-CA-CB	5.88	109.42	103.25
13	6	48	ASP	N-CA-C	-5.88	104.05	111.92
26	Z	829	GLN	CA-C-O	-5.88	114.32	120.55
27	N	567	ALA	CA-C-O	-5.88	114.32	120.55
28	S	449	LEU	CA-C-N	5.88	130.51	122.34
28	S	449	LEU	C-N-CA	5.88	130.51	122.34
17	K	294	ARG	CA-C-N	5.88	127.96	120.56
17	K	294	ARG	C-N-CA	5.88	127.96	120.56
26	Z	935	THR	N-CA-CB	5.88	119.16	109.88
30	Q	147	GLN	CA-C-O	5.88	126.61	119.38
4	D	103	THR	O-C-N	-5.87	115.93	122.86
19	M	55	ASN	CA-C-O	-5.87	114.65	120.82
21	W	75	GLY	N-CA-C	-5.87	105.50	113.37
27	N	863	SER	N-CA-C	-5.87	105.88	113.16
28	S	142	VAL	CB-CA-C	-5.87	104.45	111.97
16	I	122	SER	O-C-N	-5.87	114.57	121.32
23	T	130	ASP	CA-CB-CG	-5.87	106.73	112.60
32	U	233	PHE	CA-CB-CG	-5.87	107.93	113.80
9	2	137	VAL	N-CA-C	-5.87	105.01	110.53
19	M	57	VAL	N-CA-C	-5.87	105.01	110.53
20	J	45	GLU	CA-C-N	5.87	128.62	120.29
20	J	45	GLU	C-N-CA	5.87	128.62	120.29
26	Z	859	LYS	N-CA-C	-5.87	99.78	108.99
32	U	173	HIS	CA-CB-CG	5.87	119.67	113.80
7	g	154	TRP	CE2-CD2-CE3	5.87	124.67	118.80
27	N	199	ASN	OD1-CG-ND2	5.87	128.47	122.60
1	a	145	ILE	N-CA-CB	5.86	119.80	111.82
12	l	196	LEU	CA-C-O	-5.86	114.20	120.42
14	7	129	TYR	CA-C-N	5.86	130.67	122.23
14	7	129	TYR	C-N-CA	5.86	130.67	122.23
20	J	146	THR	CA-C-N	5.86	129.22	120.31
20	J	146	THR	C-N-CA	5.86	129.22	120.31
32	U	259	ASN	N-CA-C	-5.86	104.81	111.14
1	a	166	GLN	CG-CD-OE1	-5.86	109.08	120.80
1	A	75	ASN	CA-C-O	5.86	126.57	120.30
23	T	19	ASP	CA-C-O	-5.86	114.31	120.58
30	Q	78	ILE	CA-C-O	-5.86	113.87	118.85
14	n	226	LYS	CA-C-O	5.86	127.90	121.40
2	B	94	HIS	ND1-CE1-NE2	5.86	114.26	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	189	TYR	CA-C-N	5.86	126.27	119.47
8	1	189	TYR	C-N-CA	5.86	126.27	119.47
24	X	111	LEU	CA-C-N	5.86	129.16	120.90
24	X	111	LEU	C-N-CA	5.86	129.16	120.90
8	1	193	TYR	CB-CG-CD2	-5.86	112.01	120.80
19	M	141	LYS	O-C-N	-5.86	116.38	121.71
29	P	177	ILE	CA-C-O	-5.86	114.86	120.95
33	O	101	ASP	O-C-N	5.86	128.42	122.09
1	a	225	PHE	CB-CG-CD2	-5.86	110.75	120.70
1	A	141	LEU	N-CA-C	-5.86	106.14	113.28
16	I	227	THR	CA-CB-OG1	5.85	118.38	109.60
2	b	142	PHE	CA-C-O	-5.85	114.22	120.42
19	M	375	ASN	OD1-CG-ND2	5.85	128.45	122.60
28	S	101	LYS	N-CA-CB	5.85	120.38	110.49
33	O	283	HIS	CB-CG-CD2	-5.85	123.59	131.20
17	K	204	ASP	CA-CB-CG	-5.85	106.75	112.60
28	S	420	GLU	CB-CA-C	-5.85	101.08	110.79
1	a	173	LEU	CA-C-O	-5.85	114.35	120.55
5	e	137	ALA	O-C-N	-5.85	115.63	123.23
7	G	105	ILE	N-CA-CB	5.85	114.19	110.50
23	T	78	PHE	CA-CB-CG	5.85	119.65	113.80
23	T	116	GLN	N-CA-CB	5.85	119.64	110.46
5	e	143	ASP	O-C-N	-5.85	115.29	122.25
12	l	89	GLN	N-CA-CB	5.85	118.72	110.12
2	B	92	VAL	N-CA-CB	5.85	117.39	110.55
7	G	86	ASN	CA-C-N	5.85	128.12	120.28
7	G	86	ASN	C-N-CA	5.85	128.12	120.28
16	I	68	HIS	CB-CG-CD2	-5.85	123.60	131.20
20	J	301	ASP	CA-C-O	-5.85	114.09	120.17
25	Y	22	GLU	CB-CA-C	-5.85	101.70	110.88
27	N	269	LEU	CA-C-N	5.85	128.12	120.28
27	N	269	LEU	C-N-CA	5.85	128.12	120.28
27	N	657	MET	CG-SD-CE	-5.85	88.03	100.90
13	m	164	THR	N-CA-C	-5.84	104.38	112.03
14	7	164	ASP	N-CA-C	-5.84	106.19	113.38
22	V	157	ARG	CA-C-N	5.84	130.68	121.56
22	V	157	ARG	C-N-CA	5.84	130.68	121.56
31	R	210	TYR	CA-C-N	5.84	128.11	120.28
31	R	210	TYR	C-N-CA	5.84	128.11	120.28
11	k	83	PHE	CB-CG-CD1	5.84	130.63	120.70
5	E	80	MET	N-CA-CB	5.84	118.81	110.16
13	6	203	GLU	N-CA-C	-5.84	97.80	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	164	LEU	CB-CA-C	-5.84	100.92	110.85
24	X	85	ARG	N-CA-C	5.84	119.49	111.54
7	g	135	GLY	O-C-N	-5.84	118.11	123.78
4	D	182	PRO	CA-C-O	-5.84	112.09	120.56
16	I	77	SER	O-C-N	5.84	128.34	122.03
27	N	579	SER	N-CA-C	5.84	117.73	111.36
29	P	189	LEU	N-CA-C	-5.84	105.04	111.82
31	R	185	LEU	O-C-N	5.84	128.81	122.15
2	B	19	GLY	CA-C-N	5.84	128.10	120.28
2	B	19	GLY	C-N-CA	5.84	128.10	120.28
26	Z	118	VAL	CA-C-O	-5.84	114.88	120.95
13	m	36	ASN	N-CA-C	-5.84	104.87	112.23
9	i	199	LYS	CA-C-O	5.84	126.79	120.95
11	k	141	PHE	CA-CB-CG	-5.84	107.96	113.80
4	D	117	ARG	NE-CZ-NH2	5.84	124.45	119.20
16	I	378	GLU	CB-CA-C	-5.84	100.93	110.85
31	R	134	TRP	CE3-CZ3-CH2	5.83	128.69	121.10
3	c	93	HIS	CG-CD2-NE2	5.83	113.03	107.20
7	g	238	PHE	N-CA-C	-5.83	104.92	111.28
29	P	263	HIS	CA-C-O	-5.83	114.37	120.55
1	a	237	VAL	N-CA-C	-5.83	104.67	110.62
12	l	202	GLU	N-CA-CB	5.83	118.69	110.12
14	n	59	ASP	CA-CB-CG	5.83	118.43	112.60
22	V	250	GLN	N-CA-CB	5.83	119.32	110.28
27	N	363	ALA	CA-C-N	5.83	129.17	120.31
27	N	363	ALA	C-N-CA	5.83	129.17	120.31
13	m	176	SER	N-CA-CB	5.83	119.28	110.42
29	P	279	ASP	CA-C-N	5.83	128.37	120.44
29	P	279	ASP	C-N-CA	5.83	128.37	120.44
5	e	187	GLU	CB-CA-C	-5.83	101.11	110.79
7	g	240	GLN	CB-CG-CD	-5.83	102.69	112.60
4	D	199	GLU	CB-CA-C	-5.83	101.48	110.81
15	H	57	LYS	N-CA-CB	5.83	118.69	110.12
19	M	409	SER	CA-C-N	5.83	128.31	120.50
19	M	409	SER	C-N-CA	5.83	128.31	120.50
23	T	213	ASN	CA-CB-CG	-5.83	106.77	112.60
7	g	50	ILE	CB-CA-C	5.83	119.47	111.31
4	D	238	LYS	CA-C-N	5.83	128.56	120.29
4	D	238	LYS	C-N-CA	5.83	128.56	120.29
7	G	197	TYR	N-CA-CB	5.83	118.69	110.12
7	G	90	GLU	CB-CA-C	-5.83	100.94	110.85
18	L	325	MET	N-CA-C	-5.83	99.69	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	593	HIS	CB-CA-C	-5.83	103.65	110.76
31	R	207	ARG	CA-C-N	5.83	128.09	120.28
31	R	207	ARG	C-N-CA	5.83	128.09	120.28
31	R	338	TYR	CB-CA-C	-5.83	100.95	110.85
32	U	227	GLY	CA-C-N	5.83	128.09	120.28
32	U	227	GLY	C-N-CA	5.83	128.09	120.28
19	M	389	ALA	CA-C-N	5.82	128.08	120.28
19	M	389	ALA	C-N-CA	5.82	128.08	120.28
23	T	164	LEU	N-CA-CB	5.82	118.68	110.12
31	R	96	GLN	N-CA-CB	5.82	120.06	110.39
1	A	8	THR	O-C-N	-5.82	115.95	122.12
14	7	125	GLN	OE1-CD-NE2	-5.82	116.78	122.60
5	E	85	ARG	CA-C-N	5.82	128.01	120.44
5	E	85	ARG	C-N-CA	5.82	128.01	120.44
8	1	195	GLN	O-C-N	5.82	128.06	122.07
28	S	286	TYR	N-CA-CB	5.82	119.09	110.53
33	O	288	ARG	NE-CZ-NH1	5.82	127.32	121.50
5	e	189	GLU	CB-CA-C	-5.82	101.13	110.79
12	l	106	ARG	CA-C-N	5.82	128.55	120.29
12	l	106	ARG	C-N-CA	5.82	128.55	120.29
1	A	53	LYS	N-CA-C	-5.82	105.68	112.89
16	I	349	LEU	N-CA-CB	5.82	119.90	110.42
25	Y	38	PHE	O-C-N	-5.82	114.94	120.70
9	i	88	PHE	N-CA-CB	5.82	118.67	110.12
21	W	193	GLU	CA-C-O	-5.82	114.87	120.92
26	Z	751	ASP	N-CA-C	-5.82	104.86	111.14
4	d	124	VAL	N-CA-C	-5.81	99.39	108.81
12	l	9	GLN	N-CA-CB	5.81	118.78	110.06
20	J	68	PRO	CA-C-N	5.81	129.43	120.07
20	J	68	PRO	C-N-CA	5.81	129.43	120.07
24	X	31	GLY	N-CA-C	5.81	121.61	111.78
32	U	29	GLU	CA-C-N	5.81	130.83	122.40
32	U	29	GLU	C-N-CA	5.81	130.83	122.40
5	e	138	GLY	N-CA-C	-5.81	102.60	110.80
10	j	139	GLY	CA-C-N	5.81	128.54	120.29
10	j	139	GLY	C-N-CA	5.81	128.54	120.29
12	l	128	CYS	CA-C-O	-5.81	113.87	120.32
6	F	52	ALA	N-CA-C	5.81	117.70	111.36
27	N	96	GLN	O-C-N	-5.81	115.81	122.09
27	N	489	MET	N-CA-C	-5.81	105.77	112.92
27	N	673	PRO	CA-N-CD	5.81	120.14	112.00
1	a	178	LYS	N-CA-C	-5.81	104.86	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	33	ILE	N-CA-C	-5.81	100.11	108.53
33	O	353	VAL	O-C-N	5.81	129.21	122.99
14	n	110	LEU	N-CA-CB	5.81	119.01	110.35
2	B	90	ARG	CA-C-O	-5.81	114.72	120.82
14	7	154	LEU	CA-C-N	5.81	128.06	120.28
14	7	154	LEU	C-N-CA	5.81	128.06	120.28
23	T	88	TYR	CA-C-N	5.81	129.14	120.31
23	T	88	TYR	C-N-CA	5.81	129.14	120.31
27	N	790	GLU	CA-C-N	5.81	128.06	120.28
27	N	790	GLU	C-N-CA	5.81	128.06	120.28
9	i	195	VAL	CA-C-O	-5.81	115.57	121.67
2	B	207	ASP	CA-C-O	5.81	126.68	120.70
3	C	208	ASP	CA-C-O	5.81	126.31	119.28
15	H	192	ASP	O-C-N	-5.81	114.64	121.32
20	J	226	GLY	N-CA-C	-5.81	107.71	115.32
27	N	296	CYS	CA-C-O	-5.81	114.27	120.42
30	Q	378	SER	CA-C-N	5.81	128.53	120.29
30	Q	378	SER	C-N-CA	5.81	128.53	120.29
13	6	145	LEU	N-CA-C	-5.80	104.55	111.69
27	N	236	GLY	CA-C-O	-5.80	114.51	120.66
1	a	210	SER	N-CA-C	-5.80	101.34	109.69
23	T	251	HIS	ND1-CE1-NE2	5.80	114.20	108.40
29	P	96	MET	CA-C-N	5.80	130.13	120.62
29	P	96	MET	C-N-CA	5.80	130.13	120.62
33	O	235	HIS	CE1-NE2-CD2	-5.80	103.20	109.00
16	I	130	VAL	CB-CA-C	-5.80	103.25	111.19
2	b	190	HIS	ND1-CE1-NE2	5.80	114.20	108.40
4	d	214	LYS	CA-C-O	-5.80	114.88	120.97
9	i	203	TYR	CA-C-N	5.80	128.99	120.82
9	i	203	TYR	C-N-CA	5.80	128.99	120.82
20	J	150	VAL	CA-C-N	5.80	128.96	121.13
20	J	150	VAL	C-N-CA	5.80	128.96	121.13
31	R	69	GLU	N-CA-CB	5.80	120.01	110.39
1	a	39	LYS	N-CA-C	-5.79	104.88	111.14
5	e	23	ILE	O-C-N	5.79	127.49	121.87
17	K	384	ALA	CA-C-O	-5.79	114.41	120.55
6	F	116	GLN	N-CA-C	-5.79	104.87	111.07
16	I	103	PRO	N-CD-CG	5.79	110.75	103.80
18	L	401	PHE	CA-C-N	5.79	128.04	120.28
18	L	401	PHE	C-N-CA	5.79	128.04	120.28
21	W	80	GLN	N-CA-C	-5.79	98.84	108.34
14	7	48	ASN	N-CA-C	-5.79	105.88	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	330	VAL	CA-C-O	5.79	126.19	119.36
28	S	132	ALA	CA-C-N	5.79	128.51	120.29
28	S	132	ALA	C-N-CA	5.79	128.51	120.29
30	Q	409	TYR	CD1-CG-CD2	5.79	126.78	118.10
17	K	258	PHE	CA-CB-CG	-5.79	108.01	113.80
26	Z	590	ALA	CA-C-N	5.79	130.88	121.62
26	Z	590	ALA	C-N-CA	5.79	130.88	121.62
9	2	52	THR	CA-CB-OG1	5.79	118.28	109.60
2	B	142	PHE	CA-CB-CG	5.79	119.58	113.80
3	C	24	ALA	N-CA-C	-5.79	104.94	112.23
4	D	209	GLU	CA-C-O	5.79	126.84	120.71
24	X	61	LEU	O-C-N	5.79	130.28	122.59
5	e	157	TYR	N-CA-CB	5.78	120.00	110.69
6	F	20	GLN	CA-C-N	5.78	127.85	120.56
6	F	20	GLN	C-N-CA	5.78	127.85	120.56
26	Z	956	LEU	N-CA-CB	5.78	119.79	110.65
27	N	697	PHE	CA-C-N	5.78	126.36	120.00
27	N	697	PHE	C-N-CA	5.78	126.36	120.00
28	S	423	VAL	CA-C-N	5.78	128.03	120.28
28	S	423	VAL	C-N-CA	5.78	128.03	120.28
3	c	215	ILE	N-CA-C	-5.78	98.09	107.28
11	k	166	GLN	N-CA-C	-5.78	105.06	111.36
20	J	55	VAL	CA-C-O	-5.78	114.94	120.95
7	G	10	VAL	N-CA-C	-5.78	99.80	108.12
7	G	136	GLY	CA-C-O	-5.78	115.31	121.38
15	H	314	VAL	N-CA-CB	5.78	120.77	111.23
18	L	68	ARG	CA-C-N	5.78	128.02	120.28
18	L	68	ARG	C-N-CA	5.78	128.02	120.28
26	Z	156	HIS	ND1-CE1-NE2	5.78	114.18	108.40
27	N	325	PHE	CA-C-N	5.78	128.02	120.28
27	N	325	PHE	C-N-CA	5.78	128.02	120.28
8	h	190	PRO	N-CA-C	-5.78	106.15	114.18
11	4	100	VAL	N-CA-C	-5.78	99.73	108.17
14	7	152	ASN	CA-C-N	5.78	125.46	119.05
14	7	152	ASN	C-N-CA	5.78	125.46	119.05
15	H	414	SER	CA-C-N	5.78	130.01	120.94
15	H	414	SER	C-N-CA	5.78	130.01	120.94
19	M	388	GLY	O-C-N	5.78	127.74	122.19
7	g	141	GLY	N-CA-C	5.78	117.39	111.56
1	A	175	ASN	O-C-N	5.78	128.24	122.12
17	K	169	VAL	CA-C-N	5.78	127.95	120.44
17	K	169	VAL	C-N-CA	5.78	127.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	153	ALA	CA-C-O	-5.77	114.43	120.55
11	k	107	TYR	CA-C-O	5.77	126.54	120.36
14	7	158	VAL	CA-C-O	-5.77	115.27	121.27
18	L	108	VAL	CA-CB-CG2	-5.77	100.59	110.40
26	Z	617	ILE	CA-C-N	5.77	127.94	120.44
26	Z	617	ILE	C-N-CA	5.77	127.94	120.44
27	N	424	LYS	CA-C-N	5.77	128.49	120.29
27	N	424	LYS	C-N-CA	5.77	128.49	120.29
28	S	389	LYS	CA-C-O	5.77	126.88	120.82
31	R	244	THR	N-CA-CB	5.77	118.52	110.04
32	U	202	SER	CA-C-N	5.77	127.94	120.44
32	U	202	SER	C-N-CA	5.77	127.94	120.44
4	D	228	ASN	CA-C-N	5.77	127.94	120.44
4	D	228	ASN	C-N-CA	5.77	127.94	120.44
19	M	233	ARG	O-C-N	-5.77	115.57	122.15
22	V	234	GLU	CA-C-N	5.77	127.94	120.44
22	V	234	GLU	C-N-CA	5.77	127.94	120.44
31	R	125	GLU	N-CA-CB	5.77	120.24	110.49
10	j	135	PHE	N-CA-CB	5.77	120.50	111.56
2	B	214	ILE	N-CA-C	-5.77	97.34	109.34
17	K	379	SER	CA-C-N	5.77	127.35	120.14
17	K	379	SER	C-N-CA	5.77	127.35	120.14
15	H	374	LYS	N-CA-CB	5.77	120.50	110.81
27	N	797	GLU	N-CA-C	-5.77	104.90	111.07
28	S	38	LEU	CA-C-N	5.77	128.48	120.29
28	S	38	LEU	C-N-CA	5.77	128.48	120.29
30	Q	33	LYS	CA-C-N	5.77	127.94	120.44
30	Q	33	LYS	C-N-CA	5.77	127.94	120.44
33	O	175	ASN	O-C-N	5.77	128.23	122.12
31	R	150	ALA	N-CA-C	-5.77	104.91	111.14
6	f	54	GLU	CA-C-N	5.76	128.47	120.29
6	f	54	GLU	C-N-CA	5.76	128.47	120.29
17	K	86	VAL	CB-CA-C	-5.76	102.92	112.26
18	L	103	GLN	CA-C-O	-5.76	115.10	121.33
19	M	377	GLN	CB-CG-CD	-5.76	102.80	112.60
27	N	197	VAL	CB-CA-C	-5.76	103.31	111.21
33	O	253	GLN	CA-C-N	5.76	127.93	120.44
33	O	253	GLN	C-N-CA	5.76	127.93	120.44
3	c	133	SER	N-CA-C	-5.76	99.51	108.90
8	h	51	ASP	N-CA-C	-5.76	104.92	111.14
9	i	7	LYS	N-CA-C	-5.76	101.16	110.32
11	k	160	LEU	O-C-N	5.76	128.23	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	580	GLN	OE1-CD-NE2	-5.76	116.84	122.60
27	N	533	ASP	CA-CB-CG	-5.76	106.84	112.60
9	i	118	SER	N-CA-CB	5.76	118.53	109.83
10	3	49	PHE	N-CA-CB	5.76	120.85	110.83
11	4	193	ASP	CA-C-N	5.76	128.89	120.71
11	4	193	ASP	C-N-CA	5.76	128.89	120.71
4	d	176	ASN	CB-CA-C	-5.76	99.17	109.24
2	B	43	VAL	N-CA-C	-5.76	100.75	108.35
9	2	88	PHE	CA-CB-CG	5.76	119.56	113.80
16	I	131	SER	N-CA-C	-5.76	100.80	109.95
22	V	241	THR	CA-C-N	5.76	127.99	120.28
22	V	241	THR	C-N-CA	5.76	127.99	120.28
3	c	117	ILE	N-CA-C	-5.75	104.91	110.72
18	L	267	PHE	CA-C-N	5.75	129.06	120.31
18	L	267	PHE	C-N-CA	5.75	129.06	120.31
19	M	43	ILE	CA-C-N	5.75	127.99	120.28
19	M	43	ILE	C-N-CA	5.75	127.99	120.28
31	R	70	TYR	CG-CD1-CE1	5.75	129.83	121.20
9	i	56	THR	N-CA-CB	5.75	118.58	110.12
9	i	196	ARG	N-CA-CB	5.75	120.22	110.49
11	k	86	GLN	OE1-CD-NE2	5.75	128.35	122.60
2	B	87	ASP	CA-C-N	5.75	128.31	120.54
2	B	87	ASP	C-N-CA	5.75	128.31	120.54
8	l	123	PRO	O-C-N	5.75	130.25	122.37
16	I	134	SER	CB-CA-C	-5.75	108.94	115.79
3	c	88	ASN	OD1-CG-ND2	-5.75	116.85	122.60
7	G	237	ASP	O-C-N	5.75	127.99	122.07
8	l	164	LYS	O-C-N	5.75	128.22	122.12
16	I	266	GLN	CA-C-N	5.75	128.02	120.60
16	I	266	GLN	C-N-CA	5.75	128.02	120.60
23	T	170	ASN	CA-CB-CG	5.75	118.35	112.60
26	Z	618	GLN	N-CA-C	-5.75	104.92	111.07
27	N	653	ARG	NE-CZ-NH2	-5.75	114.02	119.20
4	d	79	ASP	N-CA-C	-5.75	105.01	111.28
9	i	99	ILE	N-CA-CB	5.75	117.94	111.21
1	a	92	ALA	O-C-N	5.75	128.21	122.12
15	H	392	HIS	ND1-CE1-NE2	5.75	114.15	108.40
23	T	38	ASN	CA-CB-CG	-5.75	106.85	112.60
23	T	105	LEU	CA-C-O	-5.75	114.33	120.42
25	Y	80	GLU	N-CA-C	-5.75	105.01	111.28
1	a	176	HIS	CE1-NE2-CD2	-5.75	103.25	109.00
6	F	156	TYR	N-CA-C	-5.75	106.81	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	31	CYS	N-CA-C	-5.75	98.56	110.80
15	H	351	VAL	N-CA-C	-5.75	99.36	107.75
27	N	669	GLU	CB-CG-CD	-5.75	102.83	112.60
33	O	326	HIS	CA-C-N	5.75	128.30	120.54
33	O	326	HIS	C-N-CA	5.75	128.30	120.54
22	V	269	ARG	N-CA-C	5.75	117.22	111.07
14	n	160	ASP	CA-CB-CG	5.74	118.34	112.60
21	W	172	LEU	O-C-N	5.74	130.05	123.27
27	N	295	THR	N-CA-CB	5.74	119.92	110.39
22	V	35	LEU	CA-C-N	5.74	129.04	120.31
22	V	35	LEU	C-N-CA	5.74	129.04	120.31
21	W	39	ALA	CA-C-N	5.74	127.97	120.28
21	W	39	ALA	C-N-CA	5.74	127.97	120.28
23	T	96	LEU	N-CA-C	-5.74	103.99	111.74
23	T	182	LYS	N-CA-CB	5.74	118.33	110.01
24	X	87	PHE	N-CA-CB	5.74	119.12	109.94
6	f	88	ARG	N-CA-CB	5.74	118.56	110.12
9	2	57	GLN	CA-C-N	5.74	128.44	120.29
9	2	57	GLN	C-N-CA	5.74	128.44	120.29
22	V	86	VAL	CA-C-N	5.74	128.44	120.29
22	V	86	VAL	C-N-CA	5.74	128.44	120.29
32	U	265	LEU	N-CA-C	-5.74	105.16	111.82
9	2	30	ASN	CA-CB-CG	-5.74	106.86	112.60
14	7	89	PRO	CA-N-CD	5.74	120.03	112.00
21	W	130	LYS	N-CA-CB	5.74	119.75	110.40
30	Q	231	ASP	N-CA-C	-5.74	100.05	109.40
9	i	134	ALA	O-C-N	5.74	128.28	122.09
1	A	25	ALA	N-CA-CB	5.74	119.05	110.22
1	A	52	ASP	N-CA-C	-5.74	101.53	110.42
17	K	310	THR	N-CA-C	-5.74	104.95	111.14
23	T	177	PHE	N-CA-C	-5.74	106.93	114.04
27	N	439	VAL	O-C-N	-5.74	116.31	121.87
5	e	206	GLU	CB-CA-C	-5.73	100.51	110.09
9	2	52	THR	N-CA-CB	5.73	118.32	110.01
15	H	64	LYS	CA-C-N	5.73	127.96	120.28
15	H	64	LYS	C-N-CA	5.73	127.96	120.28
33	O	314	SER	O-C-N	5.73	128.20	122.12
4	d	184	ALA	N-CA-C	-5.73	103.88	111.96
11	k	190	ARG	CA-C-N	5.73	131.24	122.93
11	k	190	ARG	C-N-CA	5.73	131.24	122.93
6	F	185	PRO	CA-C-N	5.73	128.24	120.44
6	F	185	PRO	C-N-CA	5.73	128.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	4	ILE	N-CA-C	-5.73	99.87	108.12
16	I	360	LYS	N-CA-CB	5.73	118.64	110.16
18	L	138	SER	N-CA-C	-5.73	106.45	113.50
27	N	319	SER	N-CA-C	5.73	117.33	111.14
4	d	52	LEU	N-CA-CB	5.73	123.13	113.10
5	e	107	SER	N-CA-C	-5.73	105.12	111.36
12	5	27	ALA	N-CA-C	-5.73	105.40	112.90
15	H	255	GLY	CA-C-N	5.73	127.96	120.28
15	H	255	GLY	C-N-CA	5.73	127.96	120.28
18	L	376	PHE	CA-C-N	5.73	127.89	120.44
18	L	376	PHE	C-N-CA	5.73	127.89	120.44
28	S	314	ASN	CA-C-N	5.73	127.95	120.28
28	S	314	ASN	C-N-CA	5.73	127.95	120.28
28	S	404	LEU	CA-C-O	5.73	126.56	119.97
1	a	221	LYS	CB-CA-C	-5.73	100.97	109.90
29	P	40	LEU	CA-C-N	5.73	128.30	120.46
29	P	40	LEU	C-N-CA	5.73	128.30	120.46
10	j	35	VAL	CA-CB-CG1	-5.72	100.67	110.40
13	m	63	ALA	N-CA-C	5.72	117.52	111.28
4	D	119	THR	CA-C-N	-5.72	111.15	120.71
4	D	119	THR	C-N-CA	-5.72	111.15	120.71
15	H	379	LEU	O-C-N	-5.72	114.74	121.32
18	L	268	ALA	CA-C-N	5.72	128.42	120.29
18	L	268	ALA	C-N-CA	5.72	128.42	120.29
26	Z	936	VAL	O-C-N	5.72	129.63	122.59
27	N	619	CYS	N-CA-C	5.72	117.60	111.36
27	N	892	PRO	CA-C-N	5.72	127.77	120.56
27	N	892	PRO	C-N-CA	5.72	127.77	120.56
28	S	206	GLN	CB-CG-CD	-5.72	102.87	112.60
30	Q	89	ALA	CA-C-O	-5.72	114.95	121.65
31	R	330	VAL	CA-C-N	5.72	127.95	120.28
31	R	330	VAL	C-N-CA	5.72	127.95	120.28
4	d	51	LYS	CB-CG-CD	5.72	124.46	111.30
11	k	107	TYR	O-C-N	-5.72	116.70	123.22
13	m	27	THR	N-CA-C	-5.72	105.96	113.17
19	M	413	GLU	CB-CA-C	-5.72	101.29	110.79
23	T	196	SER	CB-CA-C	-5.72	101.90	110.88
27	N	116	GLN	N-CA-C	-5.72	106.14	113.23
30	Q	21	ASN	N-CA-C	5.72	117.52	111.28
32	U	112	LYS	CA-C-N	5.72	128.22	120.44
32	U	112	LYS	C-N-CA	5.72	128.22	120.44
33	O	195	TYR	N-CA-C	-5.72	105.12	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	69	ILE	N-CA-C	-5.72	104.78	110.62
20	J	150	VAL	CA-C-O	-5.72	114.44	120.39
12	l	57	THR	N-CA-CB	5.72	118.62	110.16
24	X	111	LEU	O-C-N	-5.72	116.62	123.31
28	S	429	ASP	CA-CB-CG	-5.72	106.88	112.60
4	d	107	LEU	N-CA-CB	5.72	118.53	110.12
2	B	249	ALA	CB-CA-C	-5.72	100.90	110.56
26	Z	968	ASP	N-CA-CB	5.72	119.53	110.55
29	P	6	PRO	CA-N-CD	-5.72	104.00	112.00
1	A	200	HIS	CA-CB-CG	5.72	119.52	113.80
18	L	77	ARG	CA-C-O	5.72	126.48	120.42
4	D	178	ASP	N-CA-C	-5.71	100.37	109.23
19	M	340	SER	N-CA-CB	5.71	118.37	109.85
27	N	774	ASN	OD1-CG-ND2	-5.71	116.89	122.60
33	O	23	HIS	N-CA-CB	5.71	119.29	110.43
12	5	199	LYS	CA-C-N	5.71	128.29	120.46
12	5	199	LYS	C-N-CA	5.71	128.29	120.46
32	U	170	GLY	CA-C-N	5.71	128.29	120.46
32	U	170	GLY	C-N-CA	5.71	128.29	120.46
6	f	189	ILE	CA-C-N	5.71	127.94	120.28
6	f	189	ILE	C-N-CA	5.71	127.94	120.28
14	n	37	ASN	CB-CA-C	-5.71	98.46	109.37
21	W	162	ASN	CB-CA-C	-5.71	102.12	110.06
28	S	66	GLN	CA-C-O	-5.71	114.82	120.70
2	B	104	TYR	CA-C-O	-5.71	114.41	120.23
32	U	269	THR	CA-C-N	5.71	127.93	120.28
32	U	269	THR	C-N-CA	5.71	127.93	120.28
8	h	177	VAL	N-CA-C	-5.71	99.65	107.99
14	n	162	GLU	N-CA-C	-5.71	106.27	113.18
18	L	371	THR	N-CA-C	-5.71	105.90	112.92
16	I	266	GLN	N-CA-CB	5.71	118.51	110.12
26	Z	214	HIS	N-CA-C	5.71	118.44	111.82
26	Z	841	GLU	N-CA-C	-5.71	100.03	108.99
32	U	96	GLY	CA-C-O	-5.71	113.36	121.52
11	k	138	PHE	N-CA-C	5.71	117.50	111.28
4	d	50	LEU	O-C-N	-5.70	116.52	123.19
2	B	170	ALA	CA-C-N	5.70	127.92	120.28
2	B	170	ALA	C-N-CA	5.70	127.92	120.28
11	4	74	GLU	N-CA-CB	5.70	118.96	110.29
15	H	195	VAL	N-CA-C	-5.70	104.96	110.72
23	T	87	PRO	N-CA-C	5.70	121.35	113.65
27	N	706	MET	N-CA-CB	5.70	118.44	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	PHE	N-CA-C	-5.70	100.53	109.25
31	R	173	THR	CA-C-N	5.70	127.86	120.56
31	R	173	THR	C-N-CA	5.70	127.86	120.56
24	X	107	GLY	O-C-N	-5.70	116.58	122.68
1	a	176	HIS	ND1-CE1-NE2	5.70	114.10	108.40
10	3	7	ASN	CA-CB-CG	-5.70	106.90	112.60
21	W	116	SER	CA-C-O	-5.70	115.00	120.64
21	W	88	ALA	N-CA-C	-5.70	104.97	111.07
26	Z	593	HIS	CA-CB-CG	5.70	119.50	113.80
14	n	52	GLY	O-C-N	-5.70	119.22	123.61
10	3	114	LYS	N-CA-C	-5.70	106.33	113.28
26	Z	70	ALA	CA-C-N	5.70	128.23	120.54
26	Z	70	ALA	C-N-CA	5.70	128.23	120.54
30	Q	278	VAL	CA-C-N	5.70	128.38	120.29
30	Q	278	VAL	C-N-CA	5.70	128.38	120.29
8	h	122	LEU	CA-C-O	5.69	125.58	120.34
26	Z	459	ALA	CB-CA-C	-5.69	99.23	110.27
2	b	223	GLY	N-CA-C	-5.69	107.47	115.32
6	F	163	ARG	CA-C-N	5.69	130.22	120.72
6	F	163	ARG	C-N-CA	5.69	130.22	120.72
13	6	50	ILE	N-CA-CB	5.69	119.83	111.52
7	G	189	VAL	CA-C-N	5.69	127.90	120.28
7	G	189	VAL	C-N-CA	5.69	127.90	120.28
8	h	69	GLN	O-C-N	5.69	128.60	122.34
2	B	139	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
8	1	52	THR	N-CA-CB	5.69	119.09	110.28
20	J	337	LEU	CA-C-O	5.69	127.45	121.19
23	T	109	TYR	O-C-N	5.69	128.15	122.12
26	Z	865	ASP	O-C-N	5.69	130.25	122.46
27	N	276	GLU	CA-C-O	-5.69	114.85	120.82
29	P	62	ILE	CA-CB-CG1	5.69	120.07	110.40
26	Z	752	ILE	CA-C-N	5.69	127.25	120.14
26	Z	752	ILE	C-N-CA	5.69	127.25	120.14
27	N	593	PHE	N-CA-C	5.69	117.56	111.36
31	R	355	SER	CA-C-N	5.68	128.36	120.29
31	R	355	SER	C-N-CA	5.68	128.36	120.29
13	m	130	SER	N-CA-C	5.68	118.31	110.35
18	L	323	ILE	N-CA-C	-5.68	99.99	108.46
20	J	137	MET	CA-C-N	5.68	127.83	120.44
20	J	137	MET	C-N-CA	5.68	127.83	120.44
31	R	245	SER	CA-C-N	5.68	128.46	120.28
31	R	245	SER	C-N-CA	5.68	128.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	87	ILE	N-CA-C	-5.68	104.98	110.72
5	e	136	ILE	CB-CA-C	5.68	119.09	111.19
6	f	18	LEU	CA-C-N	5.68	128.36	120.29
6	f	18	LEU	C-N-CA	5.68	128.36	120.29
1	A	17	TYR	CA-C-N	5.68	128.36	120.29
1	A	17	TYR	C-N-CA	5.68	128.36	120.29
6	F	56	SER	N-CA-CB	5.68	118.72	109.69
4	d	121	SER	O-C-N	5.68	129.66	123.13
8	h	120	HIS	ND1-CE1-NE2	5.68	114.08	108.40
13	6	102	PHE	CA-CB-CG	-5.68	108.12	113.80
15	H	148	ASN	N-CA-C	-5.68	99.03	108.34
19	M	356	SER	CA-C-N	5.68	127.82	120.44
19	M	356	SER	C-N-CA	5.68	127.82	120.44
21	W	55	ALA	N-CA-C	5.68	118.08	110.35
26	Z	867	PHE	CA-C-N	5.68	127.89	120.28
26	Z	867	PHE	C-N-CA	5.68	127.89	120.28
33	O	13	THR	N-CA-CB	5.68	118.31	110.07
1	A	43	VAL	CA-C-O	5.68	126.50	120.48
14	7	210	LYS	O-C-N	5.68	129.42	123.06
7	g	243	ILE	O-C-N	5.68	129.95	122.12
14	n	21	ILE	N-CA-C	-5.68	99.94	108.12
28	S	124	GLU	CA-C-O	5.68	126.44	120.42
8	1	168	SER	N-CA-CB	5.67	119.04	110.30
18	L	229	THR	N-CA-C	-5.67	105.17	111.36
24	X	83	SER	CA-C-O	5.67	127.34	120.99
6	f	125	ARG	CA-C-O	-5.67	113.90	120.03
23	T	184	ALA	CB-CA-C	-5.67	101.37	110.79
26	Z	299	ASP	CA-C-N	5.67	128.45	120.28
26	Z	299	ASP	C-N-CA	5.67	128.45	120.28
4	d	125	ARG	CA-C-N	5.67	125.62	119.78
4	d	125	ARG	C-N-CA	5.67	125.62	119.78
13	m	22	VAL	CA-CB-CG2	5.67	120.04	110.40
5	E	25	LEU	O-C-N	5.67	128.62	122.15
5	E	78	ARG	N-CA-CB	5.67	118.65	110.20
17	K	40	LEU	CA-C-N	5.67	127.88	120.28
17	K	40	LEU	C-N-CA	5.67	127.88	120.28
27	N	133	LEU	CA-C-N	5.67	127.81	120.44
27	N	133	LEU	C-N-CA	5.67	127.81	120.44
27	N	800	ALA	N-CA-C	5.67	117.46	111.28
31	R	408	ASP	CA-CB-CG	-5.67	106.93	112.60
4	D	215	PRO	CA-C-N	5.67	130.19	122.19
4	D	215	PRO	C-N-CA	5.67	130.19	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	235	PHE	N-CA-CB	5.67	118.55	110.16
6	F	76	LEU	CB-CA-C	5.67	118.34	109.84
14	7	59	ASP	CA-C-N	5.67	127.88	120.28
14	7	59	ASP	C-N-CA	5.67	127.88	120.28
27	N	703	GLN	CA-C-N	5.67	127.22	120.14
27	N	703	GLN	C-N-CA	5.67	127.22	120.14
31	R	161	ALA	CA-C-O	5.67	126.53	120.46
31	R	332	GLU	CB-CA-C	-5.67	101.98	110.88
31	R	417	TYR	CA-C-N	5.67	126.11	119.94
31	R	417	TYR	C-N-CA	5.67	126.11	119.94
32	U	212	ASP	CB-CA-C	-5.67	101.22	110.85
12	5	38	ASN	CA-CB-CG	5.67	118.27	112.60
17	K	152	PRO	CA-C-N	5.67	127.87	120.28
17	K	152	PRO	C-N-CA	5.67	127.87	120.28
2	b	163	ALA	CA-C-N	5.66	131.70	122.69
2	b	163	ALA	C-N-CA	5.66	131.70	122.69
17	K	420	THR	CA-C-N	5.66	128.19	120.77
17	K	420	THR	C-N-CA	5.66	128.19	120.77
27	N	345	ASP	O-C-N	5.66	129.88	123.42
30	Q	9	GLU	CA-C-N	5.66	127.80	120.44
30	Q	9	GLU	C-N-CA	5.66	127.80	120.44
32	U	70	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
26	Z	257	PRO	N-CA-C	5.66	117.61	110.70
26	Z	360	SER	O-C-N	5.66	128.12	122.12
28	S	401	LYS	N-CA-C	-5.66	99.29	108.52
31	R	135	ILE	O-C-N	5.66	127.36	121.87
11	4	17	SER	CA-C-N	5.66	128.74	120.71
11	4	17	SER	C-N-CA	5.66	128.74	120.71
18	L	99	GLN	N-CA-C	-5.66	106.21	113.23
19	M	312	LEU	CA-C-N	5.66	129.14	121.05
19	M	312	LEU	C-N-CA	5.66	129.14	121.05
3	c	181	ASP	CA-CB-CG	-5.66	106.94	112.60
13	m	108	HIS	CA-CB-CG	-5.66	108.14	113.80
13	m	213	ARG	NE-CZ-NH1	5.66	127.16	121.50
8	1	128	GLY	CA-C-N	5.66	128.13	120.44
8	1	128	GLY	C-N-CA	5.66	128.13	120.44
20	J	249	GLU	N-CA-C	-5.66	98.75	110.80
23	T	81	TYR	N-CA-C	-5.66	105.03	111.14
17	K	172	ALA	CA-C-N	5.66	128.91	120.31
17	K	172	ALA	C-N-CA	5.66	128.91	120.31
20	J	40	ASN	CB-CG-ND2	5.66	124.88	116.40
2	b	6	SER	CA-C-N	5.65	128.74	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	6	SER	C-N-CA	5.65	128.74	120.71
5	E	149	HIS	N-CA-C	-5.65	99.07	108.34
11	4	183	ILE	CA-CB-CG2	-5.65	100.89	110.50
31	R	190	LYS	N-CA-CB	5.65	118.53	110.16
33	O	264	ASP	CB-CA-C	5.65	120.46	110.85
33	O	382	LYS	CA-C-N	5.65	127.79	120.44
33	O	382	LYS	C-N-CA	5.65	127.79	120.44
10	j	88	GLN	CA-C-N	5.65	127.85	120.28
10	j	88	GLN	C-N-CA	5.65	127.85	120.28
18	L	229	THR	CA-CB-OG1	5.65	118.08	109.60
20	J	163	VAL	CA-C-O	-5.65	114.66	120.71
32	U	19	LEU	N-CA-C	5.65	117.12	111.07
33	O	213	LEU	CA-C-N	5.65	127.85	120.28
33	O	213	LEU	C-N-CA	5.65	127.85	120.28
10	j	98	ARG	CA-C-O	5.65	126.59	120.55
29	P	141	LYS	CA-C-N	5.65	128.89	120.31
29	P	141	LYS	C-N-CA	5.65	128.89	120.31
6	f	189	ILE	CA-CB-CG1	5.65	120.00	110.40
6	F	217	LYS	O-C-N	5.65	127.89	122.07
11	k	82	SER	O-C-N	-5.64	116.14	122.12
13	6	145	LEU	CB-CA-C	-5.64	100.37	110.70
7	g	102	PRO	O-C-N	5.64	129.73	122.85
7	g	114	GLN	OE1-CD-NE2	5.64	128.24	122.60
8	1	92	ASN	OD1-CG-ND2	5.64	128.24	122.60
31	R	134	TRP	CB-CG-CD2	-5.64	118.90	126.80
4	d	164	ARG	NE-CZ-NH2	5.64	124.28	119.20
4	D	145	LEU	N-CA-C	-5.64	98.71	108.69
19	M	277	ILE	N-CA-CB	5.64	119.76	111.52
11	4	104	ILE	N-CA-C	-5.64	99.42	107.77
16	I	121	THR	O-C-N	-5.64	115.90	123.23
27	N	875	LEU	O-C-N	-5.64	115.11	121.43
32	U	225	ILE	N-CA-C	-5.64	104.87	110.62
9	i	217	ILE	N-CA-C	-5.64	102.25	109.30
11	k	2	ASP	N-CA-CB	5.64	118.25	109.85
16	I	225	PRO	CA-C-O	-5.64	115.12	121.43
3	c	145	TYR	N-CA-CB	5.63	118.32	110.04
7	G	7	SER	CA-C-N	5.63	128.71	120.71
7	G	7	SER	C-N-CA	5.63	128.71	120.71
9	2	210	THR	CA-C-O	-5.63	115.67	121.87
21	W	117	PRO	CA-C-O	-5.63	110.34	120.60
24	X	130	ASN	OD1-CG-ND2	5.63	128.23	122.60
26	Z	142	ASP	CA-C-O	5.63	127.52	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	268	ALA	CA-C-N	5.63	128.10	120.38
26	Z	268	ALA	C-N-CA	5.63	128.10	120.38
27	N	30	ASN	N-CA-C	-5.63	105.22	111.36
27	N	134	THR	CA-C-O	5.63	126.74	120.82
12	l	107	LYS	N-CA-C	-5.63	105.22	111.36
27	N	167	GLU	CA-C-N	5.63	128.29	120.29
27	N	167	GLU	C-N-CA	5.63	128.29	120.29
3	c	11	ILE	CA-C-N	5.63	129.25	120.75
3	c	11	ILE	C-N-CA	5.63	129.25	120.75
2	B	191	ILE	CA-C-N	5.63	128.10	120.44
2	B	191	ILE	C-N-CA	5.63	128.10	120.44
5	E	111	LEU	CA-C-O	-5.63	112.68	119.27
6	F	142	HIS	CG-ND1-CE1	-5.63	99.73	109.30
27	N	340	HIS	N-CA-C	-5.63	105.72	112.59
26	Z	511	PRO	N-CA-C	-5.63	100.60	111.69
1	a	84	ALA	CA-C-N	5.63	127.82	120.28
1	a	84	ALA	C-N-CA	5.63	127.82	120.28
6	f	104	VAL	N-CA-C	-5.63	105.02	110.42
26	Z	10	GLN	N-CA-C	-5.63	105.29	111.82
28	S	203	SER	O-C-N	5.63	128.80	122.22
28	S	434	ALA	CA-C-O	-5.63	115.15	121.40
30	Q	242	SER	CA-C-N	5.63	128.14	120.54
30	Q	242	SER	C-N-CA	5.63	128.14	120.54
33	O	270	ILE	CA-CB-CG1	5.63	119.97	110.40
6	f	219	THR	N-CA-C	-5.63	96.58	108.73
2	B	123	GLN	CA-C-N	5.63	129.34	121.24
2	B	123	GLN	C-N-CA	5.63	129.34	121.24
10	3	113	SER	N-CA-CB	5.63	119.30	110.46
17	K	64	GLN	CA-C-N	5.63	128.28	120.29
17	K	64	GLN	C-N-CA	5.63	128.28	120.29
18	L	158	ILE	O-C-N	-5.63	116.08	122.72
19	M	236	ALA	CA-C-O	-5.63	114.91	120.82
23	T	74	ASN	CA-C-N	5.63	128.14	120.54
23	T	74	ASN	C-N-CA	5.63	128.14	120.54
24	X	31	GLY	O-C-N	-5.63	116.75	122.60
14	7	7	THR	CA-C-N	5.62	128.46	122.38
14	7	7	THR	C-N-CA	5.62	128.46	122.38
28	S	199	GLU	O-C-N	5.62	129.63	123.22
1	a	58	THR	N-CA-CB	5.62	119.00	110.28
2	b	214	ILE	O-C-N	-5.62	115.51	122.88
5	e	95	TYR	CB-CA-C	-5.62	99.23	110.42
11	k	41	HIS	CE1-NE2-CD2	-5.62	103.38	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	206	THR	N-CA-C	-5.62	100.51	109.23
10	3	48	VAL	N-CA-C	-5.62	101.56	109.21
14	7	229	GLY	CA-C-O	-5.62	108.99	120.80
26	Z	608	TYR	CA-C-O	5.62	126.08	119.28
27	N	768	ILE	O-C-N	-5.62	117.07	121.46
28	S	457	PRO	CA-N-CD	5.62	119.87	112.00
33	O	26	PHE	CA-C-O	-5.62	114.59	120.55
33	O	156	THR	CA-C-N	5.62	127.81	120.28
33	O	156	THR	C-N-CA	5.62	127.81	120.28
2	B	206	GLY	CA-C-N	5.62	128.09	120.44
2	B	206	GLY	C-N-CA	5.62	128.09	120.44
30	Q	55	GLU	CB-CG-CD	-5.62	103.04	112.60
19	M	349	PHE	O-C-N	-5.62	115.91	121.19
27	N	904	VAL	CA-CB-CG2	-5.62	100.85	110.40
9	i	35	HIS	ND1-CE1-NE2	5.62	114.02	108.40
19	M	166	ARG	CA-C-N	5.62	127.75	120.56
19	M	166	ARG	C-N-CA	5.62	127.75	120.56
20	J	202	VAL	N-CA-C	-5.62	105.03	110.42
29	P	29	GLN	N-CA-CB	5.62	118.38	110.12
29	P	282	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
29	P	417	HIS	N-CA-CB	5.62	118.48	110.16
33	O	187	SER	CA-C-N	5.62	128.12	120.54
33	O	187	SER	C-N-CA	5.62	128.12	120.54
13	m	111	ILE	O-C-N	-5.62	117.14	122.98
4	d	158	SER	CB-CA-C	-5.62	102.06	110.88
4	D	25	VAL	CA-C-O	-5.62	115.43	121.27
15	H	89	GLN	N-CA-C	-5.62	105.16	112.23
27	N	293	LEU	CA-C-N	5.62	125.72	119.32
27	N	293	LEU	C-N-CA	5.62	125.72	119.32
27	N	387	ALA	CA-C-O	-5.62	112.89	118.34
6	f	51	ASN	CA-C-N	5.61	127.74	120.44
6	f	51	ASN	C-N-CA	5.61	127.74	120.44
14	7	85	GLU	N-CA-C	-5.61	105.64	112.88
26	Z	177	THR	N-CA-C	-5.61	101.34	109.59
27	N	501	MET	N-CA-CB	5.61	118.15	110.01
7	g	199	ALA	CA-C-O	5.61	126.28	119.38
9	i	62	ASN	CA-CB-CG	-5.61	106.99	112.60
10	3	72	LEU	O-C-N	-5.61	116.17	122.12
10	3	142	SER	CA-C-N	5.61	127.74	120.44
10	3	142	SER	C-N-CA	5.61	127.74	120.44
9	2	88	PHE	CA-C-N	5.61	127.80	120.28
9	2	88	PHE	C-N-CA	5.61	127.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	170	ASN	OD1-CG-ND2	-5.61	116.99	122.60
28	S	467	PHE	CA-C-O	-5.61	114.60	120.55
12	l	8	PHE	N-CA-C	-5.61	100.99	108.34
13	m	182	LYS	N-CA-CB	5.61	118.36	110.12
23	T	235	PHE	CA-C-N	5.61	128.84	120.31
23	T	235	PHE	C-N-CA	5.61	128.84	120.31
10	3	133	LYS	N-CA-C	-5.61	104.20	111.71
26	Z	76	LYS	CA-C-N	5.61	128.84	120.31
26	Z	76	LYS	C-N-CA	5.61	128.84	120.31
1	a	232	ILE	N-CA-C	-5.61	105.06	110.72
4	D	113	GLY	CA-C-N	5.61	128.38	120.42
4	D	113	GLY	C-N-CA	5.61	128.38	120.42
10	3	80	ALA	CA-C-N	5.61	128.87	120.69
10	3	80	ALA	C-N-CA	5.61	128.87	120.69
29	P	267	PHE	CA-CB-CG	-5.61	108.19	113.80
30	Q	90	LYS	N-CA-C	-5.61	101.39	108.45
27	N	451	GLY	CA-C-N	5.60	127.79	120.28
27	N	451	GLY	C-N-CA	5.60	127.79	120.28
30	Q	274	LEU	N-CA-C	-5.60	99.77	108.90
8	h	157	HIS	N-CA-CB	5.60	118.13	110.01
30	Q	166	LYS	N-CA-C	-5.60	105.32	111.82
16	I	254	GLN	OE1-CD-NE2	5.60	128.20	122.60
19	M	117	ALA	CA-C-O	5.60	126.54	120.32
21	W	67	ALA	N-CA-C	-5.60	106.33	114.12
4	d	13	GLY	N-CA-C	-5.60	107.03	115.32
12	l	178	TYR	N-CA-C	-5.60	100.20	108.99
17	K	427	TYR	N-CA-CB	5.60	118.45	111.00
27	N	204	SER	CA-C-O	-5.60	114.61	120.55
31	R	141	TYR	CA-CB-CG	-5.60	103.82	113.90
9	i	160	GLN	CA-C-O	-5.60	114.62	120.55
10	j	27	ARG	O-C-N	-5.60	116.41	123.01
2	B	174	PHE	N-CA-C	-5.60	105.08	111.07
15	H	196	THR	CA-C-O	-5.60	113.53	119.97
16	I	323	LYS	CA-C-O	-5.60	115.21	121.81
30	Q	148	LYS	CG-CD-CE	5.60	124.17	111.30
1	A	94	GLU	CA-C-N	5.60	128.82	120.31
1	A	94	GLU	C-N-CA	5.60	128.82	120.31
5	e	179	TRP	CB-CG-CD2	-5.59	118.97	126.80
6	f	35	VAL	N-CA-CB	5.59	121.12	111.39
6	f	209	ASN	N-CA-C	-5.59	106.29	113.23
9	i	86	HIS	ND1-CE1-NE2	5.59	114.00	108.40
16	I	286	ALA	CA-C-N	5.59	127.72	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	286	ALA	C-N-CA	5.59	127.72	120.56
16	I	429	GLU	CA-C-N	5.59	128.81	120.31
16	I	429	GLU	C-N-CA	5.59	128.81	120.31
13	m	43	VAL	N-CA-C	5.59	116.29	109.30
22	V	294	SER	CA-C-O	-5.59	114.95	120.82
29	P	282	HIS	CA-CB-CG	-5.59	108.21	113.80
3	c	123	GLN	CA-CB-CG	5.59	125.28	114.10
4	D	132	LEU	N-CA-C	-5.59	100.07	109.07
19	M	366	ARG	CA-C-N	5.59	127.71	120.44
19	M	366	ARG	C-N-CA	5.59	127.71	120.44
21	W	109	ARG	NE-CZ-NH2	5.59	124.23	119.20
27	N	803	VAL	O-C-N	5.59	127.39	121.91
6	f	184	ASN	CA-CB-CG	-5.59	107.01	112.60
9	2	17	ASP	N-CA-C	-5.59	103.00	110.55
9	2	116	HIS	CA-CB-CG	-5.59	108.21	113.80
12	5	25	TRP	N-CA-CB	5.59	118.50	110.06
12	5	144	TYR	O-C-N	-5.59	116.07	122.89
22	V	147	VAL	N-CA-C	-5.59	107.53	112.90
26	Z	559	LYS	CA-C-N	5.59	128.23	120.29
26	Z	559	LYS	C-N-CA	5.59	128.23	120.29
28	S	205	ASN	O-C-N	5.59	128.52	122.15
1	a	101	TYR	CA-C-N	5.59	129.19	120.75
1	a	101	TYR	C-N-CA	5.59	129.19	120.75
6	F	61	LYS	N-CA-C	-5.59	107.46	114.56
5	e	10	GLU	CB-CA-C	-5.59	101.87	110.81
12	5	75	SER	CA-C-N	5.59	128.11	120.46
12	5	75	SER	C-N-CA	5.59	128.11	120.46
17	K	415	VAL	N-CA-CB	5.59	120.45	111.23
23	T	148	LEU	N-CA-CB	5.59	118.11	110.01
29	P	216	LEU	CA-C-N	5.59	128.04	120.44
29	P	216	LEU	C-N-CA	5.59	128.04	120.44
8	h	3	ILE	N-CA-CB	5.58	120.52	111.36
8	h	68	SER	CA-C-O	-5.58	113.55	119.97
23	T	91	SER	N-CA-C	-5.58	98.90	110.80
2	B	17	LYS	CA-C-N	5.58	128.77	120.90
2	B	17	LYS	C-N-CA	5.58	128.77	120.90
16	I	413	ALA	CA-C-N	5.58	127.76	120.28
16	I	413	ALA	C-N-CA	5.58	127.76	120.28
17	K	204	ASP	CA-C-O	-5.58	114.36	120.17
14	n	115	ILE	N-CA-C	-5.58	100.08	108.12
11	4	84	VAL	N-CA-C	-5.58	104.93	110.62
32	U	214	VAL	O-C-N	-5.58	116.08	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	161	GLN	CG-CD-NE2	5.58	124.77	116.40
19	M	171	GLU	CA-C-N	5.58	132.01	121.97
19	M	171	GLU	C-N-CA	5.58	132.01	121.97
26	Z	7	LYS	N-CA-CB	5.58	119.22	110.46
27	N	740	TRP	CA-C-N	5.58	130.03	120.71
27	N	740	TRP	C-N-CA	5.58	130.03	120.71
14	n	116	VAL	CB-CA-C	-5.58	103.50	111.31
9	2	6	VAL	CA-C-N	5.58	129.48	121.50
9	2	6	VAL	C-N-CA	5.58	129.48	121.50
18	L	50	GLN	CA-C-N	5.58	128.76	120.95
18	L	50	GLN	C-N-CA	5.58	128.76	120.95
23	T	109	TYR	CA-C-O	-5.58	114.64	120.55
26	Z	407	VAL	CA-C-N	5.58	130.16	120.68
26	Z	407	VAL	C-N-CA	5.58	130.16	120.68
28	S	180	ASN	OD1-CG-ND2	5.58	128.18	122.60
29	P	266	TYR	CB-CA-C	-5.58	102.12	110.88
13	m	220	LYS	N-CA-CB	5.58	118.22	109.69
2	B	3	ASP	N-CA-CB	5.58	118.25	109.83
2	B	60	THR	N-CA-C	-5.58	106.31	113.23
15	H	237	THR	N-CA-CB	5.58	118.89	110.30
26	Z	128	GLU	CA-C-O	5.58	126.33	120.42
14	n	130	VAL	CA-CB-CG2	5.58	119.88	110.40
27	N	745	LEU	CA-C-N	5.58	127.75	120.28
27	N	745	LEU	C-N-CA	5.58	127.75	120.28
32	U	101	ALA	CB-CA-C	-5.58	100.78	110.09
33	O	43	GLU	N-CA-C	5.58	117.03	111.07
6	F	2	ARG	N-CA-C	-5.57	99.28	108.48
6	F	218	ASP	N-CA-C	-5.57	106.47	113.72
10	3	197	ARG	CA-C-N	5.57	129.39	121.42
10	3	197	ARG	C-N-CA	5.57	129.39	121.42
20	J	270	ARG	N-CA-C	5.57	117.36	111.28
21	W	60	ARG	NE-CZ-NH1	-5.57	115.93	121.50
27	N	158	LEU	O-C-N	5.57	128.03	122.12
9	i	51	ASP	N-CA-CB	5.57	118.31	110.12
9	i	116	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
31	R	345	TYR	CA-C-N	5.57	128.20	120.29
31	R	345	TYR	C-N-CA	5.57	128.20	120.29
3	c	76	VAL	N-CA-C	-5.57	100.45	108.53
4	d	222	LEU	CB-CA-C	-5.57	99.65	109.62
5	e	149	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
26	Z	29	ASP	N-CA-C	-5.57	104.71	112.45
27	N	692	GLU	CA-C-N	5.57	126.16	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	692	GLU	C-N-CA	5.57	126.16	119.98
30	Q	158	ILE	N-CA-C	-5.57	105.09	110.72
30	Q	232	TYR	N-CA-C	-5.57	105.09	113.89
10	j	173	ALA	N-CA-C	5.57	117.35	111.28
27	N	89	PHE	N-CA-C	-5.57	106.38	114.12
2	b	93	ALA	CA-C-O	-5.57	114.65	120.55
6	f	88	ARG	NE-CZ-NH2	5.57	124.21	119.20
10	j	171	LEU	CB-CA-C	-5.57	102.14	110.88
11	k	160	LEU	N-CA-C	5.57	117.35	111.28
16	I	340	ARG	CA-C-N	5.57	126.80	119.84
16	I	340	ARG	C-N-CA	5.57	126.80	119.84
20	J	227	SER	N-CA-C	5.57	117.15	111.14
28	S	204	ASP	CA-CB-CG	-5.57	107.03	112.60
31	R	226	GLU	CA-C-O	-5.57	114.06	120.24
32	U	178	VAL	CA-C-N	5.57	132.17	121.54
32	U	178	VAL	C-N-CA	5.57	132.17	121.54
16	I	95	GLN	CA-C-N	5.57	127.74	120.28
16	I	95	GLN	C-N-CA	5.57	127.74	120.28
26	Z	42	ASP	O-C-N	-5.56	116.34	122.07
32	U	293	GLU	N-CA-C	5.56	118.27	111.82
15	H	444	LEU	CA-C-O	5.56	126.32	120.42
12	l	196	LEU	O-C-N	5.56	128.49	122.15
16	I	131	SER	CA-C-O	5.56	127.44	121.16
23	T	99	SER	N-CA-C	-5.56	98.95	110.80
28	S	75	CYS	CA-C-N	5.56	127.73	120.28
28	S	75	CYS	C-N-CA	5.56	127.73	120.28
29	P	364	ARG	CA-C-N	5.56	127.73	120.28
29	P	364	ARG	C-N-CA	5.56	127.73	120.28
13	m	102	PHE	N-CA-C	-5.56	105.30	111.36
2	B	163	ALA	N-CA-C	-5.56	99.97	108.76
18	L	364	HIS	CG-CD2-NE2	5.56	112.76	107.20
23	T	14	ALA	CB-CA-C	-5.56	100.35	110.63
26	Z	804	ASP	N-CA-C	5.56	117.71	110.43
27	N	668	THR	CB-CA-C	5.56	119.16	109.65
8	h	149	GLU	N-CA-C	-5.56	105.22	111.28
13	m	92	ASN	N-CA-CB	5.56	118.38	110.16
16	I	361	ILE	CA-C-N	5.56	127.73	120.28
16	I	361	ILE	C-N-CA	5.56	127.73	120.28
25	Y	76	GLU	CA-C-O	5.56	126.85	120.90
28	S	368	LYS	CB-CA-C	-5.56	102.16	110.88
6	f	88	ARG	NH1-CZ-NH2	-5.56	112.08	119.30
17	K	284	ALA	N-CA-C	-5.56	105.43	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	52	ASN	OD1-CG-ND2	5.56	128.16	122.60
31	R	291	SER	CB-CA-C	5.56	120.30	110.85
11	k	112	ASN	OD1-CG-ND2	5.55	128.16	122.60
4	D	144	LYS	N-CA-C	-5.55	99.97	109.24
11	4	7	ILE	N-CA-C	-5.55	100.06	108.17
13	6	219	LEU	N-CA-C	-5.55	100.85	109.24
23	T	237	ASN	CA-C-N	5.55	127.72	120.28
23	T	237	ASN	C-N-CA	5.55	127.72	120.28
9	i	117	GLY	CA-C-N	5.55	128.59	120.71
9	i	117	GLY	C-N-CA	5.55	128.59	120.71
21	W	182	TYR	CA-C-O	5.55	126.37	120.10
31	R	413	LYS	CA-C-N	5.55	127.66	120.44
31	R	413	LYS	C-N-CA	5.55	127.66	120.44
1	a	225	PHE	CB-CG-CD1	5.55	130.14	120.70
28	S	196	ARG	N-CA-C	-5.55	105.24	112.23
31	R	30	ALA	CA-C-N	5.55	127.72	120.28
31	R	30	ALA	C-N-CA	5.55	127.72	120.28
6	f	228	ALA	N-CA-CB	5.55	118.28	110.12
28	S	21	SER	CA-C-N	5.55	127.72	120.28
28	S	21	SER	C-N-CA	5.55	127.72	120.28
28	S	26	ALA	CA-C-N	5.55	127.72	120.28
28	S	26	ALA	C-N-CA	5.55	127.72	120.28
29	P	52	LEU	N-CA-C	-5.55	105.31	111.36
29	P	417	HIS	N-CA-C	5.55	117.41	111.36
12	l	55	TRP	CG-CD2-CE3	-5.55	128.35	133.90
15	H	229	LEU	CA-C-N	5.55	128.17	120.29
15	H	229	LEU	C-N-CA	5.55	128.17	120.29
26	Z	397	ASP	N-CA-C	-5.55	104.76	112.03
8	h	139	ASP	CA-C-O	5.55	126.43	120.55
19	M	141	LYS	N-CA-CB	5.55	116.92	111.10
26	Z	175	ASP	CA-CB-CG	5.55	118.15	112.60
30	Q	357	VAL	CB-CA-C	5.55	119.22	111.34
31	R	189	GLU	CA-C-N	5.55	128.16	120.29
31	R	189	GLU	C-N-CA	5.55	128.16	120.29
33	O	200	GLU	CB-CA-C	-5.55	100.59	109.69
14	n	67	LEU	N-CA-CB	5.54	118.27	110.12
27	N	210	SER	CA-C-N	5.54	128.26	120.28
27	N	210	SER	C-N-CA	5.54	128.26	120.28
3	c	145	TYR	CA-CB-CG	-5.54	103.92	113.90
4	d	110	TYR	CA-C-N	5.54	128.29	120.42
4	d	110	TYR	C-N-CA	5.54	128.29	120.42
23	T	109	TYR	N-CA-C	5.54	117.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	371	GLN	N-CA-CB	5.54	118.36	110.16
31	R	55	LYS	CA-C-O	-5.54	114.54	120.42
7	g	78	ILE	CB-CA-C	-5.54	106.74	114.00
19	M	157	ASP	CA-CB-CG	5.54	118.14	112.60
26	Z	357	ILE	CA-CB-CG1	5.54	119.82	110.40
9	i	116	HIS	CB-CG-CD2	5.54	138.40	131.20
18	L	420	ARG	CA-C-O	5.54	126.41	120.70
32	U	186	LEU	CA-C-O	-5.54	114.68	120.55
8	h	51	ASP	CA-C-O	-5.54	115.00	120.70
9	i	172	ASN	CA-CB-CG	-5.54	107.06	112.60
16	I	204	HIS	O-C-N	-5.54	116.84	121.44
27	N	666	GLN	CB-CG-CD	-5.54	103.19	112.60
17	K	343	LEU	N-CA-C	-5.54	104.75	112.45
26	Z	123	ALA	CA-C-N	5.54	127.64	120.44
26	Z	123	ALA	C-N-CA	5.54	127.64	120.44
28	S	429	ASP	N-CA-C	-5.54	106.53	113.28
7	G	16	ARG	CA-C-N	5.54	130.20	121.56
7	G	16	ARG	C-N-CA	5.54	130.20	121.56
15	H	51	GLN	N-CA-CB	5.54	118.26	110.12
17	K	200	GLN	N-CA-C	5.54	117.39	111.36
20	J	86	VAL	N-CA-C	-5.54	100.48	108.89
27	N	441	VAL	N-CA-C	5.54	116.27	110.62
28	S	258	GLU	N-CA-C	-5.54	106.19	113.17
9	i	114	HIS	ND1-CE1-NE2	5.53	113.93	108.40
19	M	351	LEU	CA-C-N	5.53	126.76	119.84
19	M	351	LEU	C-N-CA	5.53	126.76	119.84
20	J	265	ASP	CA-C-N	5.53	128.15	120.29
20	J	265	ASP	C-N-CA	5.53	128.15	120.29
22	V	104	VAL	CA-C-O	-5.53	114.17	120.98
1	a	28	GLN	CB-CG-CD	-5.53	103.19	112.60
5	e	9	PRO	O-C-N	5.53	130.11	122.64
3	C	4	ARG	N-CA-CB	5.53	118.44	110.20
4	D	126	PRO	CA-N-CD	5.53	119.75	112.00
5	E	38	VAL	N-CA-C	-5.53	100.61	108.58
26	Z	294	ILE	CA-CB-CG1	5.53	119.80	110.40
9	i	60	GLY	CA-C-N	5.53	127.63	120.44
9	i	60	GLY	C-N-CA	5.53	127.63	120.44
12	l	155	TYR	CA-C-N	5.53	127.69	120.28
12	l	155	TYR	C-N-CA	5.53	127.69	120.28
11	4	100	VAL	O-C-N	-5.53	117.10	123.07
13	6	48	ASP	CA-C-N	5.53	130.26	122.46
13	6	48	ASP	C-N-CA	5.53	130.26	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	67	ASP	N-CA-CB	5.53	118.34	110.16
16	I	331	ILE	N-CA-C	-5.53	106.44	112.80
27	N	408	LEU	CA-C-O	-5.53	114.56	120.42
28	S	161	LYS	CA-C-N	5.53	127.64	120.56
28	S	161	LYS	C-N-CA	5.53	127.64	120.56
28	S	428	ARG	CA-C-O	5.53	126.41	120.55
26	Z	727	GLU	O-C-N	5.53	129.06	122.20
7	g	208	PHE	CA-C-N	5.53	131.25	122.74
7	g	208	PHE	C-N-CA	5.53	131.25	122.74
7	G	239	ALA	O-C-N	5.53	129.07	122.27
9	2	202	SER	N-CA-CB	5.53	118.13	110.17
26	Z	484	LYS	O-C-N	-5.53	116.38	122.07
30	Q	140	LYS	CA-C-N	5.53	128.14	120.29
30	Q	140	LYS	C-N-CA	5.53	128.14	120.29
1	a	172	ASN	CB-CG-ND2	-5.53	108.11	116.40
12	l	101	ILE	CA-CB-CG2	-5.53	101.11	110.50
8	1	6	VAL	CA-C-O	-5.53	114.69	120.27
17	K	109	ILE	CA-C-O	5.53	126.86	120.67
26	Z	279	THR	N-CA-C	-5.53	105.34	111.36
29	P	424	GLU	CA-C-N	5.53	127.68	120.28
29	P	424	GLU	C-N-CA	5.53	127.68	120.28
8	h	113	ILE	CA-C-N	5.52	126.75	119.84
8	h	113	ILE	C-N-CA	5.52	126.75	119.84
11	k	190	ARG	CA-C-O	-5.52	115.16	121.40
26	Z	376	SER	O-C-N	5.52	129.94	122.59
13	m	208	THR	N-CA-C	-5.52	101.34	109.18
15	H	201	GLU	N-CA-C	-5.52	100.40	109.40
24	X	103	GLU	N-CA-C	-5.52	101.20	109.15
31	R	116	LYS	CA-C-O	-5.52	115.00	121.07
13	m	215	GLU	N-CA-C	-5.52	100.67	109.23
26	Z	903	MET	N-CA-C	5.52	118.46	109.24
4	d	18	VAL	CA-C-N	5.52	128.13	120.29
4	d	18	VAL	C-N-CA	5.52	128.13	120.29
1	A	200	HIS	CE1-NE2-CD2	-5.52	103.48	109.00
4	D	12	ASP	CA-C-N	5.52	132.23	121.41
4	D	12	ASP	C-N-CA	5.52	132.23	121.41
5	E	158	ARG	O-C-N	-5.52	116.72	122.96
16	I	206	GLU	CA-C-N	5.52	127.94	120.44
16	I	206	GLU	C-N-CA	5.52	127.94	120.44
21	W	113	PHE	CA-CB-CG	-5.52	108.28	113.80
22	V	131	GLN	N-CA-CB	5.52	118.23	110.12
7	g	154	TRP	CA-C-N	5.52	126.76	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	154	TRP	C-N-CA	5.52	126.76	120.53
7	G	230	ASP	CA-CB-CG	-5.52	107.08	112.60
8	1	156	LYS	CA-C-O	5.52	126.40	120.55
11	4	13	VAL	N-CA-C	-5.52	100.18	108.12
18	L	208	GLN	CA-C-N	5.52	127.67	120.28
18	L	208	GLN	C-N-CA	5.52	127.67	120.28
31	R	21	VAL	CA-CB-CG2	-5.52	101.02	110.40
33	O	381	GLY	CA-C-N	5.52	128.12	120.29
33	O	381	GLY	C-N-CA	5.52	128.12	120.29
27	N	15	GLU	O-C-N	5.52	130.35	123.01
2	b	69	PRO	N-CD-CG	5.51	111.47	103.20
7	g	37	LYS	N-CA-CB	5.51	119.43	110.17
7	g	158	GLY	O-C-N	5.51	127.46	123.27
10	3	173	ALA	CA-C-N	5.51	127.67	120.28
10	3	173	ALA	C-N-CA	5.51	127.67	120.28
15	H	68	GLY	O-C-N	5.51	128.84	122.61
33	O	48	PHE	CA-CB-CG	-5.51	108.29	113.80
2	b	179	TRP	CG-CD2-CE3	-5.51	128.39	133.90
14	n	68	LYS	CA-C-N	5.51	127.67	120.28
14	n	68	LYS	C-N-CA	5.51	127.67	120.28
20	J	268	VAL	N-CA-CB	5.51	118.03	110.54
26	Z	524	ALA	N-CA-C	-5.51	105.35	111.36
7	g	232	LEU	CA-C-N	5.51	127.66	120.28
7	g	232	LEU	C-N-CA	5.51	127.66	120.28
14	n	225	ILE	N-CA-C	-5.51	99.80	108.23
26	Z	238	ASP	N-CA-CB	5.51	118.15	109.94
2	B	89	SER	CB-CA-C	-5.51	101.65	110.79
15	H	400	ARG	NE-CZ-NH2	5.51	124.16	119.20
20	J	359	LYS	CA-C-N	5.51	126.09	119.98
20	J	359	LYS	C-N-CA	5.51	126.09	119.98
27	N	11	ALA	CB-CA-C	5.51	120.21	110.85
33	O	121	ASP	CB-CA-C	5.51	119.29	109.38
2	B	151	ASP	CA-C-O	-5.51	115.64	120.60
14	7	177	ILE	N-CA-C	5.51	116.24	110.62
27	N	347	SER	N-CA-CB	5.51	118.31	110.16
33	O	173	SER	CA-C-N	5.51	127.60	120.44
33	O	173	SER	C-N-CA	5.51	127.60	120.44
6	f	81	ARG	NH1-CZ-NH2	5.50	126.46	119.30
7	g	85	VAL	O-C-N	-5.50	116.16	121.83
8	h	93	LEU	N-CA-CB	5.50	119.19	110.55
9	i	66	HIS	CG-CD2-NE2	5.50	112.70	107.20
29	P	337	HIS	CA-C-O	5.50	125.46	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	39	ALA	O-C-N	-5.50	115.88	122.15
29	P	268	LEU	CA-C-N	5.50	128.24	120.42
29	P	268	LEU	C-N-CA	5.50	128.24	120.42
31	R	100	ASN	CA-C-N	5.50	129.94	121.19
31	R	100	ASN	C-N-CA	5.50	129.94	121.19
31	R	116	LYS	N-CA-CB	5.50	118.19	109.82
11	k	152	MET	CG-SD-CE	-5.50	88.80	100.90
20	J	94	TYR	CA-CB-CG	-5.50	104.00	113.90
27	N	347	SER	CB-CA-C	-5.50	101.50	110.85
3	c	192	ALA	N-CA-CB	5.50	117.98	110.01
6	f	101	LYS	CB-CA-C	-5.50	100.25	109.65
4	D	194	VAL	CA-C-N	5.50	127.59	120.44
4	D	194	VAL	C-N-CA	5.50	127.59	120.44
29	P	180	ILE	CA-C-N	5.50	127.65	120.28
29	P	180	ILE	C-N-CA	5.50	127.65	120.28
10	j	89	LEU	N-CA-CB	5.50	118.20	110.12
3	C	21	VAL	O-C-N	-5.50	116.54	121.87
14	7	203	ASN	CA-C-O	-5.50	114.14	120.24
16	I	170	VAL	N-CA-C	5.50	116.23	110.62
16	I	376	ASN	CA-C-O	-5.50	112.65	120.51
9	i	140	SER	N-CA-CB	-5.50	101.67	110.19
12	l	72	GLU	N-CA-CB	5.50	119.98	111.24
28	S	423	VAL	N-CA-CB	5.50	116.98	110.55
6	f	131	LEU	CB-CA-C	-5.49	98.23	109.38
9	i	52	THR	CA-CB-OG1	5.49	117.84	109.60
9	i	93	HIS	CB-CG-ND1	5.49	130.94	122.70
16	I	419	ALA	N-CA-CB	5.49	118.29	110.16
18	L	404	ARG	O-C-N	5.49	128.65	122.22
29	P	366	ASN	CB-CA-C	-5.49	101.34	110.68
12	l	51	ASP	CB-CA-C	-5.49	102.22	110.90
33	O	23	HIS	CA-C-O	-5.49	113.01	118.34
5	e	100	ASN	O-C-N	-5.49	116.18	122.93
7	G	83	HIS	ND1-CE1-NE2	5.49	113.89	108.40
15	H	289	ARG	NE-CZ-NH1	5.49	126.99	121.50
27	N	393	SER	N-CA-C	-5.49	106.25	113.17
17	K	168	ASP	CA-CB-CG	5.49	118.09	112.60
22	V	63	VAL	O-C-N	-5.49	117.33	123.26
33	O	230	PHE	N-CA-CB	5.49	119.76	110.49
12	l	66	HIS	CB-CG-CD2	-5.49	124.07	131.20
16	I	364	ILE	CA-C-N	5.49	127.90	120.44
16	I	364	ILE	C-N-CA	5.49	127.90	120.44
28	S	370	LEU	CA-C-O	5.49	126.37	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	199	GLU	CB-CG-CD	-5.48	103.28	112.60
6	f	136	TYR	CA-CB-CG	-5.48	104.03	113.90
10	j	149	CYS	N-CA-C	5.48	117.34	111.36
14	n	195	PHE	CA-CB-CG	-5.48	108.32	113.80
11	4	39	SER	N-CA-C	-5.48	101.84	108.14
3	c	9	THR	CA-C-N	5.48	130.14	122.41
3	c	9	THR	C-N-CA	5.48	130.14	122.41
7	g	112	LEU	CA-C-N	5.48	125.91	119.94
7	g	112	LEU	C-N-CA	5.48	125.91	119.94
9	i	199	LYS	CA-C-N	5.48	128.07	120.29
9	i	199	LYS	C-N-CA	5.48	128.07	120.29
10	j	57	THR	N-CA-CB	5.48	118.27	110.16
17	K	405	SER	CB-CA-C	-5.48	101.53	110.85
14	7	207	THR	N-CA-C	-5.48	99.59	108.52
21	W	160	ALA	CA-C-N	5.48	127.97	120.46
21	W	160	ALA	C-N-CA	5.48	127.97	120.46
26	Z	722	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	99	TYR	N-CA-C	-5.48	106.60	113.72
5	E	81	ILE	CA-C-O	-5.48	115.04	120.85
29	P	279	ASP	N-CA-CB	5.48	118.77	110.28
30	Q	366	ILE	N-CA-C	-5.48	105.19	110.72
33	O	63	ASP	N-CA-C	5.48	117.68	111.11
12	l	117	SER	CA-C-N	5.48	128.07	120.29
12	l	117	SER	C-N-CA	5.48	128.07	120.29
17	K	64	GLN	CA-C-O	5.48	126.29	120.10
27	N	107	GLU	CA-C-O	5.48	126.22	120.42
5	e	43	GLU	CA-C-N	5.47	128.06	120.29
5	e	43	GLU	C-N-CA	5.47	128.06	120.29
8	1	148	LYS	CA-C-N	5.47	127.62	120.28
8	1	148	LYS	C-N-CA	5.47	127.62	120.28
26	Z	775	MET	N-CA-C	5.47	118.08	111.40
14	n	95	TYR	CA-CB-CG	-5.47	104.05	113.90
1	A	196	PHE	N-CA-C	-5.47	99.14	110.80
16	I	152	LYS	CB-CA-C	-5.47	102.29	110.88
28	S	298	ARG	CA-C-N	5.47	128.06	120.29
28	S	298	ARG	C-N-CA	5.47	128.06	120.29
31	R	185	LEU	CA-C-O	-5.47	114.62	120.42
32	U	21	HIS	CA-C-N	5.47	127.61	120.28
32	U	21	HIS	C-N-CA	5.47	127.61	120.28
32	U	279	SER	CA-C-N	5.47	127.61	120.28
32	U	279	SER	C-N-CA	5.47	127.61	120.28
3	c	128	ARG	CD-NE-CZ	5.47	132.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	120	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
14	n	208	PHE	CA-CB-CG	-5.47	108.33	113.80
13	6	115	ASP	CA-C-N	5.47	127.88	120.44
13	6	115	ASP	C-N-CA	5.47	127.88	120.44
16	I	305	THR	CA-C-N	5.47	127.61	120.28
16	I	305	THR	C-N-CA	5.47	127.61	120.28
18	L	225	GLY	CA-C-O	5.47	125.06	119.10
19	M	347	ILE	CA-C-O	5.47	126.38	120.53
19	M	137	PRO	CA-C-N	5.47	128.06	120.29
19	M	137	PRO	C-N-CA	5.47	128.06	120.29
30	Q	324	GLU	CA-C-N	5.47	127.61	120.28
30	Q	324	GLU	C-N-CA	5.47	127.61	120.28
4	d	8	ILE	N-CA-CB	5.47	120.43	111.58
4	d	213	VAL	N-CA-CB	5.47	118.79	111.90
16	I	68	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
5	E	152	PRO	CA-N-CD	5.46	119.65	112.00
22	V	257	GLU	N-CA-C	-5.46	99.78	108.30
23	T	270	ILE	CA-C-O	5.46	126.64	120.85
27	N	228	VAL	CA-C-N	5.46	127.44	120.56
27	N	228	VAL	C-N-CA	5.46	127.44	120.56
32	U	111	LYS	N-CA-C	-5.46	106.11	112.89
33	O	83	LEU	CA-C-O	5.46	126.56	120.82
33	O	328	VAL	CA-C-N	5.46	127.54	120.44
33	O	328	VAL	C-N-CA	5.46	127.54	120.44
5	e	172	GLN	N-CA-C	5.46	117.99	111.71
9	i	13	VAL	N-CA-CB	5.46	118.94	111.41
26	Z	545	SER	CA-C-N	5.46	127.55	120.56
26	Z	545	SER	C-N-CA	5.46	127.55	120.56
1	A	63	ILE	CA-C-O	-5.46	114.61	121.11
26	Z	926	ASN	CA-C-N	5.46	131.05	122.70
26	Z	926	ASN	C-N-CA	5.46	131.05	122.70
29	P	206	LYS	CA-C-N	5.46	128.61	120.31
29	P	206	LYS	C-N-CA	5.46	128.61	120.31
6	f	12	PHE	N-CA-CB	5.46	117.99	109.97
6	f	179	ILE	CA-C-O	-5.46	114.58	120.47
10	3	187	TYR	O-C-N	5.46	130.14	123.21
27	N	873	ARG	NE-CZ-NH1	5.46	126.96	121.50
28	S	193	THR	CA-C-N	5.46	127.59	120.28
28	S	193	THR	C-N-CA	5.46	127.59	120.28
4	d	216	ASP	CA-C-N	5.46	130.57	122.82
4	d	216	ASP	C-N-CA	5.46	130.57	122.82
5	e	48	SER	O-C-N	-5.46	116.75	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	85	LEU	O-C-N	5.46	128.37	122.15
10	j	165	THR	N-CA-C	-5.46	105.25	111.14
15	H	337	ILE	CB-CA-C	-5.46	104.77	112.14
26	Z	487	SER	N-CA-CB	5.46	118.24	110.16
29	P	246	GLN	CA-C-O	-5.46	112.67	119.38
9	i	82	MET	CG-SD-CE	-5.46	88.90	100.90
17	K	348	GLU	CB-CA-C	-5.46	101.73	110.79
33	O	362	GLN	CA-C-N	5.46	127.93	120.46
33	O	362	GLN	C-N-CA	5.46	127.93	120.46
2	b	54	PRO	CA-C-N	5.45	127.59	120.28
2	b	54	PRO	C-N-CA	5.45	127.59	120.28
7	g	144	LEU	CA-C-O	5.45	126.25	120.36
14	n	108	ASN	CA-CB-CG	-5.45	107.15	112.60
23	T	182	LYS	N-CA-C	-5.45	105.23	111.07
29	P	52	LEU	O-C-N	-5.45	115.93	122.15
29	P	84	LYS	N-CA-C	5.45	117.30	111.36
10	j	21	ALA	CA-C-O	-5.45	114.88	120.99
12	l	66	HIS	CA-CB-CG	-5.45	108.35	113.80
13	m	76	HIS	O-C-N	-5.45	116.34	122.12
22	V	174	THR	N-CA-CB	5.45	117.98	109.97
3	c	5	TYR	N-CA-CB	5.45	118.38	110.26
13	m	213	ARG	CB-CG-CD	5.45	123.84	111.30
14	7	77	ASP	CA-C-N	5.45	128.97	120.68
14	7	77	ASP	C-N-CA	5.45	128.97	120.68
11	k	169	GLU	N-CA-C	-5.45	105.24	111.07
5	E	24	LYS	N-CA-C	-5.45	105.34	111.28
20	J	331	HIS	CA-C-N	5.45	127.58	120.28
20	J	331	HIS	C-N-CA	5.45	127.58	120.28
26	Z	230	ILE	N-CA-C	-5.45	105.41	110.53
27	N	649	VAL	CA-C-N	5.45	127.58	120.28
27	N	649	VAL	C-N-CA	5.45	127.58	120.28
3	c	151	ASN	CA-C-N	5.45	125.92	120.04
3	c	151	ASN	C-N-CA	5.45	125.92	120.04
6	f	167	ALA	N-CA-CB	5.45	118.22	110.16
16	I	419	ALA	CA-C-O	-5.45	114.65	120.42
14	7	172	VAL	CB-CA-C	-5.45	104.79	112.14
19	M	266	ALA	CA-C-N	5.45	128.02	120.29
19	M	266	ALA	C-N-CA	5.45	128.02	120.29
26	Z	463	HIS	N-CA-CB	5.45	118.69	110.30
27	N	906	ARG	N-CA-C	-5.45	100.83	109.76
19	M	40	GLU	CA-C-N	5.44	127.92	120.46
19	M	40	GLU	C-N-CA	5.44	127.92	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	135	VAL	N-CA-CB	5.44	117.05	110.95
21	W	140	ASP	N-CA-C	-5.44	100.31	109.07
8	h	174	ARG	N-CA-C	-5.44	100.84	109.76
12	l	146	TRP	CE2-CD2-CE3	5.44	124.24	118.80
5	E	187	GLU	N-CA-C	5.44	117.21	111.28
20	J	255	SER	CA-C-N	5.44	128.58	120.31
20	J	255	SER	C-N-CA	5.44	128.58	120.31
20	J	283	GLU	CA-C-O	-5.44	115.09	120.70
23	T	77	SER	CA-C-N	5.44	127.52	120.44
23	T	77	SER	C-N-CA	5.44	127.52	120.44
26	Z	930	GLY	CA-C-N	5.44	128.97	120.75
26	Z	930	GLY	C-N-CA	5.44	128.97	120.75
27	N	446	ALA	CA-C-N	5.44	128.02	120.29
27	N	446	ALA	C-N-CA	5.44	128.02	120.29
33	O	157	LEU	O-C-N	5.44	127.89	122.12
4	d	91	ALA	CA-C-O	-5.44	115.11	120.82
13	m	98	TYR	CA-C-O	-5.44	114.65	120.42
4	D	223	SER	N-CA-CB	5.44	118.04	110.04
7	G	221	ASN	CA-C-N	5.44	131.32	120.77
7	G	221	ASN	C-N-CA	5.44	131.32	120.77
17	K	152	PRO	N-CA-C	-5.44	106.31	113.65
20	J	116	ARG	N-CA-C	-5.44	101.43	109.86
23	T	84	GLN	N-CA-C	5.44	117.21	111.28
24	X	85	ARG	CA-C-O	5.44	127.85	121.54
6	f	93	TYR	CB-CG-CD1	5.44	128.96	120.80
9	i	42	TRP	CA-C-O	5.44	127.30	121.16
15	H	199	THR	N-CA-CB	5.44	118.11	110.12
17	K	133	PRO	N-CA-CB	5.44	108.08	103.19
27	N	42	GLU	CA-C-O	5.44	126.53	119.95
33	O	235	HIS	CG-CD2-NE2	5.44	112.64	107.20
1	a	217	GLY	CA-C-O	5.44	125.97	120.64
4	d	72	SER	O-C-N	-5.44	116.12	123.19
23	T	213	ASN	CA-C-N	5.44	128.01	120.29
23	T	213	ASN	C-N-CA	5.44	128.01	120.29
33	O	176	SER	CA-C-N	5.44	127.51	120.44
33	O	176	SER	C-N-CA	5.44	127.51	120.44
14	n	75	ALA	CA-C-N	5.43	128.56	120.90
14	n	75	ALA	C-N-CA	5.43	128.56	120.90
13	6	217	TYR	O-C-N	-5.43	116.83	123.30
18	L	119	VAL	CA-CB-CG2	5.43	119.64	110.40
20	J	118	ASP	N-CA-C	-5.43	106.69	113.38
31	R	179	PHE	CA-C-O	-5.43	114.79	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	59	LEU	CA-C-N	5.43	128.57	120.31
33	O	59	LEU	C-N-CA	5.43	128.57	120.31
33	O	331	ALA	CA-C-N	5.43	127.41	120.56
33	O	331	ALA	C-N-CA	5.43	127.41	120.56
33	O	354	GLN	CA-C-N	5.43	126.63	119.84
33	O	354	GLN	C-N-CA	5.43	126.63	119.84
2	B	207	ASP	O-C-N	-5.43	116.22	122.09
5	E	80	MET	CB-CA-C	-5.43	101.61	110.85
6	F	127	TYR	N-CA-CB	5.43	118.51	109.60
7	G	142	ALA	CB-CA-C	-5.43	100.36	109.65
8	1	132	THR	CA-C-O	5.43	126.31	120.55
23	T	188	GLU	N-CA-CB	5.43	118.11	110.12
26	Z	754	LYS	CA-C-N	5.43	127.56	120.28
26	Z	754	LYS	C-N-CA	5.43	127.56	120.28
27	N	900	ASN	CA-CB-CG	-5.43	107.17	112.60
28	S	34	LEU	CA-C-N	5.43	127.56	120.28
28	S	34	LEU	C-N-CA	5.43	127.56	120.28
32	U	287	ALA	CA-C-O	-5.43	114.66	120.42
4	d	40	VAL	N-CA-C	-5.43	100.30	108.12
12	5	109	GLY	O-C-N	-5.43	116.34	121.77
12	l	166	HIS	ND1-CE1-NE2	5.43	113.83	108.40
5	E	179	TRP	N-CA-CB	5.43	118.03	109.83
23	T	93	ASN	CA-CB-CG	-5.43	107.17	112.60
23	T	238	GLN	CA-C-N	5.43	127.87	120.54
23	T	238	GLN	C-N-CA	5.43	127.87	120.54
26	Z	281	ALA	CB-CA-C	-5.43	101.78	110.79
15	H	351	VAL	CA-C-O	5.43	126.03	120.39
33	O	89	SER	CA-C-O	5.43	127.05	120.81
2	b	220	ASP	N-CA-C	5.43	117.27	111.36
12	l	66	HIS	N-CA-C	-5.43	105.28	111.14
26	Z	548	ASP	N-CA-CB	5.43	119.24	110.40
28	S	271	ARG	CA-C-N	5.43	127.55	120.28
28	S	271	ARG	C-N-CA	5.43	127.55	120.28
28	S	484	ASP	CA-C-O	-5.43	115.12	120.82
33	O	278	PRO	CA-C-N	5.43	127.50	120.56
33	O	278	PRO	C-N-CA	5.43	127.50	120.56
2	b	154	GLY	N-CA-C	-5.42	107.19	115.00
8	1	10	ASP	CA-CB-CG	-5.42	107.18	112.60
11	4	188	GLY	N-CA-C	-5.42	100.32	113.18
22	V	218	LYS	N-CA-C	-5.42	106.71	113.38
23	T	94	HIS	CA-C-N	5.42	130.06	122.08
23	T	94	HIS	C-N-CA	5.42	130.06	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	717	LEU	N-CA-CB	5.42	117.94	110.07
29	P	69	ARG	CA-C-O	-5.42	112.78	119.18
31	R	21	VAL	CB-CA-C	-5.42	106.89	114.00
32	U	273	LEU	CB-CA-C	-5.42	102.13	110.81
7	G	57	PRO	CA-C-N	5.42	131.02	122.78
7	G	57	PRO	C-N-CA	5.42	131.02	122.78
1	a	89	LYS	N-CA-CB	5.42	118.18	110.16
11	k	105	GLY	O-C-N	-5.42	118.81	123.80
4	D	68	HIS	CB-CG-CD2	-5.42	124.15	131.20
19	M	73	ARG	CA-C-N	5.42	128.80	121.05
19	M	73	ARG	C-N-CA	5.42	128.80	121.05
4	d	14	HIS	ND1-CE1-NE2	5.42	113.82	108.40
4	D	151	SER	N-CA-C	-5.42	106.67	113.28
16	I	119	ILE	CA-C-O	-5.42	114.75	120.39
20	J	257	ARG	NE-CZ-NH1	5.42	126.92	121.50
33	O	69	PHE	CB-CG-CD1	5.42	129.91	120.70
26	Z	496	ALA	N-CA-CB	5.42	118.01	109.94
32	U	143	VAL	CB-CA-C	-5.42	104.74	111.08
7	g	179	HIS	CA-CB-CG	-5.42	108.38	113.80
13	6	30	ILE	N-CA-C	-5.42	101.20	108.35
27	N	19	SER	CA-C-N	5.42	128.11	120.42
27	N	19	SER	C-N-CA	5.42	128.11	120.42
33	O	306	ARG	N-CA-C	-5.42	102.31	110.06
27	N	620	GLY	N-CA-C	-5.42	107.95	114.66
28	S	163	VAL	CA-C-O	-5.42	114.62	120.47
7	g	31	THR	N-CA-CB	5.41	118.58	109.92
12	l	152	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	64	PHE	N-CA-CB	5.41	119.69	110.71
26	Z	64	TYR	CA-C-N	5.41	128.31	120.79
26	Z	64	TYR	C-N-CA	5.41	128.31	120.79
30	Q	267	LEU	CA-C-N	5.41	127.53	120.28
30	Q	267	LEU	C-N-CA	5.41	127.53	120.28
1	a	161	ALA	CA-C-O	5.41	127.09	120.60
19	M	150	LYS	N-CA-C	5.41	118.10	111.82
26	Z	289	GLY	N-CA-C	-5.41	108.17	115.21
30	Q	143	THR	CA-C-N	5.41	128.54	120.31
30	Q	143	THR	C-N-CA	5.41	128.54	120.31
5	e	39	VAL	N-CA-CB	5.41	118.61	111.25
6	f	88	ARG	CB-CA-C	-5.41	101.81	110.79
14	n	226	LYS	N-CA-CB	5.41	120.34	111.31
26	Z	248	TYR	CA-C-O	-5.41	114.81	120.55
26	Z	732	ILE	N-CA-C	-5.41	105.26	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	136	ILE	N-CA-C	-5.41	105.23	110.42
29	P	76	ASN	CA-C-O	5.41	126.28	120.55
5	e	191	LEU	O-C-N	-5.41	116.50	122.07
5	e	198	GLN	N-CA-CB	5.41	117.85	110.01
7	g	54	LEU	N-CA-C	-5.41	106.45	113.16
13	m	152	ASN	N-CA-C	-5.41	105.47	111.36
19	M	204	ALA	N-CA-C	5.41	118.67	111.75
21	W	3	LEU	CA-C-O	5.41	128.24	120.51
22	V	221	TRP	N-CA-C	-5.41	106.85	113.50
27	N	61	ALA	O-C-N	-5.41	115.98	122.15
29	P	42	LEU	N-CA-C	5.41	117.18	111.28
32	U	5	HIS	CA-CB-CG	5.41	119.21	113.80
19	M	302	GLN	O-C-N	5.41	127.64	122.07
4	d	58	THR	N-CA-C	-5.41	102.97	109.83
8	h	97	ILE	CA-C-N	-5.41	116.12	122.93
8	h	97	ILE	C-N-CA	-5.41	116.12	122.93
9	2	9	ASN	N-CA-C	5.41	119.36	112.87
9	2	51	ASP	N-CA-CB	5.41	118.66	110.28
14	7	28	GLY	N-CA-C	-5.41	100.37	113.18
19	M	350	PRO	N-CA-C	-5.41	102.06	112.01
21	W	103	ASN	CA-CB-CG	-5.41	107.19	112.60
30	Q	56	THR	CA-C-N	5.41	127.47	120.44
30	Q	56	THR	C-N-CA	5.41	127.47	120.44
7	g	8	ASN	CA-C-N	5.40	131.86	121.54
7	g	8	ASN	C-N-CA	5.40	131.86	121.54
29	P	162	GLU	CB-CA-C	-5.40	101.49	110.68
6	f	198	GLN	N-CA-C	-5.40	105.47	111.36
13	m	121	ALA	O-C-N	-5.40	116.68	123.27
7	G	183	LEU	CA-C-N	5.40	128.91	120.75
7	G	183	LEU	C-N-CA	5.40	128.91	120.75
12	5	79	ALA	O-C-N	-5.40	115.99	122.15
27	N	603	PRO	O-C-N	5.40	129.48	122.24
1	a	184	HIS	ND1-CE1-NE2	5.40	113.80	108.40
3	c	78	GLY	CA-C-N	5.40	128.43	120.82
3	c	78	GLY	C-N-CA	5.40	128.43	120.82
10	j	60	THR	N-CA-CB	5.40	118.15	110.16
3	C	40	SER	O-C-N	-5.40	116.39	122.12
5	E	195	ILE	CA-C-N	5.40	127.52	120.28
5	E	195	ILE	C-N-CA	5.40	127.52	120.28
20	J	299	ILE	N-CA-CB	5.40	118.76	112.33
27	N	662	MET	CA-C-O	5.40	126.16	119.79
32	U	7	LYS	CA-C-O	-5.40	115.01	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	125	VAL	N-CA-C	-5.40	107.54	113.43
3	c	216	ARG	CA-C-O	5.40	126.43	120.71
5	e	91	HIS	O-C-N	5.40	127.84	122.12
11	k	187	ASP	CA-C-N	5.40	129.76	122.42
11	k	187	ASP	C-N-CA	5.40	129.76	122.42
13	m	81	ASP	CA-CB-CG	-5.40	107.20	112.60
5	E	184	THR	CA-C-O	-5.40	114.71	121.46
16	I	303	GLN	CA-C-N	5.40	127.95	120.29
16	I	303	GLN	C-N-CA	5.40	127.95	120.29
17	K	297	ILE	CA-C-N	5.40	127.51	120.28
17	K	297	ILE	C-N-CA	5.40	127.51	120.28
17	K	408	GLU	N-CA-C	5.40	117.16	111.28
20	J	249	GLU	N-CA-CB	5.40	119.61	110.49
21	W	84	LYS	CA-C-O	5.40	126.87	120.66
26	Z	263	ALA	CA-C-O	-5.40	114.70	120.42
27	N	74	GLU	CA-C-O	-5.40	115.83	122.36
33	O	303	LYS	CA-C-N	5.40	127.95	120.29
33	O	303	LYS	C-N-CA	5.40	127.95	120.29
9	i	166	ASP	CA-CB-CG	-5.40	107.20	112.60
10	j	64	GLU	CA-C-O	5.40	126.27	120.55
3	C	122	THR	N-CA-C	-5.40	106.70	113.72
3	c	152	PRO	N-CA-C	-5.39	106.99	114.27
7	G	56	VAL	N-CA-CB	-5.39	104.59	111.23
25	Y	88	ASN	OD1-CG-ND2	-5.39	117.21	122.60
12	l	141	ASP	N-CA-CB	5.39	117.89	110.07
3	C	100	THR	CA-C-O	5.39	126.14	120.42
7	G	119	HIS	N-CA-C	-5.39	106.20	112.89
19	M	134	LEU	N-CA-C	-5.39	105.06	111.69
26	Z	259	PRO	N-CA-CB	5.39	108.69	103.51
26	Z	795	THR	CB-CA-C	-5.39	100.83	110.70
3	c	155	ASN	CB-CG-OD1	5.39	131.58	120.80
2	B	178	ARG	NE-CZ-NH2	-5.39	114.35	119.20
9	2	25	ILE	O-C-N	5.39	129.10	122.95
15	H	49	LEU	CA-C-N	5.39	127.45	120.44
15	H	49	LEU	C-N-CA	5.39	127.45	120.44
17	K	421	VAL	O-C-N	5.39	127.78	121.96
18	L	173	PHE	CA-CB-CG	-5.39	108.41	113.80
26	Z	939	ALA	O-C-N	5.39	129.76	122.59
29	P	262	SER	N-CA-C	-5.39	105.48	111.36
3	c	202	SER	CA-C-N	5.39	127.82	120.54
3	c	202	SER	C-N-CA	5.39	127.82	120.54
5	e	51	LEU	N-CA-CB	5.39	118.03	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	358	LYS	CA-C-N	-5.39	112.64	120.29
16	I	358	LYS	C-N-CA	-5.39	112.64	120.29
17	K	334	LEU	N-CA-CB	5.39	119.60	110.49
26	Z	361	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
31	R	311	THR	CA-C-N	5.39	127.94	120.29
31	R	311	THR	C-N-CA	5.39	127.94	120.29
33	O	250	TRP	CG-CD2-CE3	-5.39	128.51	133.90
8	h	5	ALA	O-C-N	5.39	129.61	123.31
14	7	78	ASN	CA-CB-CG	-5.39	107.21	112.60
21	W	129	ALA	O-C-N	5.39	128.90	122.27
6	f	142	HIS	ND1-CE1-NE2	5.38	113.78	108.40
7	g	123	ASN	N-CA-C	-5.38	105.53	113.61
5	E	83	HIS	ND1-CE1-NE2	5.38	113.78	108.40
23	T	249	MET	N-CA-C	-5.38	99.96	108.14
26	Z	65	GLU	CA-C-N	5.38	127.50	120.28
26	Z	65	GLU	C-N-CA	5.38	127.50	120.28
4	d	81	ARG	CA-C-O	-5.38	114.84	120.55
15	H	286	GLU	CA-C-O	5.38	126.13	120.42
3	c	43	ILE	CA-C-N	5.38	129.86	123.19
3	c	43	ILE	C-N-CA	5.38	129.86	123.19
9	i	38	SER	O-C-N	-5.38	116.97	121.54
11	k	176	PHE	CA-C-O	5.38	124.69	118.55
2	B	87	ASP	N-CA-CB	5.38	117.81	110.01
27	N	702	ALA	N-CA-C	5.38	117.14	111.28
33	O	310	PHE	CA-C-N	5.38	127.44	120.44
33	O	310	PHE	C-N-CA	5.38	127.44	120.44
1	a	187	GLU	N-CA-CB	5.38	117.87	109.85
11	4	172	MET	O-C-N	-5.38	113.74	121.54
20	J	96	VAL	CG1-CB-CG2	5.38	122.64	110.80
27	N	913	PRO	CA-C-O	-5.38	114.85	121.31
32	U	100	ARG	NE-CZ-NH1	5.38	126.88	121.50
4	d	183	PRO	O-C-N	5.38	129.19	123.01
7	g	199	ALA	N-CA-C	-5.38	105.98	112.54
11	k	146	HIS	CA-CB-CG	5.38	119.18	113.80
2	B	214	ILE	CA-C-O	5.38	127.50	120.78
12	5	200	VAL	O-C-N	5.38	127.09	121.87
18	L	56	ALA	CB-CA-C	-5.38	102.21	110.81
19	M	270	ALA	CB-CA-C	-5.38	101.86	110.79
26	Z	457	ILE	O-C-N	5.38	127.09	121.87
30	Q	179	LEU	CA-C-N	5.38	127.49	120.28
30	Q	179	LEU	C-N-CA	5.38	127.49	120.28
11	k	97	PRO	CB-CA-C	-5.38	102.35	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	57	ASP	CA-C-O	5.38	127.05	120.55
27	N	430	ASN	N-CA-C	5.38	118.85	112.72
7	g	215	CYS	CA-C-O	-5.38	114.56	120.36
14	n	40	GLU	N-CA-CB	5.38	117.87	109.97
15	H	294	LEU	N-CA-C	5.38	117.22	111.36
26	Z	891	PRO	CA-C-O	-5.38	114.86	121.31
32	U	197	LEU	N-CA-C	-5.38	105.32	111.07
4	d	221	ALA	CA-C-N	5.37	128.86	120.75
4	d	221	ALA	C-N-CA	5.37	128.86	120.75
2	B	181	ASP	N-CA-C	-5.37	105.08	111.69
7	G	66	VAL	O-C-N	5.37	128.90	123.20
15	H	311	ILE	N-CA-C	-5.37	105.76	113.07
16	I	306	MET	CA-C-N	5.37	127.92	120.29
16	I	306	MET	C-N-CA	5.37	127.92	120.29
21	W	30	ILE	O-C-N	5.37	127.18	121.91
21	W	58	ASN	CB-CA-C	5.37	115.49	110.17
2	b	119	GLN	N-CA-C	5.37	117.14	111.28
2	b	172	LYS	O-C-N	5.37	127.81	122.12
2	b	192	ALA	CA-C-O	-5.37	114.86	120.55
14	7	99	VAL	CA-C-O	-5.37	115.16	120.85
30	Q	128	GLU	N-CA-C	-5.37	104.92	112.12
31	R	120	LEU	CA-C-N	5.37	127.48	120.28
31	R	120	LEU	C-N-CA	5.37	127.48	120.28
2	b	233	PRO	N-CA-CB	5.37	108.10	103.27
7	g	83	HIS	CA-C-N	5.37	127.47	120.28
7	g	83	HIS	C-N-CA	5.37	127.47	120.28
9	i	82	MET	CA-C-N	5.37	127.47	120.28
9	i	82	MET	C-N-CA	5.37	127.47	120.28
15	H	434	ARG	NE-CZ-NH1	5.37	126.87	121.50
26	Z	865	ASP	CA-C-O	-5.37	112.99	119.27
5	e	44	LYS	N-CA-C	-5.37	105.51	111.36
21	W	154	LEU	N-CA-CB	5.37	118.49	110.22
29	P	223	LEU	N-CA-CB	5.37	118.56	110.30
8	h	86	CYS	CA-C-N	5.37	127.42	120.44
8	h	86	CYS	C-N-CA	5.37	127.42	120.44
26	Z	102	ILE	CA-C-O	5.37	124.89	119.20
1	a	78	ILE	CA-C-O	-5.36	112.76	119.95
7	g	54	LEU	N-CA-CB	5.36	118.64	110.44
1	A	238	ALA	N-CA-C	-5.36	105.51	111.36
27	N	407	GLY	CA-C-N	5.36	127.91	120.29
27	N	407	GLY	C-N-CA	5.36	127.91	120.29
30	Q	403	PRO	O-C-N	-5.36	115.40	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	219	ALA	O-C-N	-5.36	115.46	122.59
6	f	89	GLN	CA-C-O	-5.36	115.19	120.82
1	A	40	ASP	CA-CB-CG	5.36	117.96	112.60
14	7	8	GLY	N-CA-C	-5.36	101.21	112.04
16	I	235	ALA	CB-CA-C	-5.36	102.70	110.96
25	Y	79	ALA	CA-C-N	5.36	127.47	120.28
25	Y	79	ALA	C-N-CA	5.36	127.47	120.28
30	Q	71	LYS	CA-C-N	5.36	127.47	120.28
30	Q	71	LYS	C-N-CA	5.36	127.47	120.28
30	Q	211	PRO	CA-C-O	-5.36	115.30	121.36
33	O	23	HIS	CB-CG-ND1	-5.36	114.66	122.70
4	d	179	ARG	N-CA-C	-5.36	105.52	111.36
11	k	98	TYR	N-CA-C	-5.36	99.70	108.76
1	A	50	VAL	CA-CB-CG1	-5.36	101.29	110.40
6	F	46	VAL	CA-C-O	5.36	125.68	120.27
15	H	372	ASP	N-CA-C	-5.36	107.11	113.97
18	L	295	THR	CA-C-O	-5.36	115.97	121.87
4	d	127	PHE	CA-C-O	-5.36	115.72	121.56
1	a	158	LYS	CA-C-N	5.36	131.78	121.54
1	a	158	LYS	C-N-CA	5.36	131.78	121.54
15	H	146	VAL	CB-CA-C	-5.36	103.64	110.98
20	J	116	ARG	N-CA-CB	5.36	118.91	110.39
31	R	161	ALA	O-C-N	-5.36	116.38	123.13
1	a	32	ASN	CA-CB-CG	-5.36	107.25	112.60
7	g	225	LYS	CB-CA-C	-5.36	98.29	110.07
10	3	124	ASP	N-CA-C	-5.36	100.93	109.07
12	5	109	GLY	CA-C-N	5.36	125.28	119.76
12	5	109	GLY	C-N-CA	5.36	125.28	119.76
17	K	421	VAL	CA-C-O	-5.36	115.84	121.41
28	S	166	ASN	CA-C-O	-5.36	114.74	120.42
33	O	94	GLU	CA-C-N	5.36	127.46	120.28
33	O	94	GLU	C-N-CA	5.36	127.46	120.28
22	V	267	LYS	N-CA-C	5.35	117.87	111.71
24	X	75	TRP	N-CA-CB	5.35	119.15	110.42
3	c	117	ILE	O-C-N	5.35	127.34	121.83
14	n	60	MET	N-CA-C	-5.35	105.44	111.28
8	1	85	LEU	CA-C-O	5.35	126.22	120.55
9	2	221	CYS	CA-C-N	5.35	128.69	120.82
9	2	221	CYS	C-N-CA	5.35	128.69	120.82
26	Z	760	HIS	N-CA-C	-5.35	105.61	111.82
29	P	68	SER	N-CA-C	5.35	117.78	110.55
26	Z	218	GLU	CA-C-N	5.35	128.44	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	218	GLU	C-N-CA	5.35	128.44	120.31
29	P	336	HIS	CA-C-N	5.35	131.56	122.36
29	P	336	HIS	C-N-CA	5.35	131.56	122.36
2	b	104	TYR	N-CA-CB	5.35	117.92	110.11
5	E	59	ILE	CA-C-O	5.35	126.15	120.48
9	2	48	THR	CA-C-N	5.35	128.44	120.31
9	2	48	THR	C-N-CA	5.35	128.44	120.31
14	7	112	ASN	OD1-CG-ND2	5.35	127.95	122.60
19	M	64	ASP	CA-C-N	5.35	127.45	120.28
19	M	64	ASP	C-N-CA	5.35	127.45	120.28
22	V	257	GLU	CA-C-N	5.35	130.33	122.63
22	V	257	GLU	C-N-CA	5.35	130.33	122.63
26	Z	278	LEU	N-CA-C	-5.35	106.34	112.92
27	N	796	VAL	CA-C-N	5.35	127.39	120.44
27	N	796	VAL	C-N-CA	5.35	127.39	120.44
29	P	282	HIS	CG-CD2-NE2	5.35	112.55	107.20
29	P	405	PRO	CA-N-CD	5.35	119.49	112.00
5	e	106	GLN	CB-CA-C	-5.35	101.91	110.79
2	B	73	ALA	CA-C-O	5.35	126.77	120.89
2	B	244	ASN	CB-CG-ND2	5.35	124.42	116.40
16	I	139	GLU	CA-C-O	-5.35	114.88	120.55
27	N	783	SER	CA-C-O	-5.35	115.67	121.87
28	S	186	TYR	CA-CB-CG	-5.35	104.28	113.90
6	F	79	ASP	O-C-N	5.35	128.24	122.15
10	3	99	PHE	CA-CB-CG	-5.35	108.45	113.80
21	W	192	LEU	N-CA-C	-5.35	106.14	113.30
27	N	438	ASP	CA-C-N	5.35	127.78	120.46
27	N	438	ASP	C-N-CA	5.35	127.78	120.46
29	P	118	VAL	CB-CA-C	-5.35	104.84	112.22
31	R	350	LEU	N-CA-C	-5.35	105.53	111.36
13	m	198	VAL	CB-CA-C	5.34	118.93	111.34
9	2	151	ALA	N-CA-C	-5.34	105.53	111.36
12	5	37	ILE	N-CA-C	-5.34	105.51	110.53
27	N	117	TYR	CB-CG-CD2	-5.34	112.78	120.80
31	R	349	SER	N-CA-CB	5.34	118.54	110.42
3	C	96	ASN	CB-CA-C	-5.34	101.92	110.79
7	g	101	THR	O-C-N	-5.34	115.86	122.16
12	l	29	GLN	N-CA-C	-5.34	106.54	113.16
12	l	37	ILE	O-C-N	5.34	127.33	121.83
13	m	77	PHE	O-C-N	-5.34	116.46	122.12
1	A	111	ARG	NE-CZ-NH1	-5.34	116.16	121.50
11	4	165	VAL	O-C-N	-5.34	116.69	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	406	LEU	N-CA-C	-5.34	105.37	111.14
17	K	148	ASP	CA-CB-CG	5.34	117.94	112.60
26	Z	622	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
28	S	444	GLU	CB-CG-CD	-5.34	103.52	112.60
30	Q	433	LEU	N-CA-CB	-5.34	102.25	110.16
2	b	110	LEU	CA-C-N	5.34	127.78	120.46
2	b	110	LEU	C-N-CA	5.34	127.78	120.46
2	b	165	GLY	N-CA-C	-5.34	106.17	111.56
7	g	44	PHE	N-CA-C	-5.34	100.47	109.07
13	m	200	ASP	CA-C-N	5.34	126.53	121.46
13	m	200	ASP	C-N-CA	5.34	126.53	121.46
1	A	127	PRO	CA-C-N	5.34	128.35	120.82
1	A	127	PRO	C-N-CA	5.34	128.35	120.82
9	2	2	THR	N-CA-CB	5.34	119.58	110.71
9	2	134	ALA	CA-C-N	5.34	127.75	120.54
9	2	134	ALA	C-N-CA	5.34	127.75	120.54
10	3	151	SER	CA-C-N	5.34	128.43	120.31
10	3	151	SER	C-N-CA	5.34	128.43	120.31
16	I	68	HIS	CA-C-N	5.34	127.38	120.44
16	I	68	HIS	C-N-CA	5.34	127.38	120.44
19	M	237	ALA	CA-C-O	-5.34	114.31	120.24
26	Z	226	GLU	N-CA-C	5.34	117.10	111.28
26	Z	457	ILE	CA-C-O	-5.34	115.40	120.95
30	Q	54	GLN	N-CA-C	5.34	117.10	111.28
7	g	190	LYS	CB-CG-CD	5.34	123.58	111.30
10	j	194	VAL	N-CA-CB	5.34	118.58	111.64
1	A	13	GLU	N-CA-CB	5.34	118.55	110.28
9	2	80	LEU	N-CA-C	-5.34	105.46	111.28
1	a	97	TYR	CA-C-N	5.34	127.87	120.29
1	a	97	TYR	C-N-CA	5.34	127.87	120.29
8	h	60	GLN	O-C-N	5.34	127.64	122.09
1	A	116	SER	N-CA-C	5.34	117.10	111.28
7	G	90	GLU	CA-C-N	5.34	129.71	120.58
7	G	90	GLU	C-N-CA	5.34	129.71	120.58
11	4	146	HIS	CA-CB-CG	-5.34	108.46	113.80
16	I	75	PHE	CA-CB-CG	5.34	119.14	113.80
19	M	135	VAL	CA-C-N	5.34	128.77	120.60
19	M	135	VAL	C-N-CA	5.34	128.77	120.60
19	M	411	LYS	CA-C-N	5.34	127.96	120.28
19	M	411	LYS	C-N-CA	5.34	127.96	120.28
22	V	189	ILE	CB-CA-C	-5.34	104.94	112.14
27	N	339	MET	N-CA-CB	5.34	118.06	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	812	ALA	N-CA-CB	5.34	118.06	110.16
28	S	140	LEU	N-CA-CB	5.34	117.75	110.01
29	P	217	LYS	CA-C-N	5.34	127.70	120.44
29	P	217	LYS	C-N-CA	5.34	127.70	120.44
30	Q	301	ALA	O-C-N	5.34	129.17	122.23
10	3	82	GLU	CA-C-O	-5.33	115.14	120.63
16	I	112	ILE	CA-C-N	5.33	130.13	123.14
16	I	112	ILE	C-N-CA	5.33	130.13	123.14
10	j	43	PHE	CA-CB-CG	-5.33	108.47	113.80
19	M	177	THR	O-C-N	-5.33	115.50	122.59
23	T	199	PHE	CA-CB-CG	-5.33	108.47	113.80
26	Z	938	GLN	CA-C-N	5.33	131.72	121.54
26	Z	938	GLN	C-N-CA	5.33	131.72	121.54
27	N	866	TYR	CB-CG-CD2	-5.33	112.80	120.80
33	O	152	ASP	CA-C-N	5.33	127.86	120.29
33	O	152	ASP	C-N-CA	5.33	127.86	120.29
11	k	8	ARG	NE-CZ-NH2	-5.33	114.40	119.20
13	m	18	GLU	N-CA-C	-5.33	106.71	114.12
15	H	392	HIS	CA-C-N	5.33	128.41	120.31
15	H	392	HIS	C-N-CA	5.33	128.41	120.31
19	M	228	LYS	CA-C-N	5.33	131.72	121.54
19	M	228	LYS	C-N-CA	5.33	131.72	121.54
1	a	181	LYS	N-CA-CB	5.33	119.50	110.49
13	m	169	LYS	N-CA-C	-5.33	102.86	110.59
20	J	364	GLU	CA-C-N	5.33	127.86	120.29
20	J	364	GLU	C-N-CA	5.33	127.86	120.29
27	N	370	SER	N-CA-CB	5.33	117.95	110.12
28	S	362	SER	CB-CA-C	-5.33	102.51	110.88
7	g	189	VAL	CB-CA-C	-5.33	104.95	112.14
13	m	141	ALA	CB-CA-C	-5.33	101.79	110.85
18	L	393	ASN	CA-CB-CG	-5.33	107.27	112.60
25	Y	28	SER	CB-CA-C	-5.33	100.78	110.63
29	P	377	GLU	N-CA-CB	5.33	117.73	110.01
3	c	121	TYR	CB-CA-C	-5.33	99.18	110.31
17	K	181	LYS	N-CA-CB	5.33	118.04	110.16
19	M	174	GLU	N-CA-CB	5.33	119.49	110.49
27	N	443	LEU	CA-C-O	5.33	125.91	119.31
33	O	242	ILE	N-CA-CB	-5.33	105.28	112.10
9	i	100	VAL	N-CA-CB	5.32	118.38	111.67
9	i	116	HIS	CG-CD2-NE2	5.32	112.52	107.20
5	E	54	ASP	N-CA-C	-5.32	104.91	111.40
8	1	132	THR	O-C-N	-5.32	116.48	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	66	ALA	O-C-N	5.32	127.76	122.12
6	f	172	GLU	O-C-N	5.32	128.22	122.15
11	k	72	ASP	CA-C-O	-5.32	114.95	121.28
7	G	169	LYS	O-C-N	5.32	127.55	122.07
15	H	218	ILE	CA-C-O	-5.32	114.72	120.47
31	R	273	SER	O-C-N	-5.32	115.96	121.28
32	U	173	HIS	CG-CD2-NE2	5.32	112.52	107.20
1	A	42	THR	N-CA-C	-5.32	99.61	108.34
14	7	68	LYS	CA-C-O	5.32	126.41	120.82
20	J	190	PRO	CA-C-O	-5.32	112.84	120.56
28	S	122	ASN	CA-CB-CG	-5.32	107.28	112.60
3	C	59	ASP	CA-C-N	-5.32	112.74	120.29
3	C	59	ASP	C-N-CA	-5.32	112.74	120.29
15	H	403	ARG	N-CA-CB	5.32	119.15	110.37
16	I	188	GLU	N-CA-C	5.32	117.51	111.02
26	Z	320	SER	CA-C-N	5.32	127.41	120.28
26	Z	320	SER	C-N-CA	5.32	127.41	120.28
26	Z	581	VAL	N-CA-C	-5.32	104.85	112.35
7	g	242	GLU	CB-CA-C	-5.32	101.81	110.85
3	C	181	ASP	O-C-N	5.32	127.75	122.12
7	G	34	ILE	CA-CB-CG2	-5.32	101.46	110.50
16	I	113	ILE	O-C-N	-5.32	117.52	123.26
19	M	344	ASP	CB-CA-C	-5.32	110.43	116.54
24	X	54	GLU	CB-CG-CD	-5.32	103.56	112.60
26	Z	338	HIS	CB-CG-CD2	-5.32	124.29	131.20
15	H	430	ALA	CA-C-N	5.31	127.74	120.46
15	H	430	ALA	C-N-CA	5.31	127.74	120.46
2	b	92	VAL	CA-CB-CG1	5.31	119.43	110.40
3	C	9	THR	CA-C-O	-5.31	113.32	119.59
9	2	203	TYR	CA-C-N	5.31	128.31	120.82
9	2	203	TYR	C-N-CA	5.31	128.31	120.82
13	6	35	ILE	N-CA-CB	-5.31	104.94	111.00
13	6	144	SER	CB-CA-C	-5.31	99.21	110.31
17	K	293	GLN	OE1-CD-NE2	5.31	127.91	122.60
18	L	253	ASP	CA-C-N	5.31	127.35	120.44
18	L	253	ASP	C-N-CA	5.31	127.35	120.44
27	N	409	GLY	N-CA-C	-5.31	106.25	113.37
27	N	417	ARG	N-CA-C	-5.31	106.85	113.38
14	n	199	ILE	CA-C-O	5.31	126.11	120.48
15	H	57	LYS	CB-CA-C	-5.31	101.97	110.79
23	T	210	PHE	CB-CA-C	-5.31	105.02	111.82
26	Z	958	ASN	CB-CG-OD1	5.31	131.42	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	132	GLY	CA-C-O	5.31	125.79	119.10
7	G	109	ALA	CA-C-N	5.31	127.34	120.44
7	G	109	ALA	C-N-CA	5.31	127.34	120.44
19	M	378	GLU	N-CA-C	-5.31	105.57	111.36
29	P	53	ALA	CA-C-N	5.31	129.71	120.68
29	P	53	ALA	C-N-CA	5.31	129.71	120.68
11	k	192	VAL	N-CA-C	-5.31	98.32	107.24
13	6	64	LEU	CA-C-N	5.31	127.25	120.56
13	6	64	LEU	C-N-CA	5.31	127.25	120.56
14	7	175	GLU	CA-C-N	5.31	127.83	120.29
14	7	175	GLU	C-N-CA	5.31	127.83	120.29
28	S	229	THR	N-CA-C	-5.31	105.58	111.36
33	O	209	GLU	CA-C-O	5.31	126.17	120.55
9	i	109	HIS	CA-C-N	5.31	131.12	121.89
9	i	109	HIS	C-N-CA	5.31	131.12	121.89
10	j	59	VAL	O-C-N	5.31	127.11	121.91
1	A	212	ASN	CB-CA-C	-5.31	102.55	110.88
11	4	97	PRO	N-CA-CB	5.31	108.03	103.31
19	M	381	ARG	CB-CA-C	-5.31	101.83	110.85
26	Z	424	SER	CA-C-N	5.31	129.00	120.30
26	Z	424	SER	C-N-CA	5.31	129.00	120.30
27	N	797	GLU	CB-CA-C	5.31	119.21	110.88
17	K	337	LYS	N-CA-C	-5.30	99.45	108.26
23	T	79	GLU	CA-C-O	-5.30	115.25	120.82
26	Z	112	LYS	O-C-N	-5.30	116.36	122.09
26	Z	488	ALA	CB-CA-C	-5.30	101.83	110.85
27	N	102	VAL	N-CA-CB	-5.30	104.34	110.55
33	O	353	VAL	CA-C-N	5.30	128.02	120.49
33	O	353	VAL	C-N-CA	5.30	128.02	120.49
11	k	176	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	198	ILE	CA-C-N	5.30	127.39	120.28
1	A	198	ILE	C-N-CA	5.30	127.39	120.28
11	4	9	VAL	CA-C-N	5.30	127.64	120.38
11	4	9	VAL	C-N-CA	5.30	127.64	120.38
17	K	366	ALA	CA-C-N	5.30	131.67	121.54
17	K	366	ALA	C-N-CA	5.30	131.67	121.54
19	M	138	ASP	N-CA-C	5.30	117.14	111.36
9	i	141	HIS	CA-CB-CG	-5.30	108.50	113.80
14	n	119	VAL	O-C-N	5.30	128.93	123.20
17	K	192	LEU	CA-C-O	5.30	126.12	120.24
23	T	70	ILE	N-CA-C	5.30	116.03	110.62
23	T	241	GLU	N-CA-C	5.30	117.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	677	ASP	N-CA-CB	5.30	118.01	110.16
29	P	123	ARG	O-C-N	-5.30	116.50	122.12
31	R	366	ASN	CA-C-O	-5.30	114.93	120.55
2	b	211	LEU	N-CA-CB	5.30	119.41	110.77
29	P	13	TYR	CA-CB-CG	5.30	123.44	113.90
14	n	110	LEU	CB-CA-C	-5.30	102.30	111.30
2	B	17	LYS	N-CA-CB	5.30	119.44	110.49
5	E	140	ASP	CA-CB-CG	-5.30	107.30	112.60
20	J	33	LYS	CA-C-N	5.30	127.72	120.46
20	J	33	LYS	C-N-CA	5.30	127.72	120.46
20	J	64	LEU	CA-C-O	-5.30	115.26	120.82
21	W	70	GLY	N-CA-C	5.30	120.47	113.37
23	T	21	ALA	N-CA-CB	5.30	117.69	110.01
27	N	494	LYS	O-C-N	5.30	126.01	121.30
2	B	54	PRO	CA-N-CD	5.29	119.41	112.00
3	C	54	THR	CA-CB-OG1	5.29	117.54	109.60
8	1	57	ASP	CA-C-N	5.29	127.23	120.56
8	1	57	ASP	C-N-CA	5.29	127.23	120.56
20	J	213	VAL	CA-C-O	5.29	126.30	120.48
28	S	129	GLU	CB-CA-C	-5.29	99.26	109.37
9	i	99	ILE	CA-CB-CG1	5.29	119.40	110.40
9	2	123	TYR	CB-CG-CD1	-5.29	112.86	120.80
17	K	260	LEU	N-CA-CB	5.29	118.00	110.16
26	Z	405	ASN	O-C-N	5.29	127.52	122.07
1	a	93	ALA	N-CA-C	5.29	117.05	111.28
12	l	114	TYR	CA-C-N	5.29	130.36	123.06
12	l	114	TYR	C-N-CA	5.29	130.36	123.06
2	B	45	ILE	N-CA-C	-5.29	100.58	108.46
7	G	200	HIS	N-CA-C	-5.29	106.50	113.17
20	J	120	TYR	CA-CB-CG	-5.29	104.38	113.90
20	J	252	SER	CB-CA-C	-5.29	102.41	111.46
13	m	86	ILE	O-C-N	5.29	127.78	121.80
8	1	162	ALA	CA-C-N	5.29	127.93	120.42
8	1	162	ALA	C-N-CA	5.29	127.93	120.42
13	6	34	SER	N-CA-CB	5.29	118.88	110.57
18	L	88	TYR	CA-C-N	5.29	127.80	120.29
18	L	88	TYR	C-N-CA	5.29	127.80	120.29
18	L	329	ARG	NE-CZ-NH2	-5.29	114.44	119.20
20	J	131	ASP	CA-C-N	5.29	125.10	119.28
20	J	131	ASP	C-N-CA	5.29	125.10	119.28
23	T	107	SER	N-CA-CB	5.29	117.90	110.12
26	Z	714	ASP	CA-CB-CG	-5.29	107.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	312	ASP	CA-C-N	5.29	127.93	120.42
33	O	312	ASP	C-N-CA	5.29	127.93	120.42
5	e	137	ALA	N-CA-C	-5.29	100.78	109.40
12	l	140	LEU	CA-C-N	5.29	127.63	120.44
12	l	140	LEU	C-N-CA	5.29	127.63	120.44
22	V	111	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
26	Z	538	CYS	N-CA-CB	5.29	117.33	109.19
31	R	63	TYR	CB-CG-CD1	-5.29	112.87	120.80
31	R	211	LYS	CA-C-O	-5.29	114.94	120.55
4	D	140	ASP	N-CA-C	-5.29	101.03	109.07
26	Z	439	TYR	N-CA-C	5.29	117.04	111.28
29	P	428	THR	CA-C-O	5.29	126.03	120.42
30	Q	85	MET	N-CA-C	-5.29	105.52	111.28
20	J	235	VAL	CA-CB-CG2	-5.29	101.41	110.40
26	Z	743	ILE	N-CA-C	-5.29	105.35	110.42
31	R	134	TRP	CE2-CD2-CE3	5.29	124.08	118.80
3	c	79	LEU	N-CA-C	-5.28	102.23	110.10
3	c	143	TYR	N-CA-CB	-5.28	102.93	110.80
5	e	151	GLU	N-CA-C	-5.28	102.84	110.40
1	A	217	GLY	CA-C-N	5.28	130.48	122.98
1	A	217	GLY	C-N-CA	5.28	130.48	122.98
16	I	75	PHE	O-C-N	-5.28	116.63	122.07
28	S	39	ASN	N-CA-CB	5.28	117.98	110.16
15	H	55	ASP	CA-CB-CG	-5.28	107.32	112.60
23	T	40	LEU	N-CA-C	-5.28	105.60	111.36
26	Z	64	TYR	N-CA-C	-5.28	106.89	113.55
28	S	485	LYS	O-C-N	5.28	127.51	122.07
29	P	142	ASP	CA-C-O	-5.28	113.90	119.97
10	j	147	GLY	N-CA-C	-5.28	106.37	112.50
3	C	239	VAL	CA-C-O	-5.28	115.19	121.05
17	K	186	GLU	N-CA-C	5.28	116.72	111.07
19	M	357	ARG	CA-C-N	5.28	127.36	120.28
19	M	357	ARG	C-N-CA	5.28	127.36	120.28
25	Y	39	PRO	CA-C-N	5.28	127.32	120.56
25	Y	39	PRO	C-N-CA	5.28	127.32	120.56
8	1	169	SER	CB-CA-C	-5.28	100.48	109.51
9	2	70	THR	CA-C-N	5.28	129.86	122.36
9	2	70	THR	C-N-CA	5.28	129.86	122.36
26	Z	716	THR	N-CA-CB	5.28	117.62	109.91
27	N	788	TYR	CA-CB-CG	-5.28	104.40	113.90
29	P	289	ASN	CA-CB-CG	-5.28	107.32	112.60
6	f	65	CYS	N-CA-C	-5.28	106.52	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	89	ALA	N-CA-CB	5.28	117.97	110.16
19	M	402	ALA	CA-C-N	5.28	127.30	120.44
19	M	402	ALA	C-N-CA	5.28	127.30	120.44
22	V	159	ILE	N-CA-C	-5.28	100.72	108.11
26	Z	880	SER	CA-C-O	5.28	126.14	120.55
31	R	134	TRP	CD2-CE2-CZ2	-5.28	117.12	122.40
18	L	64	LEU	CA-C-N	5.28	127.78	120.29
18	L	64	LEU	C-N-CA	5.28	127.78	120.29
26	Z	18	ILE	N-CA-C	-5.28	105.94	110.74
26	Z	313	ILE	CA-C-N	5.28	127.30	120.44
26	Z	313	ILE	C-N-CA	5.28	127.30	120.44
26	Z	375	ASP	CA-C-N	5.28	131.62	121.54
26	Z	375	ASP	C-N-CA	5.28	131.62	121.54
28	S	330	LEU	CA-C-N	5.28	129.04	120.60
28	S	330	LEU	C-N-CA	5.28	129.04	120.60
15	H	192	ASP	CA-C-N	5.27	125.19	119.76
15	H	192	ASP	C-N-CA	5.27	125.19	119.76
19	M	266	ALA	CB-CA-C	-5.27	102.03	110.79
6	f	141	ALA	CA-C-O	5.27	127.69	121.36
11	k	140	THR	O-C-N	-5.27	115.42	122.49
1	A	102	ASP	CA-CB-CG	-5.27	107.33	112.60
16	I	352	ASN	CA-CB-CG	-5.27	107.33	112.60
33	O	29	PHE	O-C-N	5.27	127.71	122.12
6	f	57	SER	O-C-N	5.27	129.23	123.01
9	i	31	CYS	CA-C-O	-5.27	112.97	120.51
6	F	109	HIS	CA-C-N	5.27	128.32	120.31
6	F	109	HIS	C-N-CA	5.27	128.32	120.31
15	H	228	PRO	N-CA-CB	5.27	108.57	103.51
19	M	380	ALA	N-CA-CB	5.27	117.87	110.12
23	T	149	ASP	CA-C-O	-5.27	115.26	120.90
23	T	265	ASP	CB-CA-C	-5.27	102.04	110.79
33	O	84	ALA	O-C-N	5.27	127.78	122.09
10	j	83	PRO	CB-CA-C	-5.27	103.99	112.21
14	n	45	VAL	CA-C-O	5.27	126.27	120.48
1	A	23	PHE	CB-CA-C	-5.27	100.56	110.67
14	7	120	GLN	N-CA-CB	5.27	117.97	110.44
24	X	42	GLU	CA-CB-CG	5.27	124.63	114.10
27	N	883	SER	CA-C-O	5.27	126.17	120.32
29	P	78	GLN	CA-C-N	5.27	131.60	121.54
29	P	78	GLN	C-N-CA	5.27	131.60	121.54
5	E	183	LEU	N-CA-C	5.27	117.09	110.24
26	Z	588	ILE	CA-C-O	5.27	126.89	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	16	PHE	CA-C-N	5.26	127.33	120.28
4	D	16	PHE	C-N-CA	5.26	127.33	120.28
13	6	70	ASN	CA-CB-CG	-5.26	107.33	112.60
18	L	93	ASN	OD1-CG-ND2	-5.26	117.33	122.60
20	J	397	ALA	CB-CA-C	-5.26	101.00	110.37
31	R	122	GLU	N-CA-C	-5.26	105.19	111.03
9	i	222	ASP	CA-C-N	5.26	131.44	121.97
9	i	222	ASP	C-N-CA	5.26	131.44	121.97
14	n	230	THR	O-C-N	5.26	127.49	122.07
19	M	260	ALA	CA-C-N	5.26	127.33	120.28
19	M	260	ALA	C-N-CA	5.26	127.33	120.28
27	N	336	ASN	CA-CB-CG	-5.26	107.34	112.60
27	N	647	ASP	CA-C-N	5.26	124.59	118.85
27	N	647	ASP	C-N-CA	5.26	124.59	118.85
1	a	41	CYS	CA-C-N	-5.26	115.35	122.77
1	a	41	CYS	C-N-CA	-5.26	115.35	122.77
10	3	3	PRO	O-C-N	5.26	128.81	122.23
14	7	13	SER	O-C-N	5.26	129.37	123.48
27	N	510	HIS	CG-CD2-NE2	5.26	112.46	107.20
29	P	55	SER	CA-C-N	5.26	127.33	120.28
29	P	55	SER	C-N-CA	5.26	127.33	120.28
33	O	39	PHE	CA-CB-CG	-5.26	108.54	113.80
33	O	174	THR	CA-C-N	5.26	127.33	120.28
33	O	174	THR	C-N-CA	5.26	127.33	120.28
6	F	88	ARG	N-CA-CB	5.26	117.85	110.12
8	1	193	TYR	CB-CG-CD1	5.26	128.69	120.80
9	2	180	ILE	CA-C-O	-5.26	114.06	120.69
9	i	90	TYR	CA-CB-CG	-5.26	104.44	113.90
11	k	52	ASP	CA-CB-CG	-5.26	107.34	112.60
5	E	127	SER	O-C-N	-5.26	115.60	122.59
10	3	35	VAL	N-CA-C	-5.26	107.04	111.56
20	J	36	SER	N-CA-C	-5.26	105.63	111.36
21	W	167	GLU	CB-CG-CD	-5.26	103.66	112.60
27	N	577	SER	N-CA-C	5.26	118.86	112.23
30	Q	35	SER	N-CA-C	5.26	117.01	111.28
4	d	195	ARG	O-C-N	-5.26	116.62	122.09
7	g	121	LEU	CB-CA-C	-5.26	101.91	110.85
12	l	161	ILE	CA-C-O	-5.26	114.79	120.47
21	W	184	ASN	CA-C-O	-5.26	114.85	120.42
24	X	60	GLU	O-C-N	5.26	127.69	122.12
27	N	234	ASP	CA-C-O	5.26	126.01	120.33
1	a	163	GLY	CA-C-N	5.25	125.33	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	163	GLY	C-N-CA	5.25	125.33	119.87
10	j	135	PHE	CA-C-N	5.25	130.29	122.99
10	j	135	PHE	C-N-CA	5.25	130.29	122.99
27	N	226	ASN	OD1-CG-ND2	-5.25	117.34	122.60
4	d	61	LYS	N-CA-C	-5.25	106.72	113.02
5	e	101	VAL	N-CA-CB	5.25	119.33	110.56
6	f	142	HIS	CA-CB-CG	5.25	119.05	113.80
14	n	201	ASP	N-CA-C	-5.25	102.00	110.14
7	G	9	SER	N-CA-C	5.25	118.64	111.39
13	6	7	ASP	CB-CA-C	-5.25	98.51	110.07
21	W	22	PRO	CA-C-N	5.25	131.16	121.70
21	W	22	PRO	C-N-CA	5.25	131.16	121.70
26	Z	79	THR	CA-C-O	5.25	126.12	120.55
27	N	745	LEU	N-CA-C	5.25	119.31	113.01
31	R	102	LEU	N-CA-CB	5.25	119.37	110.49
31	R	280	ILE	CA-CB-CG1	5.25	119.33	110.40
8	h	33	LYS	N-CA-C	-5.25	106.87	113.28
32	U	70	HIS	CA-C-N	5.25	127.32	120.28
32	U	70	HIS	C-N-CA	5.25	127.32	120.28
3	c	14	PRO	CA-C-N	5.25	127.27	120.44
3	c	14	PRO	C-N-CA	5.25	127.27	120.44
5	e	111	LEU	N-CA-CB	5.25	118.31	110.22
7	G	133	ILE	N-CA-CB	5.25	117.29	110.99
19	M	408	SER	O-C-N	-5.25	115.81	122.27
27	N	787	MET	N-CA-CB	5.25	118.43	109.87
31	R	205	GLU	N-CA-C	5.25	117.08	111.36
10	j	112	ASN	CA-CB-CG	-5.25	107.35	112.60
14	n	17	ASP	N-CA-C	5.25	117.00	111.28
26	Z	921	GLU	CA-C-O	-5.25	115.36	119.66
29	P	276	LEU	CA-C-N	5.25	127.62	120.54
29	P	276	LEU	C-N-CA	5.25	127.62	120.54
31	R	142	ALA	CA-C-O	-5.25	114.17	120.10
1	A	35	ALA	N-CA-C	-5.25	100.14	109.06
1	A	229	ALA	CA-C-N	5.25	127.26	120.44
1	A	229	ALA	C-N-CA	5.25	127.26	120.44
6	F	193	VAL	N-CA-CB	5.25	116.69	110.55
7	G	143	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
11	4	155	GLU	CB-CG-CD	5.25	121.52	112.60
18	L	198	GLU	O-C-N	5.25	127.76	122.09
21	W	98	LEU	N-CA-C	-5.25	106.38	112.89
22	V	247	ILE	N-CA-C	-5.25	106.77	113.22
23	T	160	ALA	N-CA-C	5.25	116.68	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	46	TRP	N-CA-CB	5.25	117.79	109.71
33	O	16	MET	O-C-N	5.25	127.47	122.07
11	4	93	ARG	CD-NE-CZ	-5.25	117.06	124.40
27	N	896	PHE	CB-CG-CD2	5.25	129.62	120.70
8	h	124	TYR	CB-CG-CD1	5.24	128.67	120.80
12	l	191	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
5	E	206	GLU	N-CA-C	-5.24	106.66	113.16
6	F	119	THR	CA-C-N	5.24	127.74	120.29
6	F	119	THR	C-N-CA	5.24	127.74	120.29
17	K	275	ASP	CA-CB-CG	5.24	117.84	112.60
17	K	302	GLN	CA-C-O	-5.24	113.94	119.97
23	T	119	THR	CA-C-N	5.24	127.62	120.54
23	T	119	THR	C-N-CA	5.24	127.62	120.54
26	Z	477	TYR	CA-C-N	-5.24	112.97	120.42
26	Z	477	TYR	C-N-CA	-5.24	112.97	120.42
27	N	497	ALA	CA-C-N	5.24	127.17	120.56
27	N	497	ALA	C-N-CA	5.24	127.17	120.56
1	a	239	ILE	CA-C-N	5.24	127.73	120.29
1	a	239	ILE	C-N-CA	5.24	127.73	120.29
10	j	58	ASP	CA-CB-CG	-5.24	107.36	112.60
14	n	216	ASN	OD1-CG-ND2	-5.24	117.36	122.60
6	f	226	GLY	CA-C-N	5.24	128.98	120.60
6	f	226	GLY	C-N-CA	5.24	128.98	120.60
18	L	378	ALA	CA-C-N	5.24	127.30	120.28
18	L	378	ALA	C-N-CA	5.24	127.30	120.28
33	O	162	SER	N-CA-C	-5.24	99.11	108.13
3	c	168	THR	CA-CB-CG2	5.24	119.41	110.50
7	g	120	THR	CA-C-O	5.24	124.90	119.14
16	I	151	HIS	O-C-N	5.24	128.12	122.15
26	Z	39	SER	N-CA-C	-5.24	105.74	111.82
31	R	172	LEU	N-CA-C	-5.24	105.65	111.36
33	O	137	TYR	N-CA-C	-5.24	105.57	111.28
33	O	318	HIS	CG-CD2-NE2	5.24	112.44	107.20
10	j	65	MET	N-CA-C	-5.24	104.99	111.33
13	m	193	GLU	N-CA-C	5.24	116.99	111.28
20	J	270	ARG	NE-CZ-NH1	-5.24	116.26	121.50
26	Z	592	GLU	CB-CG-CD	-5.24	103.70	112.60
27	N	719	ASN	N-CA-C	-5.24	99.22	108.23
28	S	269	GLU	CB-CA-C	-5.24	102.10	110.79
2	b	187	ASP	N-CA-C	-5.24	105.75	111.82
2	B	190	HIS	CA-CB-CG	-5.24	108.56	113.80
22	V	230	TYR	N-CA-C	-5.24	107.06	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	143	ASP	CB-CA-C	-5.23	101.88	110.72
4	D	82	ILE	CB-CA-C	-5.23	105.08	112.14
26	Z	211	PHE	O-C-N	5.23	127.67	122.12
27	N	768	ILE	CA-C-N	5.23	125.69	120.14
27	N	768	ILE	C-N-CA	5.23	125.69	120.14
33	O	252	PHE	CA-C-O	-5.23	115.00	120.55
5	e	91	HIS	CA-CB-CG	-5.23	108.57	113.80
5	e	207	ASN	N-CA-CB	5.23	118.51	110.61
9	i	158	ALA	N-CA-C	-5.23	105.26	111.69
10	3	151	SER	O-C-N	-5.23	116.19	122.15
10	3	182	TRP	CD2-CE2-CZ2	-5.23	117.17	122.40
11	4	114	PRO	CB-CA-C	-5.23	104.10	110.95
13	6	129	GLY	CA-C-O	-5.23	111.47	120.57
25	Y	82	ASP	N-CA-CB	5.23	117.60	110.01
26	Z	927	VAL	N-CA-CB	-5.23	104.25	111.99
27	N	637	ALA	CA-C-O	-5.23	115.01	120.55
14	n	25	ASP	CA-CB-CG	-5.23	107.37	112.60
26	Z	510	LEU	CA-C-O	-5.23	113.77	118.79
30	Q	244	GLU	O-C-N	5.23	128.11	122.15
31	R	247	GLU	O-C-N	5.23	127.66	122.12
33	O	184	ASP	N-CA-CB	5.23	118.52	110.21
9	i	72	ARG	CA-C-N	5.23	128.60	120.60
9	i	72	ARG	C-N-CA	5.23	128.60	120.60
13	m	151	ASP	CA-CB-CG	5.23	117.83	112.60
14	n	48	ASN	N-CA-C	-5.23	106.30	113.30
1	A	66	ILE	N-CA-C	-5.23	105.30	111.00
2	B	183	LEU	CA-C-N	5.23	129.15	120.94
2	B	183	LEU	C-N-CA	5.23	129.15	120.94
3	C	168	THR	CA-C-N	5.23	127.71	120.29
3	C	168	THR	C-N-CA	5.23	127.71	120.29
1	a	212	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	b	247	LEU	CB-CA-C	-5.23	99.69	109.72
9	2	16	ALA	CA-C-N	5.23	132.29	121.32
9	2	16	ALA	C-N-CA	5.23	132.29	121.32
12	5	67	GLU	N-CA-CB	5.23	118.38	110.28
17	K	310	THR	CA-C-N	5.23	128.52	121.05
17	K	310	THR	C-N-CA	5.23	128.52	121.05
14	n	137	TYR	O-C-N	-5.22	117.83	123.42
19	M	368	MET	N-CA-CB	5.22	117.54	110.38
22	V	199	LEU	CA-C-N	5.22	131.52	121.54
22	V	199	LEU	C-N-CA	5.22	131.52	121.54
31	R	391	ASN	CA-C-O	-5.22	113.78	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	23	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
11	k	62	ALA	CB-CA-C	-5.22	102.68	110.88
7	G	185	ALA	N-CA-CB	5.22	118.38	110.28
7	G	216	SER	CA-C-N	5.22	127.71	120.29
7	G	216	SER	C-N-CA	5.22	127.71	120.29
15	H	95	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
15	H	167	ASP	CA-C-N	5.22	126.56	121.65
15	H	167	ASP	C-N-CA	5.22	126.56	121.65
15	H	244	LYS	N-CA-CB	5.22	119.31	110.49
22	V	251	TYR	CA-C-N	5.22	127.28	120.28
22	V	251	TYR	C-N-CA	5.22	127.28	120.28
7	g	77	LEU	O-C-N	5.22	129.95	123.01
9	i	8	PHE	CA-C-N	5.22	127.28	120.28
9	i	8	PHE	C-N-CA	5.22	127.28	120.28
9	i	141	HIS	CB-CA-C	-5.22	101.97	110.85
12	l	17	ASP	N-CA-CB	5.22	118.89	110.85
13	m	70	ASN	OD1-CG-ND2	5.22	127.82	122.60
21	W	137	VAL	N-CA-C	-5.22	100.13	107.75
27	N	510	HIS	ND1-CE1-NE2	5.22	113.62	108.40
1	a	12	PRO	N-CA-CB	5.22	108.52	103.51
26	Z	628	ASN	CB-CG-ND2	-5.22	108.57	116.40
7	g	177	ASP	CA-CB-CG	5.22	117.82	112.60
13	m	62	ASP	O-C-N	5.22	127.44	122.07
5	E	169	GLU	CA-C-N	5.22	125.74	120.00
5	E	169	GLU	C-N-CA	5.22	125.74	120.00
20	J	231	ARG	N-CA-C	-5.22	105.04	111.40
27	N	819	LYS	O-C-N	5.22	127.44	122.07
30	Q	63	GLN	CA-C-O	5.22	125.70	119.60
22	V	266	LEU	CA-C-O	-5.21	115.02	120.55
27	N	799	VAL	CB-CA-C	5.21	119.42	112.22
30	Q	138	SER	O-C-N	-5.21	116.21	122.15
7	g	15	GLY	CA-C-O	-5.21	113.58	120.36
15	H	197	MET	CA-C-N	5.21	128.04	120.79
15	H	197	MET	C-N-CA	5.21	128.04	120.79
8	h	70	TYR	N-CA-C	-5.21	104.96	113.19
13	m	53	SER	CA-C-O	5.21	126.95	120.54
26	Z	796	LEU	CA-C-N	5.21	127.78	120.28
26	Z	796	LEU	C-N-CA	5.21	127.78	120.28
26	Z	861	THR	N-CA-C	-5.21	107.05	113.41
29	P	145	GLU	CA-C-N	5.21	127.82	120.42
29	P	145	GLU	C-N-CA	5.21	127.82	120.42
30	Q	105	GLU	O-C-N	5.21	127.51	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	83	ALA	CA-C-O	-5.21	115.03	120.55
11	k	96	ARG	NE-CZ-NH2	5.21	123.89	119.20
14	n	6	VAL	CG1-CB-CG2	5.21	122.26	110.80
27	N	331	ALA	CA-C-N	5.21	127.82	120.42
27	N	331	ALA	C-N-CA	5.21	127.82	120.42
4	d	15	ILE	CA-C-N	5.21	128.23	120.31
4	d	15	ILE	C-N-CA	5.21	128.23	120.31
7	g	101	THR	CA-CB-CG2	5.21	119.36	110.50
17	K	427	TYR	N-CA-C	-5.21	107.95	114.56
20	J	81	ASP	CA-C-N	5.21	131.49	121.54
20	J	81	ASP	C-N-CA	5.21	131.49	121.54
20	J	340	GLY	CA-C-O	-5.21	113.50	119.80
24	X	59	ARG	CA-C-N	5.21	127.26	120.28
24	X	59	ARG	C-N-CA	5.21	127.26	120.28
26	Z	750	GLU	N-CA-CB	5.21	120.56	111.13
27	N	265	ALA	N-CA-C	5.21	117.25	110.43
30	Q	11	ALA	O-C-N	5.21	127.43	122.07
30	Q	355	GLU	N-CA-C	-5.21	99.47	108.69
33	O	117	ASN	N-CA-CB	5.21	117.87	110.16
11	4	69	ILE	O-C-N	5.21	127.31	121.90
13	6	96	LEU	N-CA-C	-5.21	105.60	111.28
7	g	237	ASP	N-CA-C	5.21	117.03	111.36
3	C	134	PHE	CA-C-O	-5.21	114.74	120.36
5	E	93	LEU	CA-C-N	5.21	127.68	120.29
5	E	93	LEU	C-N-CA	5.21	127.68	120.29
33	O	304	ASN	N-CA-CB	5.21	117.86	110.16
6	F	141	ALA	CA-C-O	-5.20	115.19	120.71
27	N	510	HIS	CA-C-N	5.20	126.83	120.22
27	N	510	HIS	C-N-CA	5.20	126.83	120.22
27	N	785	PRO	CA-C-O	-5.20	114.82	122.31
28	S	277	SER	N-CA-CB	5.20	117.69	109.94
14	n	73	GLU	CA-C-N	5.20	127.68	120.29
14	n	73	GLU	C-N-CA	5.20	127.68	120.29
15	H	436	LYS	N-CA-C	-5.20	106.52	112.92
27	N	776	TYR	N-CA-C	-5.20	101.66	109.15
32	U	193	GLN	N-CA-C	-5.20	105.61	111.28
7	g	231	LEU	CA-C-N	5.20	127.20	120.44
7	g	231	LEU	C-N-CA	5.20	127.20	120.44
9	i	90	TYR	CB-CG-CD1	-5.20	113.00	120.80
11	4	168	LEU	N-CA-C	5.20	116.95	111.28
17	K	285	GLN	N-CA-C	-5.20	105.51	111.07
27	N	30	ASN	CA-C-N	5.20	130.93	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	30	ASN	C-N-CA	5.20	130.93	122.76
9	i	12	VAL	N-CA-C	-5.20	101.49	108.35
10	j	105	GLY	CA-C-O	-5.20	114.09	121.52
13	m	189	THR	N-CA-C	-5.20	105.69	111.36
1	A	227	LEU	N-CA-CB	5.20	118.65	110.23
16	I	161	GLN	CG-CD-OE1	-5.20	110.40	120.80
23	T	185	ILE	CA-C-N	5.20	127.25	120.28
23	T	185	ILE	C-N-CA	5.20	127.25	120.28
27	N	675	VAL	CA-CB-CG2	-5.20	101.56	110.40
31	R	324	ARG	O-C-N	5.20	127.63	122.12
32	U	107	ASN	CB-CA-C	-5.20	102.16	110.79
5	E	219	GLY	N-CA-C	-5.20	103.18	112.22
13	6	119	LYS	N-CA-CB	5.20	118.35	110.45
15	H	242	PRO	CB-CA-C	-5.20	104.58	110.92
17	K	282	PHE	CA-CB-CG	-5.20	108.60	113.80
20	J	235	VAL	N-CA-CB	5.20	117.61	110.54
21	W	160	ALA	CB-CA-C	-5.20	102.02	110.85
26	Z	739	ALA	N-CA-C	5.20	116.63	111.07
6	F	182	ASP	CA-C-N	5.20	130.99	121.85
6	F	182	ASP	C-N-CA	5.20	130.99	121.85
16	I	89	GLN	CA-C-N	5.20	127.50	120.38
16	I	89	GLN	C-N-CA	5.20	127.50	120.38
17	K	363	ALA	CA-C-N	5.20	126.33	119.84
17	K	363	ALA	C-N-CA	5.20	126.33	119.84
21	W	44	ASN	CA-C-N	5.20	124.70	119.19
21	W	44	ASN	C-N-CA	5.20	124.70	119.19
29	P	223	LEU	CA-C-N	5.20	127.76	120.28
29	P	223	LEU	C-N-CA	5.20	127.76	120.28
3	c	113	ARG	N-CA-C	5.19	116.63	111.07
10	j	73	TYR	N-CA-C	-5.19	105.51	111.07
15	H	105	ILE	N-CA-C	-5.19	100.28	108.23
6	f	106	ARG	CB-CA-C	-5.19	102.02	110.85
12	l	121	ARG	NE-CZ-NH2	5.19	123.87	119.20
11	4	27	VAL	N-CA-C	-5.19	99.63	107.73
12	5	169	ALA	N-CA-C	5.19	117.02	111.36
16	I	307	LEU	CA-C-N	5.19	127.66	120.29
16	I	307	LEU	C-N-CA	5.19	127.66	120.29
26	Z	263	ALA	CB-CA-C	-5.19	102.02	110.85
26	Z	358	TYR	CA-C-O	-5.19	114.92	120.42
32	U	24	ARG	NE-CZ-NH2	-5.19	114.53	119.20
33	O	65	PHE	N-CA-CB	5.19	117.75	110.12
2	b	193	LEU	N-CA-C	5.19	117.02	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	50	ALA	CB-CA-C	-5.19	102.03	110.85
10	3	151	SER	CA-C-O	5.19	125.92	120.42
15	H	180	LYS	N-CA-C	-5.19	106.18	112.88
18	L	189	GLN	N-CA-C	-5.19	105.70	111.36
20	J	217	GLU	CA-C-N	5.19	129.39	120.72
20	J	217	GLU	C-N-CA	5.19	129.39	120.72
28	S	413	LEU	O-C-N	-5.19	117.25	123.06
29	P	234	TYR	N-CA-CB	5.19	118.29	110.30
14	n	63	ILE	O-C-N	5.19	127.66	121.80
2	B	188	ALA	O-C-N	5.19	128.29	122.22
4	D	186	VAL	CA-C-O	-5.19	115.55	120.95
9	2	123	TYR	N-CA-C	-5.19	106.21	112.54
26	Z	303	ASP	N-CA-C	5.19	121.28	109.81
28	S	418	THR	N-CA-CB	5.19	117.59	110.07
33	O	194	LEU	CB-CA-C	-5.19	102.18	110.79
6	F	148	PRO	CA-N-CD	5.19	119.26	112.00
22	V	101	ASP	N-CA-C	5.19	117.55	110.24
26	Z	617	ILE	N-CA-C	5.19	117.53	111.05
2	b	85	LEU	CB-CA-C	-5.19	102.03	110.85
23	T	170	ASN	CA-C-O	-5.19	113.28	119.35
27	N	869	ASP	N-CA-C	-5.19	102.81	110.48
11	k	61	GLN	OE1-CD-NE2	-5.18	117.42	122.60
8	l	157	HIS	CG-CD2-NE2	5.18	112.38	107.20
15	H	408	SER	CA-C-N	5.18	127.23	120.28
15	H	408	SER	C-N-CA	5.18	127.23	120.28
18	L	375	ASP	N-CA-C	-5.18	106.19	112.88
26	Z	208	VAL	CA-C-O	-5.18	113.00	119.95
33	O	207	LEU	CA-C-N	5.18	127.23	120.28
33	O	207	LEU	C-N-CA	5.18	127.23	120.28
8	h	50	ALA	CB-CA-C	-5.18	102.74	110.88
8	h	132	THR	CA-C-N	5.18	127.74	120.28
8	h	132	THR	C-N-CA	5.18	127.74	120.28
10	j	72	LEU	CA-C-N	5.18	127.18	120.44
10	j	72	LEU	C-N-CA	5.18	127.18	120.44
12	l	160	SER	N-CA-CB	5.18	117.92	110.20
13	m	174	TYR	N-CA-C	-5.18	102.19	109.96
7	G	117	GLN	CA-C-N	5.18	127.23	120.28
7	G	117	GLN	C-N-CA	5.18	127.23	120.28
10	3	180	SER	N-CA-CB	5.18	117.66	109.83
27	N	10	LEU	CA-C-N	5.18	127.65	120.29
27	N	10	LEU	C-N-CA	5.18	127.65	120.29
28	S	172	ASN	N-CA-C	5.18	121.84	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	ALA	N-CA-CB	5.18	117.65	109.83
1	a	150	PRO	CB-CA-C	-5.18	104.13	112.21
6	f	118	ASN	CB-CA-C	-5.18	99.78	109.72
10	j	59	VAL	CA-C-O	-5.18	115.68	121.17
9	2	209	THR	N-CA-CB	5.18	117.92	110.20
10	3	105	GLY	CA-C-N	5.18	125.58	119.99
10	3	105	GLY	C-N-CA	5.18	125.58	119.99
20	J	213	VAL	N-CA-C	-5.18	99.05	107.28
27	N	72	LEU	CA-C-N	5.18	130.53	122.30
27	N	72	LEU	C-N-CA	5.18	130.53	122.30
4	d	222	LEU	N-CA-C	5.18	117.39	110.35
10	3	91	SER	N-CA-CB	5.18	117.52	110.01
26	Z	593	HIS	ND1-CE1-NE2	5.18	113.58	108.40
7	G	196	ILE	CA-C-N	5.18	127.22	120.28
7	G	196	ILE	C-N-CA	5.18	127.22	120.28
14	7	39	VAL	CA-C-O	5.18	127.25	120.78
17	K	140	HIS	CA-CB-CG	-5.18	108.62	113.80
18	L	307	GLU	CA-C-N	5.18	127.47	120.38
18	L	307	GLU	C-N-CA	5.18	127.47	120.38
29	P	45	LYS	N-CA-CB	5.18	117.92	109.69
30	Q	85	MET	O-C-N	-5.18	116.63	122.12
33	O	165	LEU	N-CA-CB	5.18	117.73	110.12
2	b	20	GLN	CA-C-N	5.17	127.77	120.42
2	b	20	GLN	C-N-CA	5.17	127.77	120.42
4	d	10	SER	N-CA-CB	5.17	116.29	110.03
15	H	248	LEU	CB-CA-C	-5.17	101.21	109.75
21	W	191	ILE	CA-C-O	5.17	124.69	119.20
26	Z	742	GLY	CA-C-O	-5.17	114.61	120.30
31	R	416	LYS	CB-CA-C	-5.17	102.72	110.90
13	6	11	THR	O-C-N	-5.17	117.36	123.41
29	P	417	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
9	2	133	ALA	CA-C-O	5.17	126.03	120.70
12	5	160	SER	N-CA-CB	5.17	117.57	110.07
17	K	184	ILE	N-CA-C	-5.17	105.50	110.72
19	M	55	ASN	O-C-N	5.17	127.40	122.07
19	M	139	LYS	CA-C-N	5.17	128.56	120.75
19	M	139	LYS	C-N-CA	5.17	128.56	120.75
27	N	83	LEU	N-CA-C	-5.17	106.75	113.16
28	S	208	ILE	CA-C-N	5.17	127.55	120.46
28	S	208	ILE	C-N-CA	5.17	127.55	120.46
29	P	233	GLU	O-C-N	5.17	129.23	122.87
31	R	95	ASP	N-CA-CB	5.17	119.29	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	384	VAL	CB-CA-C	-5.17	105.08	112.22
33	O	373	TRP	CB-CG-CD2	-5.17	119.56	126.80
7	g	186	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
7	G	231	LEU	CB-CA-C	-5.17	102.76	110.88
12	5	87	VAL	N-CA-CB	5.17	117.57	110.54
13	6	142	ALA	CA-C-N	5.17	127.21	120.28
13	6	142	ALA	C-N-CA	5.17	127.21	120.28
29	P	115	ARG	CA-CB-CG	5.17	124.44	114.10
6	f	208	ASP	CA-C-O	5.17	125.58	119.48
10	j	44	HIS	CA-C-O	5.17	126.80	120.60
16	I	239	GLN	CA-C-N	5.17	127.21	120.28
16	I	239	GLN	C-N-CA	5.17	127.21	120.28
5	e	84	ALA	CB-CA-C	-5.17	102.77	110.88
5	E	189	GLU	CB-CG-CD	-5.17	103.81	112.60
6	F	170	TYR	N-CA-C	5.17	116.91	111.28
19	M	393	ALA	O-C-N	-5.17	116.64	122.12
30	Q	51	ARG	CA-C-N	5.17	127.46	120.38
30	Q	51	ARG	C-N-CA	5.17	127.46	120.38
6	f	61	LYS	N-CA-CB	5.17	118.23	110.53
20	J	50	ALA	CA-C-N	5.17	127.20	120.28
20	J	50	ALA	C-N-CA	5.17	127.20	120.28
21	W	11	ASP	N-CA-C	-5.17	100.98	109.40
2	b	160	LYS	CB-CA-C	-5.16	102.22	110.79
10	j	130	ASP	CA-CB-CG	-5.16	107.44	112.60
12	l	131	SER	N-CA-C	-5.16	106.83	113.23
7	G	174	LYS	CA-C-N	5.16	127.46	120.44
7	G	174	LYS	C-N-CA	5.16	127.46	120.44
17	K	226	VAL	N-CA-CB	5.16	118.32	110.58
23	T	198	ASP	CA-CB-CG	-5.16	107.44	112.60
26	Z	548	ASP	CA-CB-CG	5.16	117.76	112.60
29	P	5	ALA	CA-C-O	-5.16	113.08	120.16
33	O	274	ILE	N-CA-C	-5.16	105.68	110.53
33	O	278	PRO	CB-CA-C	-5.16	103.24	111.04
3	c	182	ASP	N-CA-C	-5.16	106.67	113.17
13	m	162	PRO	N-CA-C	5.16	123.11	112.47
14	n	180	ALA	N-CA-C	5.16	116.99	111.36
5	E	106	GLN	CA-C-N	5.16	127.20	120.28
5	E	106	GLN	C-N-CA	5.16	127.20	120.28
26	Z	576	GLY	CA-C-O	-5.16	113.28	119.01
7	G	56	VAL	CB-CA-C	5.16	116.72	110.78
20	J	155	LYS	CA-C-N	5.16	127.62	120.29
20	J	155	LYS	C-N-CA	5.16	127.62	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	217	MET	CG-SD-CE	-5.16	89.55	100.90
27	N	528	ARG	O-C-N	-5.16	114.89	122.43
14	n	113	ALA	O-C-N	-5.16	117.27	123.31
5	E	144	GLY	CA-C-N	5.16	128.19	120.87
5	E	144	GLY	C-N-CA	5.16	128.19	120.87
6	F	167	ALA	CA-C-N	5.16	127.61	120.29
6	F	167	ALA	C-N-CA	5.16	127.61	120.29
10	3	70	THR	N-CA-CB	5.16	118.25	110.30
19	M	425	ARG	CA-C-N	5.16	128.03	120.71
19	M	425	ARG	C-N-CA	5.16	128.03	120.71
30	Q	53	GLU	O-C-N	5.16	127.45	122.09
30	Q	234	THR	N-CA-C	-5.16	105.34	111.69
8	1	141	ASN	CA-C-N	5.16	128.09	120.82
8	1	141	ASN	C-N-CA	5.16	128.09	120.82
18	L	160	PRO	N-CA-CB	5.16	107.65	103.32
26	Z	794	ASP	O-C-N	-5.16	116.65	122.12
28	S	185	PHE	CA-C-N	5.16	128.15	120.31
28	S	185	PHE	C-N-CA	5.16	128.15	120.31
10	j	156	ASN	N-CA-CB	5.16	119.20	110.49
3	C	11	ILE	N-CA-CB	5.16	117.04	110.13
4	D	62	VAL	CB-CA-C	-5.16	103.19	111.59
10	3	121	ALA	O-C-N	-5.16	117.90	123.42
4	d	182	PRO	N-CA-CB	5.15	108.08	103.08
5	e	224	ASP	CA-CB-CG	-5.15	107.45	112.60
9	i	45	GLY	O-C-N	5.15	129.16	123.49
15	H	44	PRO	N-CA-C	5.15	120.54	113.84
16	I	382	THR	N-CA-C	5.15	116.58	111.07
27	N	812	ALA	N-CA-C	-5.15	105.74	111.36
29	P	13	TYR	CA-C-N	5.15	127.14	120.44
29	P	13	TYR	C-N-CA	5.15	127.14	120.44
3	c	69	ASN	N-CA-C	-5.15	101.44	108.24
14	n	109	PRO	N-CA-CB	5.15	107.83	103.35
7	G	131	SER	CB-CA-C	-5.15	100.82	109.48
19	M	128	PHE	N-CA-C	-5.15	98.87	107.99
21	W	21	PHE	N-CA-C	-5.15	101.16	109.40
26	Z	138	ARG	N-CA-CB	5.15	118.94	110.39
26	Z	215	ASN	O-C-N	5.15	128.02	122.15
33	O	102	LEU	N-CA-C	-5.15	105.84	111.82
33	O	172	TYR	CA-C-N	5.15	127.14	120.44
33	O	172	TYR	C-N-CA	5.15	127.14	120.44
8	h	44	CYS	N-CA-C	-5.15	100.85	109.24
12	l	184	GLY	CA-C-O	-5.15	117.94	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	202	GLU	O-C-N	5.15	127.58	122.12
2	B	51	SER	CA-C-N	5.15	127.60	120.29
2	B	51	SER	C-N-CA	5.15	127.60	120.29
14	7	146	PHE	CA-C-N	5.15	126.58	120.14
14	7	146	PHE	C-N-CA	5.15	126.58	120.14
15	H	239	GLY	CA-C-N	5.15	128.27	120.13
15	H	239	GLY	C-N-CA	5.15	128.27	120.13
27	N	727	THR	N-CA-C	5.15	116.58	111.07
4	d	194	VAL	CA-C-O	5.15	126.31	120.85
10	3	63	ASN	CA-C-N	5.15	128.14	120.31
10	3	63	ASN	C-N-CA	5.15	128.14	120.31
19	M	209	ASP	CA-C-N	5.15	128.14	120.31
19	M	209	ASP	C-N-CA	5.15	128.14	120.31
2	b	79	GLY	CA-C-O	-5.15	114.16	121.52
2	B	145	PHE	CA-C-O	-5.15	115.95	121.56
4	D	227	ILE	N-CA-C	-5.15	105.69	110.53
16	I	340	ARG	CB-CA-C	5.15	120.31	110.17
19	M	334	ASP	CA-C-N	5.15	125.22	119.87
19	M	334	ASP	C-N-CA	5.15	125.22	119.87
21	W	36	ILE	CA-C-N	5.15	127.13	120.44
21	W	36	ILE	C-N-CA	5.15	127.13	120.44
26	Z	128	GLU	CA-C-N	5.15	127.18	120.28
26	Z	128	GLU	C-N-CA	5.15	127.18	120.28
27	N	50	TYR	N-CA-CB	5.15	117.78	110.16
5	e	83	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
8	l	194	GLU	N-CA-C	-5.15	105.75	111.36
19	M	56	ASN	N-CA-CB	5.15	117.68	110.12
27	N	275	THR	N-CA-CB	5.15	117.47	110.01
7	g	202	ASP	CA-CB-CG	-5.14	107.46	112.60
11	k	73	TYR	CA-CB-CG	-5.14	104.64	113.90
2	B	14	PRO	N-CA-C	-5.14	107.92	114.35
11	4	60	ILE	O-C-N	5.14	126.95	121.91
13	6	21	ALA	N-CA-CB	5.14	120.44	111.13
16	I	73	GLU	CA-C-O	-5.14	115.40	120.90
18	L	113	SER	CA-C-N	5.14	127.60	120.29
18	L	113	SER	C-N-CA	5.14	127.60	120.29
20	J	89	GLN	N-CA-CB	5.14	118.40	110.43
28	S	200	GLU	CB-CG-CD	-5.14	103.85	112.60
1	a	216	VAL	CA-C-N	5.14	127.79	122.80
1	a	216	VAL	C-N-CA	5.14	127.79	122.80
2	B	110	LEU	O-C-N	5.14	128.01	122.15
28	S	137	PHE	CA-C-N	5.14	127.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	137	PHE	C-N-CA	5.14	127.13	120.44
28	S	190	SER	N-CA-CB	5.14	117.77	110.16
30	Q	98	LYS	CA-C-N	5.14	127.13	120.44
30	Q	98	LYS	C-N-CA	5.14	127.13	120.44
9	i	42	TRP	N-CA-C	-5.14	101.78	109.95
3	C	69	ASN	N-CA-C	-5.14	101.44	108.38
14	7	214	VAL	CB-CA-C	-5.14	105.06	111.08
22	V	304	ALA	N-CA-C	-5.14	105.59	111.14
23	T	104	LYS	CB-CG-CD	5.14	123.12	111.30
10	j	80	ALA	CA-C-N	5.14	128.89	121.18
10	j	80	ALA	C-N-CA	5.14	128.89	121.18
4	D	120	GLN	CA-C-O	-5.14	115.05	120.55
11	4	190	ARG	CB-CG-CD	5.14	123.12	111.30
26	Z	347	ASN	CA-CB-CG	-5.14	107.46	112.60
14	7	3	GLN	N-CA-C	-5.14	101.23	109.04
22	V	87	PHE	CA-C-N	5.14	127.43	120.44
22	V	87	PHE	C-N-CA	5.14	127.43	120.44
26	Z	908	ILE	O-C-N	5.14	128.50	123.00
29	P	113	ASN	CA-C-O	-5.14	115.10	120.55
7	g	200	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
17	K	134	SER	N-CA-C	-5.14	102.69	110.24
19	M	358	ALA	N-CA-C	-5.14	105.68	111.28
26	Z	969	GLU	CA-C-O	5.14	126.03	120.43
6	F	185	PRO	CA-N-CD	5.13	119.19	112.00
8	1	58	ILE	CA-C-N	5.13	127.49	120.46
8	1	58	ILE	C-N-CA	5.13	127.49	120.46
23	T	125	GLU	CA-C-N	5.13	127.16	120.28
23	T	125	GLU	C-N-CA	5.13	127.16	120.28
27	N	674	GLN	CA-C-N	5.13	127.50	120.46
27	N	674	GLN	C-N-CA	5.13	127.50	120.46
29	P	436	GLU	CA-C-N	5.13	129.41	120.68
29	P	436	GLU	C-N-CA	5.13	129.41	120.68
30	Q	403	PRO	CA-C-N	-5.13	113.40	122.74
30	Q	403	PRO	C-N-CA	-5.13	113.40	122.74
11	4	71	GLU	CB-CA-C	-5.13	100.45	109.07
27	N	123	PHE	N-CA-C	-5.13	106.56	114.16
27	N	420	THR	N-CA-C	-5.13	105.69	111.28
2	b	182	GLU	N-CA-C	-5.13	105.74	112.41
4	d	137	ASP	N-CA-C	-5.13	103.06	110.40
1	A	30	ASN	OD1-CG-ND2	-5.13	117.47	122.60
6	F	174	THR	N-CA-C	-5.13	106.33	112.59
15	H	163	VAL	CA-C-N	5.13	129.07	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	163	VAL	C-N-CA	5.13	129.07	120.86
19	M	223	PRO	N-CA-CB	5.13	108.06	103.08
26	Z	106	TRP	CB-CG-CD2	-5.13	119.61	126.80
29	P	29	GLN	N-CA-C	5.13	116.87	111.28
7	g	51	THR	CB-CA-C	-5.13	102.13	110.85
14	n	66	LEU	N-CA-C	-5.13	105.77	111.36
31	R	37	LYS	O-C-N	5.13	128.00	122.15
31	R	119	LYS	O-C-N	-5.13	115.56	122.43
5	e	58	LYS	CA-C-N	5.13	129.86	123.14
5	e	58	LYS	C-N-CA	5.13	129.86	123.14
5	e	226	GLU	N-CA-CB	5.13	118.23	110.28
11	k	158	LEU	CA-C-O	-5.13	115.11	120.55
8	l	176	VAL	N-CA-C	-5.13	100.26	107.75
22	V	116	CYS	O-C-N	-5.13	115.51	122.48
28	S	121	VAL	N-CA-C	5.13	115.35	110.53
29	P	409	SER	CA-C-N	5.13	127.57	120.29
29	P	409	SER	C-N-CA	5.13	127.57	120.29
31	R	380	VAL	CA-C-O	-5.13	116.23	121.67
33	O	18	ALA	CA-C-N	5.13	128.45	120.60
33	O	18	ALA	C-N-CA	5.13	128.45	120.60
9	i	82	MET	N-CA-CB	5.13	117.44	110.01
11	k	90	LYS	N-CA-CB	5.13	117.66	110.12
6	F	19	PHE	CA-C-N	5.13	127.15	120.28
6	F	19	PHE	C-N-CA	5.13	127.15	120.28
13	6	190	SER	N-CA-C	-5.13	105.77	111.36
29	P	219	GLU	CA-C-N	5.13	127.11	120.44
29	P	219	GLU	C-N-CA	5.13	127.11	120.44
32	U	97	PRO	CA-N-CD	5.13	118.68	111.50
32	U	214	VAL	CB-CA-C	-5.13	105.14	112.22
6	f	187	GLU	N-CA-C	5.12	117.77	111.82
26	Z	280	ASP	N-CA-C	-5.12	105.39	111.69
9	i	29	LYS	N-CA-C	-5.12	105.69	111.28
3	C	60	THR	O-C-N	5.12	127.99	122.15
19	M	361	LEU	CA-C-N	5.12	127.14	120.28
19	M	361	LEU	C-N-CA	5.12	127.14	120.28
20	J	20	LYS	N-CA-CB	5.12	117.94	110.30
20	J	155	LYS	N-CA-CB	5.12	117.57	109.94
27	N	92	ASP	N-CA-C	-5.12	105.70	111.28
30	Q	93	THR	CA-CB-CG2	5.12	119.21	110.50
12	l	36	GLU	CB-CG-CD	-5.12	103.89	112.60
18	L	229	THR	CA-C-O	-5.12	114.99	120.42
21	W	150	ASN	OD1-CG-ND2	-5.12	117.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	358	LYS	O-C-N	5.12	127.99	122.15
28	S	367	TYR	N-CA-C	-5.12	106.88	112.72
9	i	90	TYR	CG-CD2-CE2	-5.12	113.52	121.20
18	L	330	PRO	CA-C-N	5.12	127.39	120.38
18	L	330	PRO	C-N-CA	5.12	127.39	120.38
3	c	69	ASN	CA-C-N	5.12	127.14	120.28
3	c	69	ASN	C-N-CA	5.12	127.14	120.28
5	e	190	LEU	O-C-N	-5.12	116.69	122.12
9	i	26	VAL	CB-CA-C	-5.12	105.70	111.23
9	i	81	GLN	OE1-CD-NE2	5.12	127.72	122.60
10	j	54	GLY	CA-C-O	-5.12	116.71	122.24
12	l	194	GLY	N-CA-C	-5.12	106.45	112.64
1	A	84	ALA	CA-C-N	5.12	127.39	120.38
1	A	84	ALA	C-N-CA	5.12	127.39	120.38
2	B	97	TYR	CA-CB-CG	-5.12	104.69	113.90
15	H	315	GLY	N-CA-C	-5.12	108.56	115.21
22	V	204	HIS	CG-CD2-NE2	5.12	112.32	107.20
23	T	191	LYS	CB-CA-C	-5.12	102.84	110.88
26	Z	258	PRO	CA-C-O	-5.12	113.14	120.56
31	R	152	LYS	O-C-N	5.12	127.34	122.07
32	U	142	GLN	CA-C-O	5.12	126.52	120.89
1	a	236	LEU	CA-C-N	5.12	127.47	120.46
1	a	236	LEU	C-N-CA	5.12	127.47	120.46
3	c	235	LYS	CA-C-O	5.12	125.97	120.55
2	B	5	TYR	CA-C-O	5.12	126.89	121.16
17	K	276	SER	CA-C-N	5.12	127.69	120.42
17	K	276	SER	C-N-CA	5.12	127.69	120.42
26	Z	910	PRO	N-CA-C	5.12	120.49	113.84
9	i	207	ARG	O-C-N	5.12	128.90	122.86
11	4	85	ARG	O-C-N	5.12	127.54	122.12
24	X	91	PHE	N-CA-C	-5.12	106.89	112.72
27	N	371	LEU	CA-C-O	-5.12	115.13	120.55
31	R	207	ARG	N-CA-CB	5.12	118.10	110.22
15	H	205	ASP	O-C-N	5.11	129.18	122.33
26	Z	186	GLY	CA-C-N	5.11	127.13	120.28
26	Z	186	GLY	C-N-CA	5.11	127.13	120.28
26	Z	496	ALA	CB-CA-C	-5.11	102.63	110.81
28	S	121	VAL	N-CA-CB	5.11	117.11	110.57
1	a	74	VAL	O-C-N	5.11	128.70	123.18
10	j	6	ILE	N-CA-C	-5.11	105.72	110.53
22	V	279	HIS	CG-CD2-NE2	5.11	112.31	107.20
26	Z	880	SER	CA-C-N	5.11	127.46	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	880	SER	C-N-CA	5.11	127.46	120.46
33	O	212	GLN	CB-CG-CD	-5.11	103.91	112.60
10	j	70	THR	N-CA-CB	5.11	117.63	110.12
13	m	145	LEU	O-C-N	-5.11	116.57	122.09
14	7	199	ILE	N-CA-C	-5.11	100.39	107.80
16	I	68	HIS	N-CA-CB	5.11	117.42	110.01
17	K	236	ARG	NE-CZ-NH2	-5.11	114.60	119.20
18	L	408	ASP	N-CA-C	-5.11	106.63	112.92
24	X	60	GLU	N-CA-CB	5.11	117.63	110.12
27	N	518	ALA	N-CA-CB	5.11	117.48	110.07
28	S	23	LYS	CA-C-N	5.11	127.55	120.29
28	S	23	LYS	C-N-CA	5.11	127.55	120.29
33	O	389	GLN	O-C-N	5.11	127.54	122.12
7	g	224	HIS	ND1-CE1-NE2	5.11	113.51	108.40
15	H	380	PRO	CA-C-N	5.11	130.04	120.95
15	H	380	PRO	C-N-CA	5.11	130.04	120.95
25	Y	41	ASP	N-CA-CB	5.11	117.48	110.07
3	c	40	SER	CA-C-O	-5.11	115.11	120.63
5	e	184	THR	CA-C-N	5.11	127.12	120.28
5	e	184	THR	C-N-CA	5.11	127.12	120.28
10	j	32	SER	CA-C-N	5.11	129.60	121.99
10	j	32	SER	C-N-CA	5.11	129.60	121.99
14	n	70	LEU	N-CA-C	5.11	116.53	111.07
16	I	254	GLN	N-CA-C	-5.11	101.14	108.60
18	L	158	ILE	CA-C-O	5.11	127.19	121.11
20	J	27	ILE	O-C-N	-5.11	116.92	121.87
6	f	154	GLU	CB-CA-C	-5.11	101.11	109.53
11	k	125	LYS	N-CA-C	5.11	118.13	109.76
11	k	147	HIS	ND1-CE1-NE2	5.11	113.51	108.40
26	Z	449	ALA	N-CA-C	-5.11	105.72	111.28
26	Z	810	ASN	CA-C-O	-5.11	115.14	120.55
33	O	229	ASN	CA-C-O	-5.11	114.94	120.81
7	G	214	TRP	CB-CG-CD2	-5.10	119.66	126.80
15	H	434	ARG	O-C-N	5.10	128.40	121.97
17	K	309	SER	N-CA-C	-5.10	102.91	110.46
26	Z	786	SER	CA-C-O	-5.10	115.46	120.82
6	f	53	ASP	N-CA-CB	5.10	119.83	111.31
8	1	124	TYR	CA-CB-CG	5.10	123.08	113.90
15	H	300	THR	N-CA-CB	5.10	117.41	110.01
15	H	367	ARG	O-C-N	-5.10	115.45	121.32
29	P	112	LEU	O-C-N	5.10	127.33	122.07
8	1	152	VAL	N-CA-C	5.10	115.32	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	173	ARG	CA-C-N	5.10	129.58	122.23
15	H	173	ARG	C-N-CA	5.10	129.58	122.23
21	W	122	ARG	O-C-N	5.10	127.32	122.07
26	Z	723	ASP	CA-C-O	-5.10	115.09	120.55
30	Q	265	MET	CA-C-N	5.10	127.07	120.44
30	Q	265	MET	C-N-CA	5.10	127.07	120.44
1	a	163	GLY	N-CA-C	-5.10	101.94	112.34
2	b	37	ILE	CA-C-O	-5.10	115.04	120.39
2	b	90	ARG	CA-C-N	5.10	127.07	120.44
2	b	90	ARG	C-N-CA	5.10	127.07	120.44
6	f	194	GLU	CA-C-O	-5.10	115.14	120.55
7	g	98	LEU	O-C-N	5.10	129.16	122.33
14	n	125	GLN	N-CA-C	-5.10	102.31	109.96
4	D	93	SER	CA-C-O	-5.10	115.02	120.42
33	O	262	ASP	CB-CA-C	5.10	118.16	109.80
4	d	195	ARG	CA-C-N	5.10	127.11	120.28
4	d	195	ARG	C-N-CA	5.10	127.11	120.28
11	k	53	THR	CA-CB-OG1	5.10	117.25	109.60
12	l	54	PHE	CA-C-O	5.10	125.82	120.42
26	Z	799	PHE	CA-C-O	-5.10	115.02	120.42
29	P	104	LEU	CA-C-N	5.10	127.07	120.44
29	P	104	LEU	C-N-CA	5.10	127.07	120.44
31	R	105	LYS	CA-C-N	5.10	131.28	121.54
31	R	105	LYS	C-N-CA	5.10	131.28	121.54
7	g	175	LEU	N-CA-CB	5.10	117.61	110.12
22	V	204	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
22	V	296	LEU	CA-C-O	5.10	125.82	120.42
27	N	39	ILE	O-C-N	5.10	127.64	122.09
2	b	247	LEU	N-CA-C	-5.09	107.06	113.28
11	k	108	ASP	CA-C-N	5.09	127.53	120.29
11	k	108	ASP	C-N-CA	5.09	127.53	120.29
14	n	9	THR	CA-CB-CG2	5.09	119.16	110.50
3	C	97	TYR	CA-C-N	5.09	127.11	120.28
3	C	97	TYR	C-N-CA	5.09	127.11	120.28
5	E	193	LEU	CA-C-N	5.09	127.11	120.28
5	E	193	LEU	C-N-CA	5.09	127.11	120.28
20	J	228	ARG	NE-CZ-NH2	-5.09	114.61	119.20
27	N	262	VAL	CA-C-O	5.09	125.97	120.47
33	O	177	GLN	CA-C-N	5.09	127.42	120.54
33	O	177	GLN	C-N-CA	5.09	127.42	120.54
6	f	106	ARG	NE-CZ-NH2	-5.09	114.62	119.20
6	f	11	THR	N-CA-C	-5.09	100.22	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	63	ASN	CB-CA-C	-5.09	102.89	110.88
14	n	2	GLN	N-CA-CB	5.09	118.54	110.55
9	2	212	VAL	CA-C-N	5.09	127.06	120.44
9	2	212	VAL	C-N-CA	5.09	127.06	120.44
10	3	3	PRO	CA-C-N	5.09	127.10	120.28
10	3	3	PRO	C-N-CA	5.09	127.10	120.28
10	3	82	GLU	N-CA-C	-5.09	103.77	110.39
11	4	59	TYR	CB-CA-C	-5.09	102.19	110.85
15	H	253	GLY	N-CA-C	-5.09	108.22	115.30
17	K	349	ARG	CA-C-N	5.09	127.10	120.28
17	K	349	ARG	C-N-CA	5.09	127.10	120.28
18	L	61	LYS	CA-C-N	5.09	127.52	120.29
18	L	61	LYS	C-N-CA	5.09	127.52	120.29
31	R	102	LEU	CA-C-O	-5.09	113.23	120.51
33	O	112	LYS	N-CA-C	5.09	116.68	111.03
3	c	192	ALA	CA-C-O	5.09	126.16	120.82
4	d	100	ASP	O-C-N	-5.09	115.47	121.32
4	d	194	VAL	N-CA-C	5.09	115.86	110.72
5	e	191	LEU	CB-CA-C	5.09	118.87	110.88
9	2	34	LEU	O-C-N	5.09	129.04	122.93
11	4	135	TYR	CA-C-N	5.09	127.10	120.28
11	4	135	TYR	C-N-CA	5.09	127.10	120.28
28	S	310	LEU	CA-C-N	5.09	127.10	120.28
28	S	310	LEU	C-N-CA	5.09	127.10	120.28
30	Q	64	LEU	O-C-N	5.09	127.95	122.15
12	5	95	LEU	N-CA-CB	5.09	117.43	109.85
27	N	222	TYR	CB-CG-CD2	5.09	128.43	120.80
27	N	700	CYS	CA-C-N	5.09	127.43	120.46
27	N	700	CYS	C-N-CA	5.09	127.43	120.46
28	S	77	THR	CA-C-O	-5.09	115.66	121.00
30	Q	238	TYR	CB-CG-CD1	-5.09	113.17	120.80
10	j	113	SER	N-CA-C	-5.09	106.58	112.89
16	I	234	LYS	CG-CD-CE	5.09	123.00	111.30
17	K	140	HIS	ND1-CE1-NE2	5.09	113.49	108.40
21	W	20	ASP	CB-CA-C	-5.09	102.35	110.79
21	W	58	ASN	CA-C-O	-5.09	115.09	119.36
21	W	194	GLU	CB-CG-CD	-5.09	103.95	112.60
22	V	164	LEU	N-CA-CB	5.09	117.69	110.16
23	T	150	ARG	O-C-N	-5.09	116.73	122.12
26	Z	93	ARG	CD-NE-CZ	-5.09	117.28	124.40
28	S	158	PHE	CA-C-N	5.09	127.10	120.28
28	S	158	PHE	C-N-CA	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	56	ALA	O-C-N	-5.08	116.73	122.12
8	h	94	THR	N-CA-C	-5.08	98.99	107.99
11	4	128	LEU	CA-C-N	5.08	125.53	120.04
11	4	128	LEU	C-N-CA	5.08	125.53	120.04
19	M	187	ASP	CA-C-O	-5.08	115.16	120.55
31	R	221	VAL	CA-C-N	5.08	127.51	120.29
31	R	221	VAL	C-N-CA	5.08	127.51	120.29
2	b	209	ILE	O-C-N	5.08	128.67	123.18
5	e	52	GLU	CA-C-O	-5.08	114.86	120.60
7	g	208	PHE	CA-C-O	5.08	127.48	121.58
9	i	54	ALA	N-CA-C	5.08	116.51	111.07
11	4	35	THR	CA-CB-CG2	5.08	119.14	110.50
15	H	280	VAL	CA-C-N	5.08	129.88	122.41
15	H	280	VAL	C-N-CA	5.08	129.88	122.41
17	K	192	LEU	O-C-N	-5.08	115.62	122.23
22	V	72	PRO	N-CA-CB	-5.08	97.91	103.25
26	Z	7	LYS	CA-C-O	5.08	125.23	119.18
26	Z	351	PRO	N-CA-C	-5.08	108.87	114.92
26	Z	553	ARG	N-CA-CB	-5.08	102.64	110.16
27	N	672	ASN	OD1-CG-ND2	5.08	127.68	122.60
33	O	24	PRO	CA-C-N	5.08	127.09	120.28
33	O	24	PRO	C-N-CA	5.08	127.09	120.28
4	d	38	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	43	VAL	O-C-N	-5.08	117.84	123.18
2	B	233	PRO	CA-C-N	5.08	127.50	120.29
2	B	233	PRO	C-N-CA	5.08	127.50	120.29
4	D	87	ALA	CA-C-N	5.08	127.51	120.29
4	D	87	ALA	C-N-CA	5.08	127.51	120.29
9	2	187	LEU	N-CA-CB	5.08	119.05	110.46
23	T	251	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
30	Q	216	ALA	CA-C-N	5.08	127.05	120.44
30	Q	216	ALA	C-N-CA	5.08	127.05	120.44
19	M	234	ALA	CA-C-N	5.08	127.35	120.44
19	M	234	ALA	C-N-CA	5.08	127.35	120.44
32	U	7	LYS	N-CA-CB	5.08	119.77	111.08
33	O	26	PHE	CA-C-N	5.08	127.04	120.44
33	O	26	PHE	C-N-CA	5.08	127.04	120.44
17	K	201	ILE	CA-C-O	-5.08	115.47	120.85
22	V	88	GLN	O-C-N	5.08	127.57	122.09
24	X	87	PHE	CA-CB-CG	-5.08	108.72	113.80
29	P	336	HIS	N-CA-C	-5.08	106.67	112.92
30	Q	343	LEU	N-CA-C	5.08	116.81	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	188	LYS	N-CA-C	5.08	116.50	111.07
31	R	347	THR	O-C-N	5.08	129.16	123.27
17	K	342	SER	CA-CB-OG	5.08	121.25	111.10
17	K	350	ARG	NE-CZ-NH2	-5.08	114.63	119.20
18	L	77	ARG	O-C-N	-5.08	116.36	122.15
5	e	228	THR	N-CA-C	-5.08	105.64	111.07
16	I	416	PHE	CA-CB-CG	-5.08	108.72	113.80
19	M	233	ARG	N-CA-C	-5.08	105.83	111.36
23	T	266	TYR	CA-C-N	5.08	127.04	120.44
23	T	266	TYR	C-N-CA	5.08	127.04	120.44
5	E	182	SER	CA-C-O	-5.07	115.04	120.42
15	H	196	THR	O-C-N	5.07	128.51	122.27
18	L	316	ASP	N-CA-C	-5.07	101.58	109.14
27	N	857	TYR	N-CA-C	-5.07	99.99	110.80
30	Q	425	GLN	CA-C-N	5.07	127.50	120.29
30	Q	425	GLN	C-N-CA	5.07	127.50	120.29
32	U	89	LEU	CA-C-O	-5.07	114.87	120.70
33	O	262	ASP	CA-C-O	5.07	126.27	120.54
6	f	156	TYR	N-CA-C	-5.07	105.83	111.36
33	O	205	ILE	CA-C-N	5.07	128.05	120.90
33	O	205	ILE	C-N-CA	5.07	128.05	120.90
6	f	81	ARG	NE-CZ-NH1	-5.07	116.43	121.50
6	F	100	ARG	CA-C-N	5.07	127.91	120.71
6	F	100	ARG	C-N-CA	5.07	127.91	120.71
16	I	420	LYS	N-CA-CB	5.07	117.36	110.01
22	V	215	ASN	N-CA-CB	5.07	117.47	110.17
26	Z	393	GLY	CA-C-N	5.07	128.53	121.02
26	Z	393	GLY	C-N-CA	5.07	128.53	121.02
27	N	256	GLN	OE1-CD-NE2	5.07	127.67	122.60
3	c	79	LEU	N-CA-CB	5.07	117.45	109.69
20	J	159	GLU	CB-CG-CD	-5.07	103.98	112.60
23	T	196	SER	N-CA-C	5.07	116.49	111.07
26	Z	179	SER	N-CA-C	-5.07	105.94	111.82
31	R	160	LYS	N-CA-CB	5.07	117.47	110.17
2	b	94	HIS	CG-CD2-NE2	5.07	112.27	107.20
2	B	90	ARG	NE-CZ-NH1	5.07	126.57	121.50
4	D	233	GLN	N-CA-C	5.07	116.49	111.07
12	5	153	ALA	CA-C-N	5.07	127.03	120.44
12	5	153	ALA	C-N-CA	5.07	127.03	120.44
26	Z	517	ASP	N-CA-CB	5.07	118.02	110.22
26	Z	924	LYS	CA-C-O	-5.07	113.15	119.18
4	d	42	LEU	CA-C-N	5.07	127.01	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	42	LEU	C-N-CA	5.07	127.01	122.20
9	i	68	LEU	CA-C-N	5.07	128.01	120.31
9	i	68	LEU	C-N-CA	5.07	128.01	120.31
3	C	180	LYS	CA-C-N	5.07	127.07	120.28
3	C	180	LYS	C-N-CA	5.07	127.07	120.28
15	H	81	LEU	CA-C-N	5.07	127.07	120.28
15	H	81	LEU	C-N-CA	5.07	127.07	120.28
16	I	80	GLU	CA-C-N	5.07	127.13	120.60
16	I	80	GLU	C-N-CA	5.07	127.13	120.60
28	S	39	ASN	CA-CB-CG	-5.07	107.53	112.60
6	f	184	ASN	N-CA-C	-5.06	97.79	108.73
20	J	287	ASN	CB-CA-C	-5.06	100.34	110.42
25	Y	28	SER	N-CA-CB	5.06	118.02	110.22
26	Z	384	SER	CB-CA-C	-5.06	102.24	110.85
7	g	123	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	A	8	THR	N-CA-C	5.06	116.80	111.28
16	I	208	TYR	CA-C-O	-5.06	115.18	120.55
17	K	314	VAL	CA-C-N	5.06	129.47	123.19
17	K	314	VAL	C-N-CA	5.06	129.47	123.19
22	V	150	LYS	N-CA-CB	5.06	119.04	110.49
27	N	195	THR	CA-CB-CG2	-5.06	101.89	110.50
14	n	222	ALA	N-CA-C	-5.06	105.85	112.23
3	C	30	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
16	I	228	GLY	CA-C-N	5.06	127.32	120.44
16	I	228	GLY	C-N-CA	5.06	127.32	120.44
25	Y	32	ASP	CB-CA-C	-5.06	109.25	116.34
28	S	45	THR	CA-CB-CG2	-5.06	101.90	110.50
14	n	178	VAL	CA-C-N	5.06	127.06	120.28
14	n	178	VAL	C-N-CA	5.06	127.06	120.28
5	E	174	GLU	CA-C-N	5.06	128.00	120.31
5	E	174	GLU	C-N-CA	5.06	128.00	120.31
20	J	205	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
27	N	109	TYR	N-CA-C	5.06	116.80	111.28
5	e	110	ASP	CA-C-O	-5.06	114.39	120.10
9	i	79	ALA	CA-C-N	5.06	127.02	120.44
9	i	79	ALA	C-N-CA	5.06	127.02	120.44
9	2	76	VAL	CB-CA-C	5.06	119.20	112.22
19	M	420	SER	N-CA-C	-5.06	106.80	113.17
27	N	360	GLN	N-CA-CB	5.06	119.25	111.46
27	N	437	GLU	CB-CA-C	-5.06	102.25	110.85
10	j	71	ASN	CB-CA-C	-5.06	102.25	110.85
13	m	201	GLY	N-CA-C	-5.06	103.16	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	88	ALA	CA-C-O	-5.06	115.51	120.82
27	N	115	LYS	CA-C-O	-5.06	115.19	120.55
14	n	131	ASN	CA-C-O	5.05	126.72	121.36
9	2	58	LEU	CA-C-N	5.05	127.60	120.42
9	2	58	LEU	C-N-CA	5.05	127.60	120.42
18	L	108	VAL	N-CA-C	-5.05	98.83	109.34
20	J	34	ILE	N-CA-C	-5.05	105.47	110.62
33	O	24	PRO	N-CA-C	5.05	120.47	113.65
7	g	116	VAL	CA-CB-CG1	5.05	118.99	110.40
14	n	204	THR	N-CA-C	-5.05	106.96	114.64
5	E	75	ALA	CB-CA-C	-5.05	102.26	110.85
6	F	42	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
14	7	50	VAL	CA-C-N	5.05	129.55	122.93
14	7	50	VAL	C-N-CA	5.05	129.55	122.93
20	J	359	LYS	CA-C-O	5.05	125.91	120.55
26	Z	211	PHE	CA-CB-CG	-5.05	108.75	113.80
5	e	124	ARG	NE-CZ-NH2	5.05	123.75	119.20
11	k	180	ILE	CA-C-O	5.05	126.70	120.84
1	A	95	PHE	CA-CB-CG	5.05	118.85	113.80
3	C	129	PRO	O-C-N	5.05	129.46	122.64
6	F	18	LEU	N-CA-C	-5.05	100.17	108.41
19	M	301	VAL	CA-C-N	5.05	127.01	120.44
19	M	301	VAL	C-N-CA	5.05	127.01	120.44
20	J	87	LYS	N-CA-C	-5.05	99.05	107.99
21	W	118	ILE	N-CA-C	5.05	117.76	109.78
27	N	739	PHE	CA-CB-CG	-5.05	108.75	113.80
33	O	170	SER	O-C-N	-5.05	116.39	122.15
11	k	110	LYS	N-CA-C	5.05	119.29	113.18
2	B	244	ASN	N-CA-CB	5.05	117.54	110.12
4	D	14	HIS	CG-CD2-NE2	5.05	112.25	107.20
4	D	101	PRO	O-C-N	-5.05	116.84	123.00
21	W	135	ASN	CA-C-N	5.05	129.90	122.63
21	W	135	ASN	C-N-CA	5.05	129.90	122.63
23	T	179	ASP	CA-CB-CG	-5.05	107.55	112.60
26	Z	5	SER	CA-C-O	-5.05	113.05	119.31
33	O	313	ILE	O-C-N	5.05	127.03	121.83
11	4	64	ILE	N-CA-C	-5.05	105.62	110.72
23	T	137	GLU	CA-C-O	5.05	124.37	118.97
6	f	95	SER	N-CA-C	-5.05	105.86	111.36
13	m	126	ASP	N-CA-CB	5.05	116.74	109.78
4	D	149	GLU	O-C-N	-5.05	117.06	121.35
26	Z	97	PRO	CB-CA-C	-5.05	104.31	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	190	ASN	O-C-N	-5.04	117.57	123.27
1	A	242	GLN	CB-CG-CD	-5.04	104.02	112.60
11	4	99	GLN	OE1-CD-NE2	5.04	127.64	122.60
28	S	414	ASP	CB-CA-C	-5.04	102.27	110.85
1	a	9	ILE	CA-C-O	5.04	127.73	122.13
12	l	57	THR	CA-CB-OG1	5.04	117.17	109.60
8	1	120	HIS	CA-C-N	5.04	128.01	120.95
8	1	120	HIS	C-N-CA	5.04	128.01	120.95
21	W	83	GLY	O-C-N	-5.04	116.11	122.82
29	P	99	LYS	CA-C-N	5.04	127.02	120.56
29	P	99	LYS	C-N-CA	5.04	127.02	120.56
30	Q	169	ASP	CB-CA-C	-5.04	102.69	110.26
32	U	55	PRO	CA-N-CD	5.04	119.06	112.00
7	g	211	GLU	CA-C-N	5.04	130.02	123.06
7	g	211	GLU	C-N-CA	5.04	130.02	123.06
12	l	64	ARG	CA-C-N	5.04	127.45	120.29
12	l	64	ARG	C-N-CA	5.04	127.45	120.29
20	J	156	GLN	CG-CD-NE2	-5.04	108.84	116.40
20	J	228	ARG	NE-CZ-NH1	5.04	126.54	121.50
21	W	130	LYS	N-CA-C	-5.04	106.64	112.89
22	V	123	VAL	N-CA-CB	5.04	118.14	110.58
26	Z	308	LYS	O-C-N	5.04	127.26	122.07
26	Z	759	ARG	CB-CA-C	-5.04	102.28	110.85
30	Q	142	ALA	CA-C-N	5.04	126.99	120.44
30	Q	142	ALA	C-N-CA	5.04	126.99	120.44
30	Q	222	SER	CA-C-N	5.04	125.54	119.94
30	Q	222	SER	C-N-CA	5.04	125.54	119.94
16	I	115	ASP	CA-C-N	5.04	129.89	122.63
16	I	115	ASP	C-N-CA	5.04	129.89	122.63
7	g	50	ILE	N-CA-C	-5.04	100.00	107.51
12	l	190	ASN	CA-C-O	5.04	125.92	120.43
5	E	237	GLU	CA-C-N	5.04	129.24	120.68
5	E	237	GLU	C-N-CA	5.04	129.24	120.68
13	6	115	ASP	CA-CB-CG	5.04	117.64	112.60
13	6	186	ASP	CA-CB-CG	5.04	117.64	112.60
15	H	399	GLU	N-CA-C	-5.04	101.54	109.25
20	J	79	VAL	N-CA-CB	5.04	120.90	112.44
26	Z	456	GLY	CA-C-N	5.04	127.36	120.46
26	Z	456	GLY	C-N-CA	5.04	127.36	120.46
27	N	307	LYS	N-CA-CB	5.04	117.40	109.69
27	N	906	ARG	CB-CA-C	5.04	117.94	109.48
28	S	46	LEU	N-CA-C	-5.04	106.44	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	268	LEU	N-CA-C	-5.04	105.87	111.36
33	O	160	LYS	N-CA-CB	5.04	117.38	109.97
33	O	359	SER	CA-C-N	5.04	125.68	119.99
33	O	359	SER	C-N-CA	5.04	125.68	119.99
20	J	132	PRO	O-C-N	5.04	128.72	122.22
24	X	57	VAL	O-C-N	-5.04	117.29	122.63
1	a	155	VAL	N-CA-C	-5.04	100.60	107.75
1	a	202	ILE	CB-CA-C	5.04	118.42	111.97
9	i	66	HIS	ND1-CE1-NE2	5.04	113.44	108.40
3	C	1	GLY	CA-C-N	5.04	131.16	121.54
3	C	1	GLY	C-N-CA	5.04	131.16	121.54
4	D	188	GLU	CA-C-O	-5.04	115.21	120.55
7	G	95	PHE	N-CA-CB	-5.04	102.72	110.12
10	3	103	PHE	CA-CB-CG	-5.04	108.76	113.80
11	4	138	PHE	CA-CB-CG	5.04	118.83	113.80
24	X	127	GLY	CA-C-N	5.04	127.01	120.56
24	X	127	GLY	C-N-CA	5.04	127.01	120.56
26	Z	218	GLU	N-CA-C	-5.04	107.14	113.28
27	N	18	ASP	CA-C-O	-5.04	115.53	120.82
3	C	20	GLN	N-CA-C	-5.03	105.79	111.28
6	F	63	ILE	N-CA-C	-5.03	100.40	107.75
18	L	386	PHE	CA-C-O	5.03	126.39	120.80
10	j	66	PHE	CB-CG-CD1	5.03	129.25	120.70
13	m	134	GLU	CA-C-O	5.03	127.62	121.68
7	G	97	LYS	CA-C-N	5.03	127.28	120.44
7	G	97	LYS	C-N-CA	5.03	127.28	120.44
17	K	173	ASP	CA-C-N	5.03	126.99	120.70
17	K	173	ASP	C-N-CA	5.03	126.99	120.70
27	N	484	GLY	CA-C-O	5.03	125.83	120.40
28	S	104	VAL	CA-C-O	-5.03	115.03	119.71
5	e	59	ILE	N-CA-C	-5.03	101.07	108.11
8	h	109	GLU	N-CA-C	-5.03	101.43	109.23
11	4	28	LEU	CA-C-O	-5.03	115.52	120.70
14	7	47	ASP	CA-CB-CG	5.03	117.63	112.60
15	H	205	ASP	CA-C-N	5.03	131.03	121.97
15	H	205	ASP	C-N-CA	5.03	131.03	121.97
19	M	272	GLU	O-C-N	5.03	127.45	122.12
26	Z	771	HIS	O-C-N	-5.03	116.79	122.12
27	N	730	VAL	N-CA-CB	5.03	116.44	110.55
28	S	106	GLY	N-CA-C	-5.03	108.18	115.27
29	P	194	SER	N-CA-C	-5.03	105.92	111.71
30	Q	43	GLY	CA-C-N	5.03	131.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	43	GLY	C-N-CA	5.03	131.15	121.54
31	R	25	GLU	CA-C-N	5.03	126.99	120.70
31	R	25	GLU	C-N-CA	5.03	126.99	120.70
5	e	149	HIS	O-C-N	5.03	129.47	123.13
5	E	128	ARG	CA-C-N	5.03	125.03	119.90
5	E	128	ARG	C-N-CA	5.03	125.03	119.90
10	3	105	GLY	CA-C-O	-5.03	114.33	121.52
19	M	28	GLN	CG-CD-NE2	-5.03	108.86	116.40
26	Z	229	SER	CA-C-N	5.03	127.00	120.56
26	Z	229	SER	C-N-CA	5.03	127.00	120.56
26	Z	745	LEU	O-C-N	5.03	127.25	122.07
26	Z	958	ASN	CB-CG-ND2	-5.03	108.86	116.40
29	P	236	GLU	CA-C-O	-5.03	115.09	120.42
31	R	181	TYR	CA-C-N	5.03	129.50	122.36
31	R	181	TYR	C-N-CA	5.03	129.50	122.36
31	R	248	SER	N-CA-CB	5.03	117.30	110.01
13	m	17	GLY	CA-C-O	5.03	127.10	121.67
5	e	86	THR	CA-C-N	5.03	127.95	120.31
5	e	86	THR	C-N-CA	5.03	127.95	120.31
7	g	203	ASN	CA-CB-CG	-5.03	107.57	112.60
10	j	66	PHE	CB-CG-CD2	-5.03	112.16	120.70
8	l	134	ILE	N-CA-C	-5.03	106.55	111.88
10	3	94	LEU	CA-C-N	5.03	128.64	120.60
10	3	94	LEU	C-N-CA	5.03	128.64	120.60
15	H	288	ALA	CA-C-N	5.03	127.01	120.28
15	H	288	ALA	C-N-CA	5.03	127.01	120.28
16	I	214	LYS	N-CA-C	-5.03	102.86	109.84
22	V	284	ALA	CA-C-N	5.03	127.43	120.29
22	V	284	ALA	C-N-CA	5.03	127.43	120.29
26	Z	593	HIS	CA-C-O	-5.03	115.99	120.56
26	Z	766	HIS	CA-C-O	-5.03	115.09	120.42
27	N	697	PHE	CA-C-O	5.03	125.88	120.55
27	N	875	LEU	N-CA-C	5.03	116.83	109.84
28	S	100	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
31	R	384	VAL	N-CA-C	5.03	115.80	110.72
7	g	185	ALA	N-CA-C	5.02	116.76	111.28
1	A	133	THR	CA-C-O	-5.02	114.24	120.57
7	G	73	VAL	N-CA-C	-5.02	101.24	108.42
17	K	196	ASP	O-C-N	5.02	127.24	122.07
26	Z	272	TYR	CB-CG-CD2	-5.02	113.27	120.80
30	Q	55	GLU	N-CA-CB	5.02	117.29	110.01
2	b	104	TYR	CA-CB-CG	-5.02	104.86	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	124	ARG	N-CA-CB	5.02	120.09	111.00
13	m	197	GLN	N-CA-CB	5.02	117.56	110.13
31	R	69	GLU	CA-C-N	-5.02	112.66	121.70
31	R	69	GLU	C-N-CA	-5.02	112.66	121.70
32	U	25	THR	CA-C-N	5.02	129.27	122.19
32	U	25	THR	C-N-CA	5.02	129.27	122.19
9	2	23	GLY	O-C-N	-5.02	116.75	121.77
30	Q	169	ASP	CA-C-N	5.02	131.13	121.54
30	Q	169	ASP	C-N-CA	5.02	131.13	121.54
1	a	194	VAL	CA-C-O	-5.02	115.53	120.85
10	3	182	TRP	NE1-CE2-CD2	5.02	113.93	107.40
14	7	99	VAL	O-C-N	5.02	127.00	121.83
27	N	107	GLU	O-C-N	-5.02	116.43	122.15
27	N	216	ASN	CA-CB-CG	-5.02	107.58	112.60
32	U	145	ASP	CA-C-N	5.02	131.13	121.54
32	U	145	ASP	C-N-CA	5.02	131.13	121.54
32	U	222	ASN	CA-CB-CG	-5.02	107.58	112.60
1	a	42	THR	N-CA-C	-5.02	100.11	108.34
7	G	138	ASP	CA-C-N	5.02	127.50	120.28
7	G	138	ASP	C-N-CA	5.02	127.50	120.28
20	J	209	LYS	N-CA-C	5.02	117.45	108.17
26	Z	196	SER	CA-C-O	-5.02	115.23	120.55
3	c	64	LYS	N-CA-CB	5.02	118.97	110.49
33	O	141	ASN	OD1-CG-ND2	5.02	127.62	122.60
14	n	120	GLN	CA-C-N	5.01	127.50	120.28
14	n	120	GLN	C-N-CA	5.01	127.50	120.28
10	3	54	GLY	CA-C-N	5.01	129.23	121.26
10	3	54	GLY	C-N-CA	5.01	129.23	121.26
18	L	223	PRO	N-CA-C	5.01	116.82	110.70
23	T	231	SER	N-CA-C	-5.01	105.20	111.92
26	Z	846	PHE	CA-C-N	5.01	130.60	122.68
26	Z	846	PHE	C-N-CA	5.01	130.60	122.68
27	N	506	GLN	CA-C-O	5.01	125.81	120.24
10	j	111	ILE	N-CA-C	-5.01	100.43	107.75
29	P	34	SER	CA-C-O	-5.01	115.11	120.42
4	D	213	VAL	CA-CB-CG1	5.01	118.92	110.40
6	F	19	PHE	N-CA-C	5.01	117.47	111.71
16	I	127	ASP	N-CA-C	-5.01	103.32	110.59
22	V	281	SER	N-CA-C	-5.01	105.90	111.36
23	T	177	PHE	CA-CB-CG	-5.01	108.79	113.80
26	Z	21	GLU	N-CA-C	-5.01	105.27	113.19
26	Z	557	GLU	CA-C-N	5.01	126.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	557	GLU	C-N-CA	5.01	126.96	120.44
27	N	695	ALA	CA-C-O	-5.01	115.56	120.82
30	Q	80	HIS	CA-CB-CG	-5.01	108.79	113.80
4	D	117	ARG	NE-CZ-NH1	-5.01	116.49	121.50
4	D	233	GLN	CA-C-O	5.01	126.08	120.82
12	5	30	THR	N-CA-CB	5.01	119.10	110.68
17	K	330	ARG	N-CA-C	-5.01	103.62	108.13
26	Z	601	VAL	O-C-N	5.01	126.73	121.87
28	S	66	GLN	OE1-CD-NE2	5.01	127.61	122.60
30	Q	358	GLU	CA-C-N	5.01	128.56	120.55
30	Q	358	GLU	C-N-CA	5.01	128.56	120.55
1	a	173	LEU	CB-CA-C	-5.01	102.48	110.79
2	b	2	THR	N-CA-CB	5.01	118.95	110.49
6	f	216	GLY	CA-C-O	5.01	126.87	121.61
11	4	32	ASP	CA-CB-CG	-5.01	107.59	112.60
15	H	101	ARG	O-C-N	5.01	129.27	123.41
20	J	211	ILE	N-CA-C	-5.01	100.05	107.51
26	Z	318	LYS	N-CA-C	-5.01	105.73	111.14
1	a	239	ILE	CA-CB-CG2	5.00	119.01	110.50
9	i	149	GLU	N-CA-CB	5.00	117.27	110.01
12	l	149	SER	N-CA-C	-5.00	102.97	110.23
2	B	5	TYR	CB-CG-CD2	-5.00	113.29	120.80
16	I	82	LEU	CA-C-O	-5.00	115.55	120.70
18	L	114	GLU	CA-C-N	5.00	129.07	120.71
18	L	114	GLU	C-N-CA	5.00	129.07	120.71
26	Z	71	LEU	CA-C-N	5.00	128.33	120.82
26	Z	71	LEU	C-N-CA	5.00	128.33	120.82
27	N	27	SER	CA-C-N	5.00	127.32	120.46
27	N	27	SER	C-N-CA	5.00	127.32	120.46
31	R	230	LEU	CB-CA-C	-5.00	102.34	110.85
32	U	123	VAL	N-CA-C	-5.00	100.05	107.51
2	b	48	GLU	N-CA-CB	5.00	118.78	110.52
4	d	50	LEU	N-CA-C	-5.00	101.55	109.76
5	E	52	GLU	N-CA-C	-5.00	100.36	108.52
9	2	97	TYR	N-CA-C	-5.00	100.25	108.41
12	5	74	ILE	CA-C-O	5.00	126.64	120.74
18	L	121	ALA	CA-C-N	5.00	126.98	120.28
18	L	121	ALA	C-N-CA	5.00	126.98	120.28
22	V	42	ARG	N-CA-CB	5.00	117.33	110.07
27	N	411	ILE	N-CA-C	-5.00	105.83	110.53
28	S	387	VAL	N-CA-C	-5.00	105.62	110.42
29	P	306	ASN	N-CA-C	-5.00	106.77	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	224	ASP	CA-C-N	5.00	126.98	120.28
5	e	224	ASP	C-N-CA	5.00	126.98	120.28
6	f	123	GLY	N-CA-C	-5.00	108.42	115.32
14	n	172	VAL	CB-CA-C	-5.00	105.57	111.97
3	C	55	LEU	CA-C-O	5.00	125.72	119.97
6	F	210	LEU	N-CA-C	-5.00	101.09	109.24

There are no chirality outliers.

All (308) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	185	ARG	Sidechain
8	1	45	ARG	Sidechain
9	2	186	TYR	Sidechain
9	2	75	ARG	Sidechain
9	2	90	TYR	Sidechain
9	2	97	TYR	Sidechain
10	3	102	TYR	Sidechain
10	3	45	TYR	Sidechain
10	3	73	TYR	Sidechain
10	3	98	ARG	Sidechain
11	4	107	TYR	Sidechain
11	4	135	TYR	Sidechain
11	4	171	ARG	Sidechain
11	4	73	TYR	Sidechain
11	4	85	ARG	Sidechain
11	4	95	ARG	Sidechain
12	5	113	TYR	Sidechain
12	5	137	TYR	Sidechain
13	6	105	TYR	Sidechain
13	6	106	TYR	Sidechain
13	6	194	ARG	Sidechain
13	6	28	ARG	Sidechain
13	6	33	TYR	Sidechain
13	6	98	TYR	Sidechain
14	7	137	TYR	Sidechain
14	7	186	TYR	Sidechain
14	7	193	ARG	Sidechain
14	7	95	TYR	Sidechain
1	A	101	TYR	Sidechain
1	A	154	TYR	Sidechain
1	A	195	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	21	TYR	Sidechain
1	A	214	LEU	Peptide
1	A	37	ARG	Sidechain
1	A	82	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	16	GLY	Mainchain
2	B	235	PHE	Sidechain
2	B	4	ARG	Sidechain
2	B	83	ARG	Sidechain
2	B	97	TYR	Sidechain
3	C	145	TYR	Sidechain
3	C	19	TYR	Sidechain
3	C	4	ARG	Sidechain
3	C	66	TYR	Sidechain
4	D	127	PHE	Sidechain
4	D	39	CYS	Peptide
5	E	128	ARG	Peptide,Sidechain
5	E	2	ARG	Sidechain
5	E	64	ARG	Sidechain
6	F	127	TYR	Sidechain
6	F	156	TYR	Sidechain
6	F	170	TYR	Sidechain
6	F	232	TYR	Sidechain
6	F	93	TYR	Sidechain
7	G	145	TYR	Sidechain
7	G	165	ARG	Sidechain
7	G	186	ARG	Sidechain
7	G	99	TYR	Sidechain
15	H	145	TYR	Sidechain
15	H	292	ARG	Sidechain
15	H	319	PHE	Sidechain
15	H	357	ARG	Sidechain
15	H	373	ARG	Sidechain
15	H	443	PHE	Sidechain
15	H	457	PHE	Sidechain
16	I	100	ARG	Peptide
16	I	128	TYR	Sidechain
16	I	182	SER	Peptide
16	I	223	GLY	Peptide
16	I	246	ARG	Sidechain
16	I	346	ARG	Sidechain

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Mol	Chain	Res	Type	Group
16	I	64	ARG	Sidechain
20	J	153	LEU	Peptide
20	J	214	SER	Peptide
20	J	22	TYR	Sidechain
20	J	222	TYR	Sidechain
20	J	228	ARG	Sidechain
20	J	310	ILE	Mainchain
20	J	71	TYR	Peptide
20	J	94	TYR	Sidechain
17	K	103	ILE	Peptide
17	K	121	ARG	Sidechain
17	K	176	GLY	Peptide
17	K	198	TYR	Sidechain
17	K	207	ARG	Sidechain
17	K	215	PRO	Peptide
17	K	246	TYR	Sidechain
17	K	329	LEU	Peptide
17	K	333	ARG	Peptide
17	K	396	ARG	Sidechain
17	K	411	TYR	Sidechain
17	K	427	TYR	Sidechain
18	L	168	TYR	Sidechain
18	L	191	ARG	Sidechain
18	L	194	ARG	Sidechain
18	L	207	PHE	Sidechain
18	L	255	TYR	Sidechain
18	L	261	ARG	Sidechain
18	L	269	TYR	Sidechain
18	L	290	ARG	Sidechain
18	L	291	PHE	Sidechain
18	L	77	ARG	Sidechain
19	M	229	THR	Mainchain
19	M	243	PHE	Sidechain
19	M	255	TYR	Sidechain
19	M	267	PHE	Sidechain
19	M	320	ARG	Peptide,Sidechain
19	M	327	THR	Peptide
19	M	354	GLU	Mainchain
19	M	366	ARG	Sidechain
19	M	381	ARG	Sidechain
19	M	432	PHE	Sidechain
19	M	45	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	M	50	ARG	Sidechain
19	M	73	ARG	Sidechain
27	N	188	TYR	Sidechain
27	N	282	TYR	Sidechain
27	N	340	HIS	Sidechain
27	N	415	PHE	Sidechain
27	N	559	TYR	Sidechain
27	N	599	TYR	Sidechain
27	N	604	ARG	Sidechain
27	N	651	PHE	Sidechain
27	N	786	ARG	Sidechain
27	N	809	ARG	Sidechain
27	N	894	ARG	Sidechain
27	N	906	ARG	Sidechain
27	N	921	ARG	Sidechain
33	O	248	TYR	Sidechain
33	O	288	ARG	Sidechain
33	O	369	ARG	Sidechain
33	O	60	ARG	Sidechain
33	O	62	TYR	Sidechain
33	O	81	TYR	Sidechain
29	P	103	TYR	Sidechain
29	P	110	LEU	Peptide
29	P	13	TYR	Sidechain
29	P	168	TYR	Sidechain
29	P	234	TYR	Sidechain
29	P	336	HIS	Sidechain
29	P	386	GLN	Peptide
29	P	79	LEU	Mainchain
30	Q	124	PHE	Peptide
30	Q	161	LEU	Peptide
30	Q	165	PHE	Sidechain
30	Q	209	TYR	Sidechain
30	Q	286	TYR	Sidechain
30	Q	383	ASP	Peptide
30	Q	400	TYR	Sidechain
30	Q	403	PRO	Peptide
30	Q	67	THR	Peptide
31	R	120	LEU	Peptide
31	R	123	ASP	Peptide
31	R	141	TYR	Sidechain
31	R	214	TYR	Sidechain

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Mol	Chain	Res	Type	Group
31	R	222	ARG	Sidechain
31	R	246	TYR	Sidechain
31	R	328	PHE	Sidechain
31	R	331	ARG	Sidechain
31	R	335	ARG	Sidechain
31	R	345	TYR	Sidechain
31	R	417	TYR	Sidechain
31	R	62	TYR	Sidechain
31	R	63	TYR	Sidechain
31	R	65	TYR	Sidechain
31	R	70	TYR	Sidechain
31	R	99	TYR	Sidechain
28	S	111	ARG	Sidechain
28	S	119	TYR	Sidechain
28	S	271	ARG	Sidechain
28	S	272	TYR	Sidechain
28	S	332	PHE	Sidechain
28	S	346	TYR	Sidechain
28	S	384	ARG	Sidechain
23	T	144	TYR	Sidechain
23	T	197	TYR	Sidechain
23	T	199	PHE	Sidechain
23	T	20	TYR	Sidechain
23	T	220	PHE	Sidechain
23	T	251	HIS	Peptide
23	T	266	TYR	Sidechain
23	T	51	TYR	Sidechain
23	T	72	THR	Peptide
23	T	91	SER	Peptide
23	T	96	LEU	Peptide,Mainchain
32	U	210	TYR	Sidechain
32	U	24	ARG	Sidechain
22	V	135	ARG	Sidechain
22	V	203	TYR	Sidechain
22	V	42	ARG	Sidechain
21	W	41	ARG	Sidechain
24	X	27	ILE	Peptide
24	X	96	ARG	Sidechain
25	Y	35	PHE	Sidechain
25	Y	86	ARG	Sidechain
26	Z	269	TYR	Sidechain
26	Z	408	TYR	Sidechain

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Mol	Chain	Res	Type	Group
26	Z	439	TYR	Sidechain
26	Z	477	TYR	Sidechain
26	Z	553	ARG	Sidechain
26	Z	564	ARG	Sidechain
26	Z	574	TYR	Sidechain
26	Z	608	TYR	Sidechain
26	Z	759	ARG	Sidechain
26	Z	773	ARG	Sidechain
26	Z	838	TYR	Sidechain
26	Z	840	ARG	Sidechain
26	Z	849	ARG	Sidechain
1	a	101	TYR	Sidechain
1	a	111	ARG	Sidechain
1	a	119	TYR	Sidechain
1	a	146	TYR	Sidechain
1	a	225	PHE	Sidechain
1	a	3	TYR	Sidechain
1	a	62	TYR	Sidechain
1	a	68	ARG	Sidechain
1	a	97	TYR	Sidechain
1	a	99	TYR	Sidechain
2	b	128	ARG	Sidechain
2	b	130	PHE	Sidechain
2	b	145	PHE	Sidechain
2	b	174	PHE	Sidechain
2	b	236	ARG	Sidechain
2	b	5	TYR	Sidechain
2	b	83	ARG	Sidechain
2	b	97	TYR	Sidechain
2	b	99	ARG	Sidechain
3	c	101	TYR	Sidechain
3	c	136	TYR	Sidechain
3	c	17	ARG	Sidechain
3	c	207	TYR	Sidechain
3	c	212	PHE	Sidechain
3	c	225	TYR	Sidechain
3	c	23	TYR	Sidechain
3	c	49	ARG	Sidechain
3	c	5	TYR	Sidechain
3	c	91	ARG	Sidechain
4	d	106	TYR	Sidechain
4	d	139	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	d	146	TYR	Sidechain
4	d	164	ARG	Sidechain
4	d	177	TYR	Sidechain
4	d	20	TYR	Sidechain
4	d	47	ARG	Sidechain
4	d	9	PHE	Sidechain
4	d	95	ARG	Sidechain
5	e	127	SER	Peptide
5	e	128	ARG	Sidechain
5	e	139	HIS	Sidechain
5	e	145	TYR	Sidechain
5	e	159	TYR	Sidechain
5	e	18	TYR	Sidechain
5	e	85	ARG	Sidechain
6	f	125	ARG	Sidechain
6	f	136	TYR	Sidechain
6	f	163	ARG	Sidechain
6	f	17	ARG	Sidechain
6	f	58	TYR	Sidechain
7	g	115	TYR	Sidechain
7	g	126	ARG	Sidechain
7	g	143	HIS	Sidechain
7	g	153	TYR	Sidechain
7	g	165	ARG	Sidechain
7	g	18	PHE	Sidechain
7	g	4	TYR	Sidechain
7	g	74	TYR	Sidechain
7	g	82	ARG	Sidechain
8	h	135	TYR	Sidechain
8	h	137	TYR	Sidechain
8	h	29	ARG	Sidechain
8	h	38	HIS	Sidechain
8	h	61	TYR	Sidechain
9	i	196	ARG	Sidechain
9	i	205	PHE	Sidechain
9	i	207	ARG	Sidechain
10	j	135	PHE	Sidechain
10	j	176	ARG	Sidechain
10	j	45	TYR	Sidechain
10	j	97	ARG	Sidechain
10	j	98	ARG	Sidechain
11	k	135	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	k	67	TYR	Sidechain
11	k	85	ARG	Sidechain
11	k	96	ARG	Sidechain
11	k	98	TYR	Sidechain
12	l	137	TYR	Sidechain
12	l	155	TYR	Sidechain
12	l	167	ARG	Sidechain
12	l	170	TYR	Sidechain
12	l	178	TYR	Sidechain
12	l	187	TYR	Sidechain
12	l	69	ARG	Sidechain
13	m	101	ARG	Sidechain
13	m	123	TYR	Sidechain
13	m	39	TYR	Sidechain
13	m	75	TYR	Sidechain
13	m	79	HIS	Sidechain
13	m	98	TYR	Sidechain
14	n	129	TYR	Sidechain
14	n	193	ARG	Sidechain
14	n	208	PHE	Sidechain
14	n	41	ARG	Sidechain
14	n	93	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1901	18	0
1	a	1907	0	1901	4	0
2	B	1915	0	1929	18	0
2	b	1915	0	1929	2	0
3	C	1904	0	1904	12	0
3	c	1904	0	1904	4	0
4	D	1881	0	1895	5	0
4	d	1881	0	1895	4	0
5	E	1861	0	1839	4	0
5	e	1861	0	1839	6	0
6	F	1795	0	1800	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	1773	0	1775	3	0
7	G	1892	0	1883	7	0
7	g	1892	0	1883	1	0
8	1	1512	0	1478	36	0
8	h	1512	0	1479	41	0
9	2	1719	0	1719	14	0
9	i	1719	0	1716	70	0
10	3	1581	0	1570	22	0
10	j	1581	0	1574	41	0
11	4	1561	0	1567	28	0
11	k	1561	0	1569	4	0
12	5	1644	0	1593	13	0
12	l	1644	0	1593	26	0
13	6	1757	0	1707	82	0
13	m	1757	0	1711	23	0
14	7	1790	0	1788	46	0
14	n	1815	0	1821	21	0
15	H	2967	0	3051	22	0
16	I	3022	0	3091	27	0
17	K	3078	0	3141	17	0
18	L	3082	0	3156	11	0
19	M	2986	0	3055	24	0
20	J	3033	0	3155	12	0
21	W	1534	0	1542	3	0
22	V	2274	0	2272	63	0
23	T	2192	0	2161	18	0
24	X	1032	0	1017	3	0
25	Y	435	0	394	2	0
26	Z	7005	0	6932	71	0
27	N	6882	0	6959	74	0
28	S	3894	0	3938	9	0
29	P	3608	0	3694	29	0
30	Q	3499	0	3524	23	0
31	R	3060	0	3083	37	0
32	U	2373	0	2403	7	0
33	O	3186	0	3213	11	0
34	H	31	0	13	3	0
34	I	31	0	13	4	0
34	J	31	0	13	8	0
34	K	31	0	13	2	0
34	L	31	0	13	0	0
35	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	I	1	0	0	0	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
36	M	27	0	12	12	0
All	All	108771	0	109020	761	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (761) 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)
22:V:117:TRP:CG	22:V:188:LEU:HD21	1.22	1.67
12:l:135:PHE:CD2	11:4:138:PHE:HE1	1.13	1.61
31:R:70:TYR:CB	31:R:70:TYR:CA	1.75	1.60
12:l:135:PHE:CG	11:4:138:PHE:CE1	1.96	1.54
12:l:135:PHE:CD2	11:4:138:PHE:CE1	1.96	1.54
10:j:182:TRP:CH2	12:5:167:ARG:NH1	1.74	1.53
22:V:117:TRP:CD1	22:V:188:LEU:CD2	1.97	1.48
22:V:186:GLN:CB	22:V:186:GLN:CA	1.95	1.45
22:V:117:TRP:NE1	22:V:188:LEU:HD23	1.22	1.45
15:H:144:LYS:O	15:H:145:TYR:CD2	1.69	1.45
9:i:167:LEU:HD11	13:6:30:ILE:CD1	0.97	1.43
12:l:135:PHE:CE2	11:4:138:PHE:HE1	1.42	1.38
9:i:167:LEU:CD1	13:6:30:ILE:HD11	0.90	1.38
9:i:164:TRP:HB2	14:7:156:ARG:CZ	1.55	1.36
22:V:186:GLN:CB	22:V:186:GLN:N	1.89	1.36
12:l:135:PHE:CE1	11:4:138:PHE:CD1	2.14	1.36
10:j:147:GLY:HA2	13:6:194:ARG:NH2	1.37	1.35
22:V:117:TRP:CE2	22:V:188:LEU:CD2	2.11	1.32
22:V:117:TRP:CD2	22:V:188:LEU:HD21	1.64	1.32
9:i:164:TRP:C	14:7:156:ARG:HH12	1.39	1.30
9:i:165:ASN:CG	14:7:153:PRO:HG3	1.55	1.30
22:V:117:TRP:NE1	22:V:188:LEU:CD2	1.93	1.28
14:n:187:ARG:HD3	9:2:139:GLU:OE2	1.17	1.28
22:V:117:TRP:CD1	22:V:188:LEU:HD21	1.58	1.28
8:h:137:TYR:CZ	8:1:140:LYS:NZ	2.01	1.28
19:M:392:LYS:HZ3	36:M:501:ADP:C4'	1.46	1.28
8:h:137:TYR:CE2	8:1:140:LYS:NZ	2.01	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:777:ALA:C	27:N:861:TYR:O	1.77	1.27
10:j:148:MET:CE	13:6:152:ASN:ND2	1.97	1.27
13:m:158:ASN:HB3	10:3:171:LEU:CD2	1.65	1.24
22:V:117:TRP:CG	22:V:188:LEU:CD2	2.12	1.23
22:V:117:TRP:CE2	22:V:188:LEU:HG	1.74	1.22
9:i:164:TRP:CB	14:7:156:ARG:CZ	2.19	1.20
22:V:117:TRP:CD1	22:V:188:LEU:HD23	1.70	1.20
9:i:209:THR:CG2	13:6:170:LYS:NZ	2.06	1.18
8:h:29:ARG:NH2	14:7:187:ARG:NH2	1.64	1.17
27:N:856:PHE:O	27:N:859:ASN:N	1.74	1.17
9:i:209:THR:HG21	13:6:170:LYS:NZ	1.59	1.17
22:V:117:TRP:CZ2	22:V:188:LEU:HG	1.77	1.17
26:Z:84:ALA:O	26:Z:86:PRO:HD2	1.40	1.17
9:i:164:TRP:C	14:7:156:ARG:NH1	2.00	1.17
10:j:148:MET:HE3	13:6:152:ASN:ND2	1.54	1.16
12:l:135:PHE:CE2	11:4:138:PHE:CE1	2.24	1.16
8:h:137:TYR:CD1	8:1:140:LYS:HD2	1.79	1.16
22:V:117:TRP:CE2	22:V:188:LEU:CG	2.29	1.15
10:j:146:PHE:O	13:6:194:ARG:CZ	1.96	1.14
9:i:203:TYR:OH	13:6:186:ASP:OD2	1.61	1.13
8:h:137:TYR:CE1	8:1:140:LYS:CD	2.30	1.13
26:Z:128:GLU:HB2	26:Z:188:ALA:HB2	1.22	1.12
8:h:187:ILE:HG13	14:7:226:LYS:NZ	1.63	1.12
12:l:135:PHE:CD1	11:4:138:PHE:CE1	2.37	1.12
12:l:135:PHE:CZ	11:4:138:PHE:CD1	2.38	1.11
10:j:146:PHE:HD1	13:6:194:ARG:HD2	1.06	1.11
10:j:135:PHE:CZ	13:6:194:ARG:HD3	1.86	1.10
13:m:158:ASN:CB	10:3:171:LEU:CD2	2.29	1.10
9:i:195:VAL:HA	13:6:220:LYS:HD3	1.30	1.09
13:m:158:ASN:CB	10:3:171:LEU:HD23	1.82	1.09
10:j:135:PHE:HZ	13:6:194:ARG:HD3	0.99	1.09
16:I:151:HIS:CE1	22:V:186:GLN:HA	1.88	1.09
8:h:190:PRO:HG2	14:7:219:TRP:CZ2	1.88	1.08
17:K:304:ASP:OD1	34:J:501:ANP:H5'2	1.52	1.08
12:l:135:PHE:CD1	11:4:138:PHE:CD1	2.42	1.07
26:Z:85:VAL:HB	26:Z:86:PRO:CD	1.84	1.07
12:l:135:PHE:CE1	11:4:138:PHE:HD1	1.58	1.06
9:i:165:ASN:OD1	14:7:153:PRO:HG3	1.53	1.06
10:j:146:PHE:CD1	13:6:194:ARG:HD2	1.92	1.05
12:l:135:PHE:CZ	11:4:138:PHE:HD1	1.74	1.05
26:Z:128:GLU:HB2	26:Z:188:ALA:CB	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:158:ASN:HB3	10:3:171:LEU:HD23	1.32	1.05
9:i:195:VAL:HA	13:6:220:LYS:CD	1.88	1.04
9:i:209:THR:HG22	13:6:170:LYS:CE	1.86	1.04
9:i:164:TRP:O	14:7:156:ARG:NH1	1.90	1.03
14:n:187:ARG:CD	9:2:139:GLU:OE2	2.05	1.03
19:M:392:LYS:HZ3	36:M:501:ADP:H4'	1.18	1.03
22:V:117:TRP:CD2	22:V:188:LEU:CD2	2.29	1.03
9:i:167:LEU:CD1	13:6:30:ILE:CD1	1.76	1.03
10:j:147:GLY:CA	13:6:194:ARG:NH2	2.21	1.02
26:Z:85:VAL:CB	26:Z:86:PRO:HD3	1.86	1.02
10:j:146:PHE:HB3	13:6:194:ARG:HE	1.24	1.02
13:m:158:ASN:HB3	10:3:171:LEU:HD21	1.42	1.01
16:I:151:HIS:HE1	22:V:186:GLN:HA	1.26	1.01
10:j:148:MET:HE1	13:6:152:ASN:ND2	1.74	1.00
19:M:392:LYS:NZ	36:M:501:ADP:C4'	2.23	1.00
20:J:310:ILE:O	20:J:310:ILE:HG22	1.20	1.00
14:n:153:PRO:HG3	9:2:165:ASN:HD22	1.27	1.00
9:i:209:THR:CG2	13:6:170:LYS:HZ1	1.67	1.00
26:Z:85:VAL:HB	26:Z:86:PRO:HD3	1.01	0.99
22:V:185:ILE:C	22:V:186:GLN:CB	2.35	0.99
1:A:242:GLN:CA	29:P:85:LYS:NZ	2.25	0.98
17:K:304:ASP:CG	34:J:501:ANP:O2A	2.06	0.98
1:A:241:GLU:C	1:A:242:GLN:C	2.31	0.98
19:M:392:LYS:NZ	36:M:501:ADP:H4'	1.77	0.98
10:j:148:MET:HE3	13:6:152:ASN:HD22	1.19	0.97
1:A:242:GLN:CA	29:P:85:LYS:HZ2	1.76	0.97
9:i:167:LEU:HD13	13:6:30:ILE:HD11	1.48	0.96
9:i:167:LEU:HD13	13:6:30:ILE:CD1	1.94	0.95
9:i:164:TRP:HB2	14:7:156:ARG:NH2	1.81	0.95
22:V:185:ILE:C	22:V:186:GLN:HB2	1.90	0.95
26:Z:84:ALA:O	26:Z:86:PRO:CD	2.15	0.94
8:h:187:ILE:CG1	14:7:226:LYS:NZ	2.30	0.94
10:j:135:PHE:HZ	13:6:194:ARG:CD	1.80	0.94
8:h:137:TYR:CE1	8:1:140:LYS:HD2	1.99	0.94
8:h:187:ILE:CG1	14:7:226:LYS:HZ1	1.81	0.94
12:l:135:PHE:CZ	11:4:138:PHE:CE1	2.55	0.93
8:h:140:LYS:HB2	8:1:161:GLN:NE2	1.83	0.93
9:i:209:THR:HG22	13:6:170:LYS:NZ	1.80	0.92
8:h:137:TYR:CE1	8:1:140:LYS:NZ	2.38	0.92
10:j:148:MET:CE	13:6:152:ASN:HD21	1.70	0.92
20:J:310:ILE:O	20:J:310:ILE:CG2	2.06	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:203:TYR:HD1	13:6:153:GLN:NE2	1.68	0.91
13:m:158:ASN:CG	10:3:171:LEU:CD2	2.44	0.91
10:j:146:PHE:O	13:6:194:ARG:NE	2.03	0.91
12:l:135:PHE:CG	11:4:138:PHE:CZ	2.58	0.91
8:h:187:ILE:HG13	14:7:226:LYS:HZ1	1.29	0.90
15:H:144:LYS:O	15:H:145:TYR:CG	2.25	0.90
8:h:187:ILE:CD1	14:7:226:LYS:NZ	2.34	0.89
1:A:242:GLN:C	29:P:85:LYS:NZ	2.31	0.89
9:i:167:LEU:HD11	13:6:30:ILE:CG1	2.01	0.89
22:V:117:TRP:CE2	22:V:188:LEU:HD23	1.88	0.89
8:h:137:TYR:CE1	8:1:140:LYS:HD3	2.05	0.89
9:i:209:THR:HG21	13:6:170:LYS:HZ2	1.30	0.89
1:A:242:GLN:C	29:P:85:LYS:HZ1	1.81	0.88
13:m:152:ASN:HD22	10:3:172:ASN:HD21	1.18	0.88
23:T:84:GLN:HB3	27:N:11:ALA:O	1.74	0.88
9:i:167:LEU:CD1	13:6:30:ILE:HD13	2.04	0.88
17:K:304:ASP:OD2	34:J:501:ANP:O2A	1.90	0.88
10:j:147:GLY:HA2	13:6:194:ARG:HH21	1.08	0.87
2:B:250:LEU:HD23	2:B:250:LEU:OXT	1.75	0.87
9:i:203:TYR:HD1	13:6:153:GLN:HE22	1.20	0.87
27:N:861:TYR:O	27:N:862:SER:O	1.93	0.87
27:N:777:ALA:HA	27:N:861:TYR:HB2	1.55	0.87
12:l:135:PHE:CE1	11:4:138:PHE:CE1	2.60	0.86
10:j:148:MET:CE	13:6:152:ASN:HD22	1.74	0.86
10:j:146:PHE:C	13:6:194:ARG:NE	2.34	0.86
1:A:242:GLN:CB	29:P:85:LYS:HZ2	1.88	0.86
31:R:70:TYR:CB	31:R:70:TYR:HA	2.00	0.86
10:j:182:TRP:HH2	12:5:167:ARG:NH1	1.37	0.86
13:m:158:ASN:CB	10:3:171:LEU:HD21	2.01	0.86
27:N:855:GLU:O	27:N:857:TYR:N	2.09	0.85
16:I:151:HIS:CE1	22:V:186:GLN:CA	2.59	0.84
22:V:117:TRP:CD2	22:V:188:LEU:CG	2.59	0.84
8:h:187:ILE:CD1	14:7:226:LYS:HZ1	1.89	0.84
8:h:137:TYR:CD2	8:1:140:LYS:NZ	2.40	0.84
22:V:117:TRP:CH2	22:V:188:LEU:HG	2.13	0.84
9:i:165:ASN:OD1	14:7:153:PRO:CG	2.25	0.84
22:V:185:ILE:HB	22:V:186:GLN:HG3	1.58	0.84
27:N:778:LYS:H	27:N:861:TYR:HA	1.43	0.84
29:P:436:GLU:CD	29:P:436:GLU:O	2.21	0.84
27:N:778:LYS:N	27:N:861:TYR:O	2.11	0.83
9:i:195:VAL:HA	13:6:220:LYS:CE	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:856:PHE:HB3	27:N:859:ASN:HB2	1.61	0.82
23:T:84:GLN:OE1	27:N:15:GLU:HB2	1.80	0.82
13:m:158:ASN:CG	10:3:171:LEU:HD21	2.04	0.82
15:H:144:LYS:O	15:H:145:TYR:HD2	1.24	0.81
27:N:536:ILE:HD13	27:N:555:ILE:HG12	1.60	0.81
27:N:856:PHE:O	27:N:857:TYR:C	2.23	0.81
8:h:137:TYR:CD1	8:1:140:LYS:CD	2.57	0.80
16:I:152:LYS:HG3	22:V:187:ALA:CA	2.12	0.80
10:j:146:PHE:HB3	13:6:194:ARG:NE	1.96	0.79
9:i:164:TRP:HB3	14:7:156:ARG:CZ	2.12	0.79
29:P:436:GLU:O	29:P:436:GLU:OE2	2.00	0.79
9:i:164:TRP:CB	14:7:156:ARG:NH1	2.44	0.79
1:A:241:GLU:O	1:A:242:GLN:C	2.26	0.78
9:i:209:THR:HG22	13:6:170:LYS:HE3	1.65	0.78
14:n:153:PRO:HG3	9:2:165:ASN:ND2	1.99	0.78
15:H:77:ALA:CB	15:H:78:PRO:CD	2.62	0.78
14:n:219:TRP:CZ3	8:1:29:ARG:NE	2.52	0.78
15:H:77:ALA:HB1	15:H:78:PRO:HD3	1.66	0.77
16:I:151:HIS:NE2	22:V:186:GLN:CA	2.47	0.77
8:h:187:ILE:HD11	14:7:226:LYS:HZ3	1.49	0.77
13:m:144:SER:O	10:3:144:GLN:OE1	2.03	0.77
10:j:147:GLY:CA	13:6:194:ARG:HH21	1.91	0.76
10:j:182:TRP:HH2	12:5:167:ARG:CZ	1.98	0.76
13:m:158:ASN:OD1	10:3:171:LEU:HG	1.85	0.76
8:h:190:PRO:HG2	14:7:219:TRP:CH2	2.20	0.76
28:S:378:GLN:OE1	28:S:378:GLN:N	2.19	0.76
8:h:190:PRO:CG	14:7:219:TRP:CZ2	2.67	0.76
9:i:165:ASN:ND2	14:7:153:PRO:HG3	2.00	0.76
9:i:167:LEU:CG	13:6:30:ILE:HD11	2.12	0.75
7:G:21:GLU:OE1	7:G:21:GLU:N	2.19	0.75
9:i:203:TYR:CD1	13:6:153:GLN:NE2	2.46	0.75
33:O:164:PRO:HD2	33:O:167:ILE:HD12	1.68	0.74
9:i:201:LYS:HE3	13:6:183:LEU:CD2	2.17	0.74
27:N:856:PHE:C	27:N:859:ASN:H	1.94	0.74
9:i:201:LYS:HE3	13:6:183:LEU:HD23	1.68	0.74
26:Z:139:LEU:HD13	26:Z:149:TRP:CE3	2.22	0.74
19:M:392:LYS:NZ	36:M:501:ADP:O2'	2.17	0.73
13:m:152:ASN:ND2	10:3:172:ASN:HD21	1.85	0.73
27:N:778:LYS:N	27:N:861:TYR:C	2.47	0.73
15:H:253:GLY:HA2	34:H:501:ANP:H5'1	1.70	0.73
8:h:136:GLY:O	8:1:161:GLN:NE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:167:LEU:HD12	13:6:30:ILE:HD11	1.53	0.72
14:n:228:TYR:CD2	8:1:53:GLN:NE2	2.55	0.72
1:A:26:THR:HG21	1:A:131:ILE:HD12	1.71	0.72
27:N:855:GLU:C	27:N:857:TYR:H	1.97	0.72
8:h:137:TYR:CE1	8:1:140:LYS:CE	2.72	0.72
26:Z:128:GLU:HA	26:Z:188:ALA:HA	1.69	0.72
9:i:209:THR:CG2	13:6:170:LYS:HZ2	1.90	0.72
22:V:117:TRP:CD2	22:V:188:LEU:HG	2.21	0.72
2:B:18:LEU:HD22	2:B:18:LEU:H	1.54	0.71
17:K:304:ASP:OD2	34:J:501:ANP:PA	2.48	0.71
10:j:146:PHE:C	13:6:194:ARG:CZ	2.63	0.71
10:j:182:TRP:CZ3	12:5:167:ARG:NH1	2.28	0.71
9:i:167:LEU:HD11	13:6:30:ILE:HD12	1.55	0.70
27:N:778:LYS:H	27:N:861:TYR:CA	2.03	0.70
8:h:187:ILE:HG13	14:7:226:LYS:HZ2	1.53	0.70
1:A:242:GLN:CA	29:P:85:LYS:HZ1	2.02	0.70
22:V:185:ILE:HA	22:V:189:ILE:HB	1.73	0.70
17:K:304:ASP:OD1	34:J:501:ANP:O2A	2.09	0.70
27:N:704:GLY:O	27:N:708:ALA:HB2	1.91	0.70
13:m:35:ILE:HD11	9:2:167:LEU:HD21	1.72	0.70
16:I:361:ILE:HD13	34:I:501:ANP:C8	2.21	0.70
26:Z:149:TRP:CE3	26:Z:153:TYR:HB3	2.26	0.70
13:m:152:ASN:HD22	10:3:172:ASN:ND2	1.90	0.70
22:V:186:GLN:N	22:V:186:GLN:CG	2.54	0.70
10:j:146:PHE:C	13:6:194:ARG:HE	1.97	0.69
15:H:77:ALA:CB	15:H:78:PRO:HD3	2.21	0.69
12:l:134:THR:HA	11:4:171:ARG:HH22	1.57	0.69
27:N:777:ALA:CA	27:N:861:TYR:O	2.40	0.69
30:Q:92:LYS:H	30:Q:92:LYS:HD3	1.58	0.69
9:i:203:TYR:CZ	13:6:186:ASP:OD2	2.45	0.69
9:i:196:ARG:HD3	13:6:193:GLU:OE2	1.93	0.69
12:l:135:PHE:CD2	11:4:138:PHE:CZ	2.79	0.69
10:j:135:PHE:CZ	13:6:194:ARG:CD	2.65	0.69
22:V:232:GLU:OE1	22:V:232:GLU:N	2.25	0.69
28:S:129:GLU:C	28:S:129:GLU:CD	2.61	0.69
25:Y:68:GLU:H	25:Y:68:GLU:CD	2.00	0.68
10:j:178:ALA:CB	12:5:170:TYR:CE2	2.76	0.68
14:n:183:VAL:HG13	9:2:139:GLU:OE1	1.94	0.68
26:Z:149:TRP:CZ3	26:Z:153:TYR:HB3	2.28	0.68
31:R:106:ASN:HA	31:R:140:TYR:OH	1.93	0.68
10:j:150:GLU:HG2	13:6:193:GLU:OE1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:151:HIS:NE2	22:V:186:GLN:HB3	2.09	0.68
26:Z:290:GLU:O	26:Z:294:ILE:HG22	1.93	0.68
27:N:778:LYS:N	27:N:861:TYR:HA	2.08	0.67
9:i:195:VAL:CA	13:6:220:LYS:CE	2.49	0.67
12:5:18:SER:HB2	12:5:31:VAL:H	1.60	0.67
1:A:241:GLU:C	29:P:85:LYS:HZ1	2.02	0.67
10:j:146:PHE:CB	13:6:194:ARG:HE	2.06	0.67
26:Z:139:LEU:HB3	26:Z:149:TRP:CE2	2.29	0.66
7:G:28:GLU:OE1	7:G:28:GLU:HA	1.95	0.66
8:h:187:ILE:CD1	14:7:226:LYS:HZ3	2.04	0.66
14:n:219:TRP:CZ3	8:1:29:ARG:CZ	2.78	0.66
1:A:185:ILE:HG22	1:A:187:GLU:H	1.58	0.66
26:Z:139:LEU:HD12	26:Z:149:TRP:CZ3	2.30	0.66
29:P:436:GLU:O	29:P:436:GLU:CG	2.43	0.66
31:R:34:THR:HG1	31:R:70:TYR:HD1	1.44	0.66
31:R:109:LYS:HD3	31:R:140:TYR:CD1	2.30	0.66
2:B:20:GLN:O	2:B:20:GLN:NE2	2.27	0.66
31:R:109:LYS:HD3	31:R:140:TYR:CE1	2.31	0.65
19:M:392:LYS:HZ2	36:M:501:ADP:C2'	2.10	0.65
5:e:59:ILE:HD13	5:e:59:ILE:H	1.63	0.65
14:n:219:TRP:CE3	8:1:29:ARG:NH2	2.65	0.64
9:i:209:THR:HG21	13:6:170:LYS:HZ1	1.30	0.64
16:I:152:LYS:HG3	22:V:187:ALA:CB	2.28	0.64
27:N:856:PHE:CB	27:N:859:ASN:HB2	2.26	0.64
1:A:242:GLN:HB3	29:P:85:LYS:HZ2	1.62	0.64
17:K:241:GLU:N	17:K:241:GLU:OE1	2.30	0.64
26:Z:767:TYR:HD1	26:Z:767:TYR:O	1.80	0.64
33:O:393:VAL:OXT	33:O:393:VAL:HG12	1.96	0.64
8:h:140:LYS:HB2	8:1:161:GLN:HE22	1.59	0.64
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.27	0.64
26:Z:139:LEU:HB2	26:Z:149:TRP:CZ2	2.33	0.64
13:m:158:ASN:CG	10:3:171:LEU:HG	2.22	0.63
27:N:570:ARG:HA	27:N:570:ARG:NE	2.14	0.63
30:Q:409:TYR:C	30:Q:409:TYR:CD2	2.76	0.63
9:i:167:LEU:HD13	13:6:30:ILE:HD13	1.72	0.63
14:n:219:TRP:CH2	8:1:29:ARG:CZ	2.81	0.63
2:B:35:LEU:HD11	2:B:46:ALA:HB3	1.78	0.63
2:B:250:LEU:OXT	2:B:250:LEU:CD2	2.44	0.63
17:K:284:ALA:HB3	20:J:257:ARG:HG2	1.80	0.63
27:N:778:LYS:N	27:N:861:TYR:CA	2.61	0.63
10:j:147:GLY:HA2	13:6:194:ARG:HH22	1.54	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:149:TRP:CE2	26:Z:153:TYR:HB3	2.34	0.62
28:S:402:ILE:O	28:S:402:ILE:HG23	2.00	0.62
6:F:37:LEU:N	6:F:37:LEU:HD23	2.15	0.62
26:Z:149:TRP:CH2	26:Z:153:TYR:CB	2.81	0.62
14:n:228:TYR:CE2	8:1:53:GLN:NE2	2.62	0.62
8:1:89:ASN:HB3	8:1:92:ASN:HD22	1.64	0.62
27:N:856:PHE:HB3	27:N:859:ASN:CB	2.28	0.62
8:h:140:LYS:HB2	8:1:161:GLN:HE21	1.61	0.62
22:V:29:ILE:HD12	22:V:201:ILE:CG2	2.28	0.62
15:H:144:LYS:O	15:H:145:TYR:CB	2.47	0.62
15:H:144:LYS:C	15:H:145:TYR:CD2	2.72	0.61
18:L:387:ASN:HB3	19:M:339:ARG:HH22	1.65	0.61
32:U:40:ASP:OD1	32:U:40:ASP:C	2.37	0.61
8:h:137:TYR:HE1	8:1:140:LYS:HD3	1.60	0.61
12:l:134:THR:HA	11:4:171:ARG:NH2	2.14	0.61
23:T:84:GLN:O	27:N:11:ALA:HB1	2.01	0.61
1:A:242:GLN:C	29:P:85:LYS:HZ3	2.08	0.61
23:T:84:GLN:HB3	27:N:11:ALA:C	2.25	0.61
20:J:183:LYS:H	20:J:311:ASP:HB3	1.64	0.61
31:R:105:LYS:HD3	31:R:109:LYS:HZ2	1.64	0.61
13:m:158:ASN:CG	10:3:171:LEU:CG	2.74	0.60
21:W:81:ILE:HD12	21:W:81:ILE:C	2.26	0.60
30:Q:67:THR:H	30:Q:68:MET:HB3	1.66	0.60
26:Z:149:TRP:CZ2	26:Z:153:TYR:HB3	2.36	0.60
26:Z:149:TRP:CH2	26:Z:153:TYR:HB2	2.35	0.60
5:E:10:GLU:OE1	5:E:10:GLU:N	2.29	0.60
22:V:117:TRP:CZ2	22:V:188:LEU:CG	2.65	0.60
9:i:164:TRP:HB3	14:7:156:ARG:NH1	2.15	0.60
9:i:165:ASN:OD1	14:7:153:PRO:HD3	2.02	0.60
26:Z:520:ILE:CG1	26:Z:522:THR:HG23	2.32	0.60
10:j:178:ALA:HB3	12:5:170:TYR:CE2	2.36	0.60
9:i:203:TYR:HD1	13:6:153:GLN:CD	2.08	0.60
19:M:129:LEU:HD22	19:M:153:TYR:O	2.01	0.60
7:G:231:LEU:HD12	7:G:231:LEU:H	1.66	0.59
16:I:188:GLU:O	16:I:191:ILE:HG22	2.02	0.59
26:Z:149:TRP:CD2	26:Z:153:TYR:HB3	2.36	0.59
10:j:150:GLU:CG	13:6:193:GLU:OE1	2.51	0.59
9:i:164:TRP:CA	14:7:156:ARG:NH1	2.65	0.59
9:i:203:TYR:CB	13:6:153:GLN:HE22	2.15	0.59
23:T:84:GLN:CD	27:N:15:GLU:HB2	2.26	0.59
22:V:69:PHE:C	22:V:69:PHE:CD1	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:165:ASN:CG	14:7:153:PRO:CG	2.51	0.59
9:i:165:ASN:OD1	14:7:153:PRO:CD	2.50	0.59
16:I:152:LYS:HE3	22:V:187:ALA:O	2.03	0.59
26:Z:520:ILE:HG13	26:Z:522:THR:HG23	1.85	0.59
13:m:158:ASN:ND2	10:3:171:LEU:HD21	2.17	0.58
27:N:861:TYR:C	27:N:862:SER:O	2.47	0.58
31:R:34:THR:HA	31:R:70:TYR:HB3	1.86	0.58
31:R:34:THR:OG1	31:R:70:TYR:HD1	1.85	0.58
8:h:133:PHE:HD1	8:1:135:TYR:HB3	1.69	0.58
8:h:137:TYR:CD1	8:1:140:LYS:NZ	2.71	0.58
22:V:185:ILE:O	22:V:186:GLN:HB2	2.04	0.58
14:n:228:TYR:HD2	8:1:53:GLN:NE2	2.01	0.58
26:Z:149:TRP:CZ3	26:Z:153:TYR:CB	2.87	0.58
26:Z:793:PHE:CD1	26:Z:793:PHE:N	2.68	0.58
32:U:40:ASP:OD1	32:U:40:ASP:O	2.22	0.57
13:m:158:ASN:HB2	10:3:171:LEU:HD23	1.84	0.57
26:Z:149:TRP:CH2	26:Z:153:TYR:HB3	2.39	0.57
30:Q:20:TYR:O	30:Q:20:TYR:CD2	2.57	0.57
22:V:185:ILE:HG22	22:V:186:GLN:H	1.69	0.57
16:I:151:HIS:NE2	22:V:186:GLN:CB	2.67	0.57
31:R:392:ARG:HB3	31:R:392:ARG:CZ	2.33	0.57
18:L:377:GLU:CD	18:L:377:GLU:H	2.12	0.57
22:V:117:TRP:HE1	22:V:188:LEU:HD23	1.53	0.57
23:T:89:TYR:CD1	23:T:89:TYR:C	2.82	0.57
11:4:3:ILE:O	11:4:3:ILE:HG23	2.04	0.57
26:Z:714:ASP:HA	26:Z:760:HIS:CD2	2.40	0.56
30:Q:50:ARG:HE	30:Q:54:GLN:HG3	1.70	0.56
32:U:10:ILE:HD13	32:U:48:VAL:HB	1.87	0.56
13:m:222:ASP:HA	9:2:164:TRP:CH2	2.40	0.56
2:B:20:GLN:HG3	2:B:129:PRO:HG2	1.88	0.56
4:D:65:ILE:HG21	4:D:107:LEU:HD21	1.87	0.56
20:J:186:ILE:HG12	20:J:310:ILE:HG23	1.86	0.56
2:B:140:ASP:OD1	2:B:140:ASP:C	2.49	0.56
31:R:42:GLN:CD	31:R:42:GLN:O	2.48	0.56
23:T:86:LYS:CB	23:T:87:PRO:HD3	2.35	0.56
14:n:219:TRP:CZ3	8:1:29:ARG:NH2	2.74	0.56
33:O:393:VAL:OXT	33:O:393:VAL:CG1	2.53	0.56
6:F:37:LEU:HD23	6:F:37:LEU:H	1.71	0.55
26:Z:149:TRP:CZ2	26:Z:153:TYR:CB	2.89	0.55
27:N:585:ARG:NH2	27:N:741:TYR:OH	2.39	0.55
31:R:42:GLN:CD	31:R:42:GLN:C	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:173:THR:HG22	22:V:197:TYR:CE1	2.42	0.55
27:N:860:LYS:HB3	27:N:861:TYR:CD2	2.41	0.55
27:N:879:SER:HA	27:N:882:ILE:CD1	2.36	0.55
10:j:35:VAL:C	12:5:167:ARG:NH2	2.63	0.55
9:i:201:LYS:CE	13:6:183:LEU:CD2	2.84	0.55
9:2:97:TYR:HB3	9:2:127:LEU:HD21	1.89	0.55
16:I:81:ILE:HG23	26:Z:632:GLU:HA	1.89	0.55
12:l:133:GLN:O	11:4:171:ARG:NH2	2.40	0.54
26:Z:519:PRO:HB3	26:Z:556:ILE:HG21	1.90	0.54
31:R:64:LYS:NZ	31:R:99:TYR:CE2	2.76	0.54
12:5:4:LEU:C	12:5:4:LEU:HD12	2.32	0.54
20:J:295:ASN:OD1	34:J:501:ANP:O3G	2.25	0.54
27:N:463:TYR:CE1	27:N:485:MET:SD	3.00	0.54
8:h:140:LYS:NZ	8:1:196:LEU:OXT	2.41	0.54
4:D:106:TYR:C	4:D:106:TYR:CD2	2.84	0.54
26:Z:139:LEU:CD1	26:Z:149:TRP:CE3	2.88	0.54
27:N:856:PHE:C	27:N:858:LYS:N	2.65	0.54
15:H:77:ALA:HB1	15:H:78:PRO:CD	2.29	0.54
27:N:555:ILE:HG23	27:N:559:TYR:HD2	1.73	0.54
27:N:707:ASN:HB3	27:N:711:ARG:HG2	1.89	0.54
32:U:114:THR:OG1	32:U:116:ASN:OD1	2.22	0.54
2:B:35:LEU:CD1	2:B:46:ALA:HB3	2.38	0.54
17:K:215:PRO:HB2	34:K:501:ANP:HNB1	1.73	0.54
9:i:164:TRP:CB	14:7:156:ARG:NE	2.67	0.54
9:i:165:ASN:ND2	14:7:153:PRO:CG	2.71	0.54
14:7:165:ILE:HB	14:7:166:PRO:HD3	1.90	0.54
23:T:84:GLN:OE1	27:N:15:GLU:CB	2.53	0.54
30:Q:243:PHE:CD2	30:Q:265:MET:HE1	2.43	0.54
26:Z:335:LEU:HD22	26:Z:345:GLU:HB3	1.90	0.53
18:L:360:ILE:HG22	18:L:391:ILE:HG21	1.90	0.53
27:N:879:SER:HA	27:N:882:ILE:HD12	1.90	0.53
19:M:199:LEU:HD23	19:M:199:LEU:C	2.34	0.53
30:Q:92:LYS:H	30:Q:92:LYS:CD	2.20	0.53
18:L:166:LEU:C	18:L:166:LEU:HD23	2.33	0.53
4:d:94:HIS:CE1	4:d:103:THR:H	2.27	0.53
2:B:157:PHE:CB	3:C:56:LEU:HD11	2.39	0.53
19:M:333:LEU:HB2	19:M:338:LEU:HD11	1.90	0.53
27:N:555:ILE:HG23	27:N:559:TYR:CD2	2.44	0.53
30:Q:409:TYR:CE1	31:R:403:LEU:HB2	2.44	0.53
9:i:203:TYR:HB3	13:6:153:GLN:HE22	1.73	0.53
17:K:215:PRO:CB	34:K:501:ANP:HNB1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:155:ALA:N	22:V:201:ILE:HD11	2.24	0.53
9:i:203:TYR:CD1	13:6:153:GLN:OE1	2.61	0.53
15:H:253:GLY:HA2	34:H:501:ANP:C5'	2.35	0.53
1:A:242:GLN:CB	29:P:85:LYS:NZ	2.68	0.53
16:I:361:ILE:CD1	34:I:501:ANP:N7	2.71	0.53
20:J:48:ARG:HD3	20:J:48:ARG:C	2.34	0.53
26:Z:139:LEU:HB2	26:Z:149:TRP:CH2	2.43	0.53
2:B:140:ASP:OD1	2:B:140:ASP:O	2.27	0.53
19:M:257:GLY:HA2	19:M:303:ARG:HH12	1.73	0.53
27:N:856:PHE:HB3	27:N:859:ASN:CA	2.39	0.53
5:e:59:ILE:HD13	5:e:59:ILE:N	2.23	0.52
2:B:157:PHE:HB2	3:C:56:LEU:HD11	1.90	0.52
19:M:392:LYS:NZ	36:M:501:ADP:C2'	2.72	0.52
6:F:37:LEU:N	6:F:37:LEU:CD2	2.73	0.52
17:K:173:ASP:HB3	17:K:222:LEU:HD23	1.92	0.52
12:l:134:THR:CA	11:4:171:ARG:HH22	2.20	0.52
9:2:166:ASP:OD1	9:2:166:ASP:C	2.47	0.52
26:Z:139:LEU:HB3	26:Z:149:TRP:CD2	2.45	0.52
27:N:855:GLU:C	27:N:857:TYR:N	2.60	0.52
9:i:203:TYR:HB3	13:6:153:GLN:NE2	2.25	0.52
9:i:203:TYR:CE2	13:6:186:ASP:OD2	2.63	0.52
26:Z:128:GLU:CB	26:Z:188:ALA:CB	2.77	0.52
8:h:11:GLY:HA2	8:h:102:TYR:CE1	2.44	0.52
8:h:187:ILE:HD12	14:7:226:LYS:HZ1	1.74	0.52
31:R:42:GLN:O	31:R:42:GLN:NE2	2.43	0.52
8:h:190:PRO:CG	14:7:219:TRP:CE2	2.92	0.52
15:H:152:ILE:O	15:H:152:ILE:HG22	2.09	0.52
3:c:97:TYR:CE2	3:c:101:TYR:CE2	2.98	0.51
9:i:201:LYS:HE3	13:6:183:LEU:HD21	1.91	0.51
12:l:132:GLY:C	11:4:138:PHE:HZ	2.18	0.51
6:F:71:LEU:HD12	6:F:71:LEU:C	2.36	0.51
29:P:436:GLU:O	29:P:436:GLU:HG3	2.08	0.51
23:T:86:LYS:HB2	23:T:87:PRO:HD3	1.90	0.51
31:R:34:THR:OG1	31:R:70:TYR:CD1	2.62	0.51
9:i:165:ASN:N	14:7:156:ARG:HH12	1.99	0.51
14:n:153:PRO:CG	9:2:165:ASN:HD22	2.12	0.51
14:n:231:GLN:OE1	8:1:57:ASP:OD1	2.28	0.51
18:L:269:TYR:CE2	18:L:273:HIS:CD2	2.99	0.51
27:N:856:PHE:O	27:N:859:ASN:CA	2.56	0.51
10:j:146:PHE:HD1	13:6:194:ARG:CD	1.99	0.51
5:e:67:GLY:HA3	5:e:220:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:512:ILE:HG12	26:Z:526:ALA:HB1	1.92	0.51
9:i:167:LEU:HD21	13:6:30:ILE:HD12	1.92	0.51
9:i:203:TYR:CD1	13:6:153:GLN:CD	2.88	0.51
6:F:233:ILE:OXT	6:F:233:ILE:HG22	2.10	0.51
27:N:739:PHE:CD1	27:N:739:PHE:C	2.88	0.51
10:j:108:VAL:HG12	10:j:109:ALA:N	2.26	0.51
12:l:135:PHE:CB	11:4:138:PHE:CZ	2.90	0.51
22:V:216:LEU:HB3	22:V:220:GLN:HG3	1.92	0.51
8:h:146:MET:HE1	8:h:154:PHE:CD2	2.46	0.51
22:V:69:PHE:CD1	22:V:69:PHE:O	2.64	0.51
16:I:81:ILE:CG2	26:Z:632:GLU:N	2.73	0.51
26:Z:139:LEU:CD1	26:Z:149:TRP:CZ3	2.94	0.51
26:Z:767:TYR:CD1	26:Z:767:TYR:C	2.89	0.51
29:P:108:LYS:NZ	29:P:142:ASP:OD2	2.43	0.51
22:V:188:LEU:HD22	22:V:188:LEU:O	2.11	0.50
12:5:55:TRP:CE3	12:5:55:TRP:HA	2.46	0.50
23:T:84:GLN:HA	27:N:11:ALA:CA	2.42	0.50
8:h:195:GLN:NE2	14:7:215:GLU:OE1	2.45	0.50
7:G:59:LYS:O	7:G:59:LYS:HG3	2.11	0.50
17:K:149:ILE:C	17:K:149:ILE:HD12	2.36	0.50
3:C:97:TYR:CD2	3:C:105:ILE:HA	2.46	0.50
28:S:88:PHE:CD1	28:S:88:PHE:N	2.74	0.50
21:W:101:ARG:HB2	21:W:104:LYS:HD3	1.93	0.50
32:U:69:ASP:C	32:U:69:ASP:OD1	2.54	0.50
9:i:164:TRP:HB2	14:7:156:ARG:NE	2.17	0.50
26:Z:767:TYR:HD1	26:Z:767:TYR:C	2.19	0.50
27:N:665:ILE:HG23	27:N:665:ILE:O	2.10	0.50
27:N:856:PHE:O	27:N:858:LYS:N	2.44	0.50
8:h:59:VAL:HG11	8:h:82:PHE:CE1	2.47	0.50
9:i:196:ARG:CD	13:6:193:GLU:OE2	2.60	0.50
15:H:144:LYS:C	15:H:145:TYR:CG	2.89	0.50
3:C:97:TYR:CE2	3:C:105:ILE:HA	2.47	0.50
29:P:240:TYR:N	29:P:240:TYR:CD1	2.75	0.50
26:Z:519:PRO:HB3	26:Z:556:ILE:HD13	1.93	0.49
31:R:119:LYS:HE3	31:R:119:LYS:HA	1.94	0.49
14:n:219:TRP:CH2	8:1:29:ARG:NE	2.80	0.49
23:T:80:ASN:HB3	27:N:16:ASN:OD1	2.11	0.49
30:Q:115:ILE:HD11	30:Q:148:LYS:HD3	1.95	0.49
2:b:7:PHE:CZ	2:b:9:LEU:HD21	2.48	0.49
13:m:222:ASP:HA	9:2:164:TRP:HH2	1.77	0.49
29:P:310:ARG:O	29:P:314:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:392:LYS:NZ	36:M:501:ADP:O4'	2.36	0.49
27:N:108:MET:SD	27:N:108:MET:C	2.95	0.49
29:P:351:ARG:HE	29:P:383:LEU:HD11	1.77	0.49
30:Q:188:LEU:O	30:Q:189:ARG:HB2	2.13	0.49
14:n:216:ASN:HB3	8:l:191:ASP:OD2	2.12	0.49
16:I:354:ASP:OD1	16:I:354:ASP:C	2.56	0.49
22:V:188:LEU:HD22	22:V:188:LEU:C	2.37	0.49
33:O:291:ILE:CG2	33:O:291:ILE:O	2.51	0.49
5:E:70:MET:HE1	5:E:78:ARG:HH11	1.78	0.49
20:J:186:ILE:HG12	20:J:310:ILE:CG2	2.42	0.49
33:O:178:TYR:CZ	33:O:182:LYS:HD2	2.47	0.49
9:i:196:ARG:HB2	13:6:193:GLU:OE2	2.13	0.49
19:M:81:ASN:OD1	19:M:81:ASN:C	2.54	0.49
2:B:98:LYS:HA	2:B:102:GLY:HA2	1.94	0.49
6:F:154:GLU:HG3	7:G:56:VAL:HG21	1.94	0.49
2:b:224:TYR:CD1	2:b:224:TYR:C	2.91	0.49
5:E:114:ARG:HH12	5:E:125:LEU:HB2	1.76	0.48
22:V:29:ILE:HD12	22:V:201:ILE:HG23	1.95	0.48
30:Q:111:LEU:HD23	30:Q:148:LYS:HG2	1.94	0.48
12:l:137:TYR:H	11:4:171:ARG:HH12	1.61	0.48
12:l:137:TYR:N	11:4:171:ARG:HH12	2.05	0.48
3:C:89:THR:HG22	3:C:93:HIS:CE1	2.48	0.48
12:5:179:HIS:HB3	12:5:188:HIS:CE1	2.48	0.48
19:M:218:ALA:HB3	19:M:324:LEU:HD22	1.95	0.48
16:I:81:ILE:HG23	26:Z:632:GLU:CA	2.43	0.48
16:I:81:ILE:HG21	26:Z:628:ASN:O	2.14	0.48
24:X:115:SER:OG	24:X:116:ALA:N	2.46	0.48
26:Z:139:LEU:CB	26:Z:149:TRP:CE2	2.94	0.48
10:j:178:ALA:CB	12:5:170:TYR:CD2	2.97	0.48
16:I:81:ILE:CG2	26:Z:631:GLY:C	2.87	0.48
31:R:60:ALA:HB1	31:R:99:TYR:CZ	2.49	0.48
17:K:428:LYS:CG	17:K:428:LYS:OXT	2.58	0.48
29:P:63:VAL:O	29:P:66:LEU:HB2	2.14	0.48
1:A:241:GLU:C	29:P:85:LYS:NZ	2.61	0.48
10:j:34:GLY:HA3	10:j:182:TRP:CH2	2.49	0.48
27:N:528:ARG:HD2	27:N:528:ARG:HA	1.75	0.48
4:D:165:ASN:C	4:D:165:ASN:OD1	2.55	0.47
16:I:151:HIS:NE2	22:V:187:ALA:N	2.61	0.47
2:B:119:GLN:C	2:B:119:GLN:OE1	2.57	0.47
19:M:392:LYS:NZ	36:M:501:ADP:C3'	2.77	0.47
30:Q:392:GLN:HB3	31:R:348:LEU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:235:PHE:N	15:H:235:PHE:CD1	2.82	0.47
29:P:52:LEU:HB2	29:P:96:MET:SD	2.54	0.47
18:L:435:GLN:C	18:L:436:LYS:O	2.53	0.47
26:Z:238:ASP:CG	26:Z:276:ASN:HD22	2.22	0.47
19:M:392:LYS:HD3	36:M:501:ADP:H1'	1.96	0.47
31:R:392:ARG:HB3	31:R:392:ARG:NH1	2.29	0.47
13:6:190:SER:HB2	13:6:194:ARG:HH22	1.79	0.47
19:M:331:ASP:OD1	19:M:332:VAL:HG23	2.15	0.47
22:V:196:TYR:CD1	22:V:196:TYR:C	2.92	0.47
27:N:156:ILE:HG23	27:N:157:ALA:N	2.30	0.47
30:Q:67:THR:H	30:Q:68:MET:CB	2.26	0.47
16:I:81:ILE:HG23	26:Z:632:GLU:N	2.30	0.47
19:M:392:LYS:CD	36:M:501:ADP:O2'	2.62	0.47
22:V:263:GLU:OE1	22:V:263:GLU:N	2.38	0.47
26:Z:85:VAL:CB	26:Z:86:PRO:CD	2.59	0.47
30:Q:111:LEU:HD22	30:Q:148:LYS:CE	2.44	0.47
31:R:60:ALA:HB1	31:R:99:TYR:CE2	2.49	0.47
12:l:26:VAL:O	10:3:176:ARG:NH2	2.47	0.47
31:R:106:ASN:CA	31:R:140:TYR:OH	2.62	0.47
4:d:106:TYR:C	4:d:106:TYR:CD2	2.92	0.47
30:Q:275:ILE:C	30:Q:275:ILE:HD12	2.40	0.47
15:H:212:GLY:H	34:H:501:ANP:C6	2.27	0.47
13:6:170:LYS:HA	13:6:171:PRO:HD3	1.84	0.46
22:V:29:ILE:HD12	22:V:201:ILE:HG21	1.95	0.46
30:Q:74:LEU:HD21	30:Q:107:VAL:HG11	1.97	0.46
33:O:165:LEU:H	33:O:165:LEU:HD23	1.80	0.46
10:j:150:GLU:OE1	13:6:193:GLU:OE1	2.33	0.46
14:7:101:TYR:HA	14:7:104:ARG:HG2	1.97	0.46
16:I:361:ILE:HD11	34:I:501:ANP:N7	2.30	0.46
17:K:428:LYS:OXT	17:K:428:LYS:HG2	2.14	0.46
26:Z:948:TRP:CD1	26:Z:948:TRP:N	2.82	0.46
27:N:677:ASP:O	27:N:680:LYS:HG2	2.15	0.46
25:Y:68:GLU:OE1	25:Y:68:GLU:N	2.32	0.46
26:Z:625:THR:HB	26:Z:626:PRO:HD3	1.96	0.46
27:N:777:ALA:HA	27:N:861:TYR:CB	2.36	0.46
33:O:291:ILE:O	33:O:291:ILE:HG22	2.04	0.46
14:7:131:ASN:ND2	14:7:133:LEU:H	2.13	0.46
22:V:263:GLU:H	22:V:263:GLU:CD	2.22	0.46
26:Z:759:ARG:HA	26:Z:792:VAL:HG22	1.97	0.46
5:e:67:GLY:HA3	5:e:220:PHE:HE2	1.79	0.46
3:C:95:GLN:HB3	10:3:68:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ARG:HG3	4:D:53:GLN:HE22	1.80	0.46
18:L:382:MET:SD	18:L:419:VAL:HG23	2.56	0.46
27:N:779:GLU:H	27:N:779:GLU:CD	2.23	0.46
26:Z:84:ALA:O	26:Z:86:PRO:N	2.49	0.46
27:N:339:MET:HG3	27:N:340:HIS:CE1	2.50	0.46
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.51	0.46
6:F:20:GLN:OE1	6:F:20:GLN:HA	2.16	0.46
26:Z:139:LEU:CB	26:Z:149:TRP:CZ2	2.98	0.46
7:G:208:PHE:H	7:G:208:PHE:HD1	1.62	0.46
11:4:106:GLY:HA2	11:4:184:VAL:HG11	1.97	0.46
31:R:99:TYR:CD1	31:R:99:TYR:N	2.82	0.46
1:a:154:TYR:CD1	1:a:154:TYR:C	2.93	0.46
26:Z:593:HIS:HB2	26:Z:596:THR:H	1.81	0.46
29:P:136:ARG:HD2	29:P:136:ARG:C	2.41	0.46
22:V:182:LYS:O	22:V:185:ILE:HD11	2.17	0.45
22:V:234:GLU:CD	22:V:234:GLU:C	2.85	0.45
24:X:46:TRP:HE1	24:X:132:SER:HA	1.82	0.45
6:f:205:LEU:HA	6:f:209:ASN:HD22	1.82	0.45
6:F:48:LEU:HD23	6:F:48:LEU:HA	1.77	0.45
15:H:191:ILE:HG13	15:H:191:ILE:O	2.16	0.45
2:B:106:PRO:HD2	2:B:109:LEU:HD12	1.98	0.45
18:L:333:LEU:HD13	18:L:334:ASP:H	1.82	0.45
23:T:84:GLN:HA	27:N:11:ALA:HB1	1.98	0.45
23:T:84:GLN:CB	27:N:11:ALA:O	2.57	0.45
2:B:18:LEU:H	2:B:18:LEU:CD2	2.28	0.45
27:N:557:LEU:HD21	27:N:734:VAL:HG21	1.98	0.45
13:m:5:TYR:CD1	13:m:106:TYR:CE1	3.04	0.45
3:C:3:ARG:HD3	6:F:122:TYR:CD2	2.52	0.45
3:C:61:SER:OG	3:C:63:GLU:OE2	2.35	0.45
22:V:185:ILE:HG23	22:V:185:ILE:HD12	1.45	0.45
26:Z:617:ILE:HG21	27:N:814:ALA:HB1	1.99	0.45
28:S:380:CYS:HA	28:S:383:LEU:HD12	1.99	0.45
2:B:83:ARG:CZ	2:B:83:ARG:HB3	2.46	0.45
16:I:253:ILE:CG1	16:I:287:ILE:HG12	2.46	0.45
18:L:377:GLU:CD	18:L:377:GLU:N	2.74	0.45
26:Z:854:LEU:HD23	26:Z:854:LEU:C	2.42	0.45
29:P:89:LEU:HB3	29:P:92:SER:HB2	1.99	0.45
16:I:361:ILE:HD13	34:I:501:ANP:N7	2.31	0.45
22:V:142:ASP:OD1	22:V:142:ASP:C	2.60	0.45
26:Z:520:ILE:HG13	26:Z:522:THR:H	1.82	0.45
27:N:525:ASN:HA	27:N:528:ARG:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:291:GLU:HA	26:Z:294:ILE:CG2	2.47	0.44
26:Z:520:ILE:HG13	26:Z:521:GLU:N	2.32	0.44
27:N:8:PRO:O	27:N:11:ALA:HB3	2.17	0.44
27:N:575:ALA:O	27:N:584:ARG:NH1	2.50	0.44
28:S:402:ILE:O	28:S:402:ILE:CG2	2.65	0.44
31:R:113:LEU:HB2	31:R:137:LEU:HD23	1.98	0.44
5:e:163:ALA:H	5:e:172:GLN:HE22	1.64	0.44
26:Z:948:TRP:CD1	26:Z:948:TRP:H	2.34	0.44
10:j:146:PHE:O	13:6:194:ARG:NH1	2.47	0.44
29:P:99:LYS:HA	29:P:99:LYS:HD3	1.81	0.44
31:R:58:GLU:HG3	31:R:102:LEU:HA	2.00	0.44
32:U:89:LEU:C	32:U:89:LEU:HD23	2.43	0.44
6:f:136:TYR:C	6:f:136:TYR:CD1	2.96	0.44
14:7:13:SER:O	14:7:155:LEU:HD13	2.18	0.44
23:T:78:PHE:O	23:T:82:PHE:HB2	2.17	0.44
26:Z:611:THR:O	26:Z:611:THR:HG23	2.16	0.44
27:N:871:MET:HG3	27:N:871:MET:O	2.18	0.44
27:N:603:PRO:HA	27:N:606:VAL:HG22	1.99	0.44
27:N:642:ASP:HB2	27:N:643:PRO:HD3	1.98	0.44
28:S:374:ASP:OD1	28:S:376:THR:OG1	2.29	0.44
33:O:238:ILE:HG23	33:O:239:MET:N	2.32	0.44
1:A:56:ASP:HB2	1:A:59:THR:HG23	1.99	0.44
31:R:238:PHE:CE1	31:R:249:ILE:HD11	2.52	0.44
6:f:134:ILE:HD12	6:f:215:VAL:HG12	1.99	0.43
12:l:75:SER:HB2	12:l:78:ALA:H	1.83	0.43
16:I:152:LYS:HG3	22:V:187:ALA:HA	1.97	0.43
29:P:284:ILE:HG22	29:P:290:LEU:HD22	2.00	0.43
29:P:326:ASP:HA	29:P:330:GLY:HA3	2.00	0.43
9:i:201:LYS:CE	13:6:183:LEU:HD23	2.43	0.43
13:m:144:SER:O	10:3:144:GLN:CD	2.61	0.43
8:1:61:TYR:CD1	8:1:61:TYR:C	2.96	0.43
19:M:378:GLU:OE1	19:M:378:GLU:HA	2.18	0.43
26:Z:23:GLN:NE2	26:Z:48:ASP:O	2.49	0.43
8:h:137:TYR:HD1	8:1:140:LYS:HD2	1.64	0.43
9:i:164:TRP:HB3	14:7:156:ARG:NE	2.33	0.43
22:V:247:ILE:O	22:V:247:ILE:HG22	2.19	0.43
26:Z:941:ARG:HB3	26:Z:942:PRO:HD3	2.00	0.43
29:P:266:TYR:CD2	29:P:328:ALA:HB1	2.53	0.43
31:R:66:LEU:HA	31:R:69:GLU:HB2	2.00	0.43
33:O:242:ILE:CG2	33:O:245:ASP:OD2	2.66	0.43
27:N:156:ILE:CG2	27:N:157:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:253:ILE:HG13	16:I:287:ILE:HG12	1.99	0.43
17:K:304:ASP:OD2	34:J:501:ANP:O1A	2.37	0.43
3:c:135:ILE:HD13	3:c:135:ILE:HA	1.78	0.43
11:k:195:PHE:HD1	11:k:195:PHE:H	1.67	0.43
17:K:346:ARG:NH1	17:K:349:ARG:HE	2.17	0.43
27:N:460:ILE:HD12	27:N:460:ILE:HA	1.89	0.43
15:H:191:ILE:O	15:H:191:ILE:HG23	2.18	0.43
15:H:191:ILE:HD12	15:H:191:ILE:HA	1.93	0.43
8:h:132:THR:O	8:l:133:PHE:HA	2.19	0.43
11:k:29:LYS:HE3	12:l:125:ASP:H	1.82	0.43
14:n:231:GLN:CD	8:l:57:ASP:OD1	2.62	0.43
26:Z:471:LEU:HD21	26:Z:504:GLU:HG3	2.00	0.43
16:I:341:PRO:O	16:I:345:ASP:N	2.46	0.43
19:M:199:LEU:HB3	19:M:200:PRO:HD3	2.01	0.43
20:J:282:PHE:CE2	20:J:290:ILE:HD11	2.53	0.43
28:S:88:PHE:CE2	28:S:162:VAL:HG11	2.53	0.43
33:O:62:TYR:HD1	33:O:63:ASP:H	1.65	0.43
20:J:234:PHE:C	20:J:234:PHE:CD2	2.96	0.43
22:V:184:ASN:HB3	22:V:188:LEU:HD12	2.01	0.43
22:V:263:GLU:N	22:V:263:GLU:CD	2.77	0.43
26:Z:294:ILE:HG13	26:Z:330:ILE:CD1	2.49	0.43
17:K:421:VAL:HG23	17:K:422:ASP:H	1.83	0.42
22:V:228:TYR:CD1	22:V:228:TYR:N	2.86	0.42
31:R:106:ASN:O	31:R:110:ILE:N	2.48	0.42
9:i:201:LYS:CE	13:6:183:LEU:HD21	2.48	0.42
11:k:107:TYR:HA	11:k:114:PRO:HA	2.02	0.42
16:I:81:ILE:HG22	26:Z:631:GLY:HA3	2.02	0.42
27:N:508:THR:HG21	27:N:513:ILE:HB	2.00	0.42
8:h:190:PRO:HD2	14:7:219:TRP:CE3	2.55	0.42
10:j:146:PHE:HB3	13:6:194:ARG:CD	2.50	0.42
3:C:48:GLU:O	3:C:48:GLU:HG3	2.19	0.42
1:A:66:ILE:HD12	1:A:88:ALA:HB3	2.01	0.42
2:B:158:PRO:O	3:C:56:LEU:HD12	2.19	0.42
4:D:165:ASN:O	4:D:165:ASN:CG	2.61	0.42
6:F:129:VAL:O	6:F:129:VAL:HG23	2.19	0.42
23:T:28:PRO:HB2	23:T:29:PRO:HD3	2.02	0.42
14:n:17:ASP:HB3	14:n:166:PRO:HA	2.00	0.42
7:G:243:ILE:C	7:G:244:ASN:O	2.60	0.42
27:N:401:LYS:HB3	27:N:442:LEU:HD13	2.02	0.42
3:C:25:LEU:HA	3:C:28:ILE:HD12	2.02	0.42
8:l:64:GLU:HA	8:l:64:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:152:ASN:HB2	14:7:153:PRO:HD3	2.01	0.42
15:H:172:MET:HG3	15:H:189:PRO:HG3	2.02	0.42
19:M:392:LYS:NZ	36:M:501:ADP:C1'	2.83	0.42
30:Q:20:TYR:O	30:Q:20:TYR:CG	2.72	0.42
30:Q:409:TYR:OH	31:R:402:LEU:HB2	2.20	0.42
15:H:77:ALA:HB3	15:H:78:PRO:HD2	1.98	0.42
5:e:115:PHE:CD2	5:e:129:PRO:HD3	2.55	0.42
7:g:226:PHE:CE2	14:n:79:PRO:HG3	2.55	0.42
2:B:159:TRP:CE2	3:C:56:LEU:HD13	2.55	0.42
11:4:191:GLN:HE22	11:4:193:ASP:HA	1.84	0.42
19:M:283:LEU:H	19:M:327:THR:HB	1.85	0.42
30:Q:361:HIS:NE2	30:Q:365:ILE:HD11	2.35	0.42
1:a:47:GLN:HE22	1:a:213:ASP:HB3	1.85	0.41
10:3:166:ILE:HD13	10:3:166:ILE:HA	1.83	0.41
20:J:282:PHE:CZ	20:J:288:ILE:HG21	2.55	0.41
23:T:86:LYS:CB	23:T:87:PRO:CD	2.98	0.41
23:T:87:PRO:HB3	27:N:7:ALA:HB1	2.02	0.41
30:Q:111:LEU:HD22	30:Q:148:LYS:HE3	2.00	0.41
1:A:119:TYR:CD1	1:A:119:TYR:N	2.85	0.41
11:4:85:ARG:HG2	11:4:85:ARG:HH11	1.85	0.41
30:Q:94:VAL:HG13	30:Q:95:LYS:N	2.34	0.41
26:Z:335:LEU:HD22	26:Z:345:GLU:CB	2.50	0.41
27:N:860:LYS:HB3	27:N:861:TYR:HD2	1.85	0.41
31:R:60:ALA:HA	31:R:63:TYR:HB3	2.00	0.41
13:m:222:ASP:CA	9:2:164:TRP:HH2	2.34	0.41
9:2:143:LYS:O	9:2:143:LYS:HG3	2.20	0.41
18:L:137:ARG:NE	18:L:137:ARG:HA	2.36	0.41
31:R:34:THR:HA	31:R:70:TYR:HA	2.02	0.41
31:R:392:ARG:HH11	31:R:392:ARG:CA	2.32	0.41
3:c:160:LYS:HB3	3:c:179:TYR:CE2	2.56	0.41
9:2:36:ARG:HG3	9:2:38:SER:O	2.20	0.41
29:P:393:VAL:HG22	29:P:400:VAL:HG23	2.03	0.41
31:R:58:GLU:CD	31:R:102:LEU:HA	2.45	0.41
14:7:48:ASN:ND2	14:7:48:ASN:H	2.18	0.41
5:E:115:PHE:H	5:E:124:ARG:NH1	2.19	0.41
13:6:75:TYR:CD1	13:6:84:LEU:HD13	2.56	0.41
33:O:252:PHE:HA	33:O:255:LEU:HD12	2.03	0.41
8:h:137:TYR:CD1	8:1:140:LYS:CE	3.02	0.41
17:K:304:ASP:CG	34:J:501:ANP:PA	3.02	0.41
21:W:81:ILE:C	21:W:81:ILE:CD1	2.94	0.41
27:N:654:GLN:HG3	27:N:698:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:64:PHE:HB2	1:a:72:MET:HE2	2.03	0.41
4:d:227:ILE:HA	4:d:230:TYR:CD2	2.56	0.41
18:L:98:LEU:HA	18:L:98:LEU:HD23	1.84	0.41
23:T:84:GLN:HA	27:N:11:ALA:HA	2.02	0.41
26:Z:369:PHE:CD1	26:Z:399:LEU:HD12	2.56	0.41
26:Z:938:GLN:CD	26:Z:938:GLN:H	2.29	0.41
27:N:211:PHE:CD1	27:N:225:LEU:HD22	2.56	0.41
27:N:525:ASN:HA	27:N:528:ARG:HG2	2.03	0.41
28:S:327:ILE:HG23	28:S:349:THR:HG23	2.02	0.41
9:i:167:LEU:HD21	13:6:35:ILE:CG1	2.50	0.41
14:n:137:TYR:CD1	14:n:137:TYR:C	2.99	0.41
6:F:233:ILE:OXT	6:F:233:ILE:CG2	2.68	0.41
11:4:22:THR:O	11:4:23:ARG:HD3	2.21	0.41
12:5:58:TRP:CZ3	12:5:86:LEU:HD22	2.56	0.41
14:7:74:ASN:HD21	14:7:87:LEU:HD21	1.86	0.41
20:J:186:ILE:HG13	20:J:310:ILE:HD13	2.03	0.41
27:N:885:ILE:HG22	27:N:888:ASP:H	1.86	0.41
29:P:66:LEU:O	29:P:66:LEU:HG	2.21	0.41
31:R:33:LEU:HD23	31:R:70:TYR:CE2	2.56	0.41
1:a:50:VAL:HG22	1:a:60:VAL:HG21	2.02	0.40
22:V:61:TYR:O	22:V:61:TYR:CG	2.71	0.40
24:X:27:ILE:HA	24:X:28:PRO:HD3	1.93	0.40
26:Z:428:TRP:CD1	26:Z:428:TRP:O	2.74	0.40
26:Z:941:ARG:HD2	26:Z:941:ARG:C	2.46	0.40
30:Q:241:GLU:OE1	30:Q:241:GLU:HA	2.20	0.40
31:R:96:GLN:HA	31:R:99:TYR:HD1	1.86	0.40
30:Q:352:GLU:HB2	30:Q:353:PRO:HD3	2.03	0.40
3:c:125:GLY:H	4:d:2:TYR:HB2	1.85	0.40
6:F:76:LEU:O	6:F:129:VAL:HG12	2.20	0.40
10:3:14:MET:HB3	10:3:166:ILE:HD11	2.02	0.40
9:i:201:LYS:NZ	13:6:183:LEU:HD21	2.37	0.40
31:R:212:THR:HG22	31:R:234:SER:HB2	2.04	0.40
31:R:403:LEU:HD21	32:U:260:ASN:HD21	1.85	0.40
15:H:144:LYS:HA	15:H:158:GLY:HA2	2.03	0.40
19:M:129:LEU:HA	19:M:129:LEU:HD23	1.73	0.40
22:V:200:ASN:OD1	22:V:200:ASN:C	2.64	0.40
27:N:59:GLU:CD	27:N:59:GLU:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	226 (95%)	10 (4%)	3 (1%)	9	42
1	a	239/252 (95%)	230 (96%)	8 (3%)	1 (0%)	30	67
2	B	248/250 (99%)	238 (96%)	7 (3%)	3 (1%)	10	44
2	b	248/250 (99%)	236 (95%)	8 (3%)	4 (2%)	7	38
3	C	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	67
3	c	242/258 (94%)	230 (95%)	11 (4%)	1 (0%)	30	67
4	D	238/254 (94%)	222 (93%)	12 (5%)	4 (2%)	7	36
4	d	238/254 (94%)	227 (95%)	10 (4%)	1 (0%)	30	67
5	E	240/260 (92%)	225 (94%)	11 (5%)	4 (2%)	7	36
5	e	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	9	42
6	F	231/234 (99%)	219 (95%)	9 (4%)	3 (1%)	9	42
6	f	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
7	G	241/288 (84%)	230 (95%)	7 (3%)	4 (2%)	7	36
7	g	241/288 (84%)	231 (96%)	8 (3%)	2 (1%)	16	54
8	1	194/215 (90%)	185 (95%)	8 (4%)	1 (0%)	24	63
8	h	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
9	2	224/261 (86%)	211 (94%)	11 (5%)	2 (1%)	14	51
9	i	224/261 (86%)	207 (92%)	14 (6%)	3 (1%)	9	42
10	3	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	12	49
10	j	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
11	4	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	63
11	k	193/198 (98%)	181 (94%)	12 (6%)	0	100	100
12	5	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
12	l	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	24	63
13	6	220/241 (91%)	209 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	24	63
14	7	227/266 (85%)	210 (92%)	12 (5%)	5 (2%)	5	29
14	n	230/266 (86%)	215 (94%)	15 (6%)	0	100	100
15	H	376/467 (80%)	340 (90%)	25 (7%)	11 (3%)	3	23
16	I	383/437 (88%)	349 (91%)	28 (7%)	6 (2%)	7	38
17	K	387/428 (90%)	354 (92%)	23 (6%)	10 (3%)	4	25
18	L	386/437 (88%)	362 (94%)	19 (5%)	5 (1%)	9	42
19	M	377/434 (87%)	342 (91%)	25 (7%)	10 (3%)	4	25
20	J	384/405 (95%)	354 (92%)	21 (6%)	9 (2%)	5	28
21	W	195/268 (73%)	184 (94%)	8 (4%)	3 (2%)	8	40
22	V	287/306 (94%)	263 (92%)	17 (6%)	7 (2%)	4	27
23	T	264/274 (96%)	241 (91%)	17 (6%)	6 (2%)	5	28
24	X	125/156 (80%)	99 (79%)	23 (18%)	3 (2%)	4	27
25	Y	47/89 (53%)	39 (83%)	7 (15%)	1 (2%)	5	30
26	Z	902/993 (91%)	835 (93%)	52 (6%)	15 (2%)	7	36
27	N	886/945 (94%)	837 (94%)	42 (5%)	7 (1%)	16	54
28	S	473/523 (90%)	441 (93%)	21 (4%)	11 (2%)	5	28
29	P	438/445 (98%)	410 (94%)	19 (4%)	9 (2%)	5	30
30	Q	432/434 (100%)	388 (90%)	28 (6%)	16 (4%)	2	20
31	R	377/429 (88%)	358 (95%)	16 (4%)	3 (1%)	16	54
32	U	296/338 (88%)	283 (96%)	8 (3%)	5 (2%)	7	36
33	O	386/393 (98%)	377 (98%)	6 (2%)	3 (1%)	16	54
All	All	13700/15139 (90%)	12845 (94%)	665 (5%)	190 (1%)	11	40

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	GLU
2	B	93	ALA
5	E	114	ARG
11	4	25	ILE
15	H	77	ALA
15	H	145	TYR
15	H	206	VAL

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Mol	Chain	Res	Type
16	I	115	ASP
17	K	104	ASP
17	K	334	LEU
17	K	398	ASN
17	K	416	LYS
17	K	418	ASP
17	K	419	ASN
18	L	432	ILE
19	M	172	VAL
19	M	177	THR
19	M	180	TYR
19	M	230	LEU
20	J	72	VAL
20	J	312	ARG
20	J	341	ILE
22	V	200	ASN
23	T	97	SER
23	T	173	GLU
24	X	29	VAL
26	Z	82	MET
26	Z	85	VAL
26	Z	728	LYS
27	N	856	PHE
27	N	862	SER
28	S	47	THR
28	S	101	LYS
28	S	150	LYS
28	S	172	ASN
29	P	89	LEU
30	Q	44	ALA
30	Q	68	MET
30	Q	384	LYS
31	R	125	GLU
31	R	280	ILE
32	U	146	ASP
1	a	159	ALA
7	g	9	SER
2	B	94	HIS
4	D	30	CYS
5	E	120	SER
5	E	125	LEU
7	G	59	LYS

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Mol	Chain	Res	Type
7	G	68	ARG
14	7	83	ALA
15	H	456	LYS
17	K	177	LEU
18	L	101	ILE
18	L	406	ASP
19	M	321	VAL
22	V	115	GLY
23	T	91	SER
23	T	99	SER
23	T	258	ASN
24	X	115	SER
26	Z	309	GLN
26	Z	339	PHE
27	N	359	ALA
28	S	153	GLU
28	S	303	ASN
29	P	111	ASP
29	P	126	THR
30	Q	46	VAL
30	Q	49	LYS
30	Q	51	ARG
30	Q	75	ARG
30	Q	170	ASP
30	Q	387	TYR
30	Q	406	ASP
32	U	6	GLU
2	b	226	GLY
7	g	221	ASN
9	i	183	ASP
12	l	206	SER
13	m	19	ASP
1	A	159	ALA
1	A	181	LYS
4	D	205	ALA
5	E	116	GLY
6	F	4	ASN
9	2	91	GLN
9	2	166	ASP
14	7	27	LEU
14	7	81	ALA
16	I	337	ALA

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Mol	Chain	Res	Type
17	K	171	TYR
17	K	342	SER
19	M	318	ASP
19	M	355	ASP
20	J	70	SER
20	J	82	LYS
20	J	249	GLU
20	J	335	MET
21	W	144	PHE
24	X	41	GLU
25	Y	31	GLU
26	Z	76	LYS
26	Z	376	SER
26	Z	611	THR
26	Z	887	GLY
26	Z	947	GLY
27	N	174	LEU
27	N	490	LEU
27	N	560	ALA
28	S	44	THR
29	P	88	GLN
29	P	132	VAL
29	P	328	ALA
29	P	397	ALA
30	Q	126	LYS
30	Q	309	ARG
32	U	5	HIS
33	O	119	SER
2	b	97	TYR
3	c	219	ALA
4	d	102	VAL
5	e	125	LEU
3	C	220	ASN
4	D	48	SER
6	F	32	SER
7	G	67	ASP
10	3	181	GLY
15	H	179	SER
15	H	181	TYR
16	I	293	ASP
17	K	49	PHE
18	L	328	ASN

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Mol	Chain	Res	Type
20	J	251	ASP
26	Z	896	LYS
26	Z	938	GLN
28	S	126	LYS
28	S	132	ALA
29	P	273	TYR
30	Q	124	PHE
30	Q	253	ASN
30	Q	286	TYR
32	U	184	GLY
33	O	243	VAL
5	e	45	ARG
9	i	171	SER
9	i	196	ARG
4	D	99	GLU
6	F	6	ASP
7	G	16	ARG
14	7	77	ASP
15	H	94	GLU
15	H	314	VAL
19	M	229	THR
19	M	432	PHE
20	J	376	HIS
21	W	149	GLN
21	W	190	ILE
22	V	184	ASN
22	V	262	THR
23	T	235	PHE
26	Z	885	ALA
26	Z	930	GLY
28	S	83	PRO
28	S	97	THR
29	P	130	ILE
30	Q	47	ASP
31	R	106	ASN
32	U	179	ARG
2	b	2	THR
8	1	48	SER
14	7	10	SER
15	H	190	ARG
16	I	83	LYS
16	I	338	LEU

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Mol	Chain	Res	Type
16	I	340	ARG
19	M	179	THR
27	N	415	PHE
5	e	129	PRO
18	L	350	PRO
22	V	185	ILE
33	O	320	PRO
15	H	203	LYS
2	b	31	GLY
10	3	183	GLY
22	V	143	PRO
26	Z	19	SER
2	B	228	PRO
22	V	112	PRO
15	H	75	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ANP	L	501	35	33,33,33	3.41	10 (30%)	45,52,52	2.28	12 (26%)
36	ADP	M	501	35	28,29,29	1.31	4 (14%)	43,45,45	1.81	13 (30%)
34	ANP	H	501	35	33,33,33	3.89	11 (33%)	45,52,52	2.22	11 (24%)
34	ANP	K	501	35	33,33,33	2.66	11 (33%)	45,52,52	2.19	12 (26%)
34	ANP	J	501	35	33,33,33	2.94	10 (30%)	45,52,52	2.20	10 (22%)
34	ANP	I	501	35	33,33,33	3.76	11 (33%)	45,52,52	2.21	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ANP	L	501	35	-	4/18/38/38	0/3/3/3
36	ADP	M	501	35	-	8/16/32/32	0/3/3/3
34	ANP	H	501	35	-	8/18/38/38	0/3/3/3
34	ANP	K	501	35	-	3/18/38/38	0/3/3/3
34	ANP	J	501	35	-	5/18/38/38	0/3/3/3
34	ANP	I	501	35	-	8/18/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	501	ANP	PB-O3A	16.05	1.79	1.59
34	I	501	ANP	PB-O3A	14.85	1.77	1.59
34	L	501	ANP	PB-O3A	14.31	1.76	1.59
34	H	501	ANP	PA-O3A	10.91	1.71	1.59
34	J	501	ANP	PB-O3A	10.44	1.72	1.59
34	I	501	ANP	PA-O3A	9.96	1.70	1.59
34	L	501	ANP	PA-O3A	8.05	1.68	1.59
34	K	501	ANP	PB-O3A	7.37	1.68	1.59
34	K	501	ANP	PA-O3A	7.12	1.67	1.59
34	J	501	ANP	PG-O1G	6.56	1.56	1.46
34	K	501	ANP	PG-O1G	6.43	1.55	1.46
34	I	501	ANP	PG-O1G	5.93	1.55	1.46
34	I	501	ANP	PB-N3B	5.28	1.77	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	501	ANP	PG-O3G	-5.07	1.43	1.56
34	L	501	ANP	PB-N3B	4.89	1.76	1.63
34	K	501	ANP	PG-N3B	4.70	1.75	1.63
34	J	501	ANP	PG-N3B	4.44	1.75	1.63
34	J	501	ANP	PB-N3B	4.42	1.74	1.63
34	J	501	ANP	PA-O3A	4.36	1.64	1.59
34	J	501	ANP	PB-O1B	4.27	1.52	1.46
34	I	501	ANP	PB-O1B	4.23	1.52	1.46
34	L	501	ANP	PB-O1B	4.10	1.52	1.46
34	I	501	ANP	C8-N9	-3.97	1.30	1.37
34	H	501	ANP	C6-N6	3.89	1.44	1.34
34	H	501	ANP	C3'-C4'	3.66	1.62	1.53
34	I	501	ANP	C4-N9	3.56	1.45	1.37
34	H	501	ANP	PB-N3B	3.56	1.72	1.63
34	L	501	ANP	PG-O1G	3.51	1.51	1.46
34	L	501	ANP	C8-N9	3.34	1.43	1.37
34	K	501	ANP	C1'-N9	3.28	1.55	1.46
36	M	501	ADP	PA-O3A	3.24	1.63	1.59
34	I	501	ANP	C6-N6	2.91	1.41	1.34
34	J	501	ANP	C6-N6	2.90	1.41	1.34
34	I	501	ANP	PG-N3B	2.90	1.70	1.63
34	K	501	ANP	PB-N3B	2.82	1.70	1.63
34	J	501	ANP	PB-O2B	-2.75	1.49	1.56
34	H	501	ANP	PB-O1B	2.73	1.50	1.46
34	J	501	ANP	C5-N7	-2.69	1.34	1.39
34	K	501	ANP	PB-O1B	2.66	1.50	1.46
34	L	501	ANP	PG-O3G	-2.61	1.49	1.56
34	K	501	ANP	PG-O3G	-2.60	1.49	1.56
34	J	501	ANP	C8-N9	-2.56	1.33	1.37
34	H	501	ANP	PG-O1G	2.50	1.50	1.46
34	L	501	ANP	PG-N3B	2.46	1.69	1.63
34	H	501	ANP	C5'-C4'	2.45	1.58	1.51
34	L	501	ANP	PG-O2G	-2.43	1.50	1.56
34	L	501	ANP	O4'-C1'	2.34	1.47	1.42
36	M	501	ADP	C4-N9	2.33	1.42	1.37
34	I	501	ANP	C5-N7	-2.30	1.34	1.39
34	H	501	ANP	PA-O2A	-2.28	1.44	1.55
34	H	501	ANP	C2'-C3'	-2.26	1.47	1.53
34	K	501	ANP	PB-O2B	-2.16	1.51	1.56
34	K	501	ANP	C2-N1	2.15	1.37	1.33
36	M	501	ADP	C1'-N9	2.09	1.52	1.46
34	K	501	ANP	C5-C4	2.03	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	501	ADP	C5-C4	-2.02	1.35	1.39
34	I	501	ANP	C2-N1	-2.00	1.30	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	J	501	ANP	O1G-PG-N3B	-9.11	98.36	111.77
34	I	501	ANP	O1G-PG-N3B	-9.03	98.48	111.77
34	L	501	ANP	O1G-PG-N3B	-7.51	100.72	111.77
34	K	501	ANP	O1G-PG-N3B	-7.26	101.07	111.77
34	H	501	ANP	O1G-PG-N3B	-6.99	101.48	111.77
34	K	501	ANP	O1B-PB-N3B	-6.16	102.70	111.77
34	K	501	ANP	O2B-PB-O1B	5.90	122.53	109.87
34	L	501	ANP	O2B-PB-O1B	5.55	121.77	109.87
34	H	501	ANP	N6-C6-N1	5.22	130.01	118.38
34	J	501	ANP	O1B-PB-N3B	-5.12	104.22	111.77
34	L	501	ANP	N6-C6-N1	4.91	129.30	118.38
34	I	501	ANP	N6-C6-N1	4.80	129.07	118.38
34	J	501	ANP	O2B-PB-O1B	4.44	119.38	109.87
34	H	501	ANP	O4'-C1'-N9	4.43	116.61	108.09
36	M	501	ADP	C4-C5-N7	-4.43	105.52	110.58
34	L	501	ANP	C6-C5-C4	4.03	122.68	117.18
36	M	501	ADP	N6-C6-N1	3.94	127.16	118.38
34	H	501	ANP	O2B-PB-O1B	3.89	118.22	109.87
34	L	501	ANP	C5-C4-N3	-3.84	121.42	126.72
36	M	501	ADP	C5-N7-C8	3.71	109.28	103.45
34	H	501	ANP	N3-C2-N1	3.71	134.20	128.58
34	H	501	ANP	C6-C5-C4	3.69	122.22	117.18
34	I	501	ANP	C5-N7-C8	3.65	109.19	103.45
34	I	501	ANP	C4-C5-N7	-3.53	106.55	110.58
36	M	501	ADP	C6-C5-C4	3.38	121.79	117.18
34	K	501	ANP	C4-C5-N7	-3.34	106.77	110.58
34	L	501	ANP	C5-C6-N6	-3.27	115.19	123.29
34	I	501	ANP	O2G-PG-O3G	3.27	116.38	107.59
34	J	501	ANP	C4-N9-C8	-3.26	102.31	105.74
34	J	501	ANP	N3-C2-N1	3.25	133.50	128.58
34	I	501	ANP	O3A-PB-N3B	-3.24	97.60	106.59
34	I	501	ANP	O2B-PB-O1B	3.23	116.80	109.87
34	L	501	ANP	O4'-C1'-N9	3.16	114.16	108.09
36	M	501	ADP	C5-C4-N9	3.15	109.25	105.81
36	M	501	ADP	C5-C4-N3	-2.93	122.68	126.72
34	H	501	ANP	O4'-C4'-C3'	-2.91	99.38	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	I	501	ANP	C4-N9-C1'	2.81	133.21	126.63
36	M	501	ADP	C2'-C3'-C4'	2.80	108.02	102.61
34	J	501	ANP	O4'-C1'-N9	2.76	113.40	108.09
34	H	501	ANP	C6-C5-N7	-2.74	126.82	132.09
34	L	501	ANP	O1B-PB-N3B	-2.69	107.81	111.77
34	H	501	ANP	C5-C6-N6	-2.69	116.62	123.29
34	J	501	ANP	N9-C8-N7	2.69	117.75	113.94
34	L	501	ANP	C6-C5-N7	-2.69	126.91	132.09
36	M	501	ADP	C5-C6-N6	-2.66	116.69	123.29
34	L	501	ANP	C5-C4-N9	2.59	108.64	105.81
34	K	501	ANP	C5-N7-C8	2.59	107.52	103.45
36	M	501	ADP	O3'-C3'-C4'	-2.57	103.69	111.08
34	L	501	ANP	O2G-PG-O3G	2.55	114.45	107.59
34	K	501	ANP	C6-C5-C4	2.51	120.61	117.18
34	L	501	ANP	O4'-C4'-C3'	-2.47	100.26	105.15
34	H	501	ANP	O1B-PB-N3B	-2.43	108.19	111.77
34	J	501	ANP	O2G-PG-O3G	2.40	114.03	107.59
36	M	501	ADP	N3-C2-N1	2.39	132.21	128.58
36	M	501	ADP	C4-N9-C8	-2.39	103.23	105.74
34	K	501	ANP	O2B-PB-O3A	2.37	112.55	104.64
36	M	501	ADP	C2-N1-C6	-2.35	114.86	118.73
34	J	501	ANP	N6-C6-N1	2.34	123.59	118.38
34	J	501	ANP	C2-N3-C4	-2.31	106.19	111.83
34	I	501	ANP	C1'-N9-C8	-2.30	122.00	127.09
34	K	501	ANP	C5-C4-N3	-2.26	123.60	126.72
34	I	501	ANP	C2-N1-C6	2.25	122.43	118.73
34	I	501	ANP	C5-C6-N1	-2.20	111.92	117.51
34	K	501	ANP	C2'-C1'-N9	2.20	118.76	113.30
34	K	501	ANP	O3'-C3'-C2'	2.12	118.61	111.82
34	I	501	ANP	O1B-PB-N3B	-2.11	108.66	111.77
36	M	501	ADP	C1'-N9-C8	2.08	131.71	127.09
34	K	501	ANP	O2A-PA-O1A	2.05	121.99	112.44
34	K	501	ANP	N9-C8-N7	-2.05	111.03	113.94
34	H	501	ANP	O2'-C2'-C1'	-2.05	103.06	110.10

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ANP	PB-N3B-PG-O1G
34	H	501	ANP	PG-N3B-PB-O1B
34	H	501	ANP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
34	H	501	ANP	C5'-O5'-PA-O3A
34	I	501	ANP	PG-N3B-PB-O3A
34	I	501	ANP	PA-O3A-PB-O2B
34	I	501	ANP	C5'-O5'-PA-O2A
34	I	501	ANP	C5'-O5'-PA-O3A
34	K	501	ANP	PB-N3B-PG-O1G
34	K	501	ANP	PG-N3B-PB-O1B
34	L	501	ANP	PB-N3B-PG-O1G
34	L	501	ANP	C5'-O5'-PA-O2A
34	L	501	ANP	C5'-O5'-PA-O3A
34	J	501	ANP	PB-N3B-PG-O1G
34	J	501	ANP	PG-N3B-PB-O1B
34	J	501	ANP	C5'-O5'-PA-O1A
34	J	501	ANP	C5'-O5'-PA-O3A
36	M	501	ADP	PA-O3A-PB-O3B
36	M	501	ADP	C5'-O5'-PA-O1A
36	M	501	ADP	C5'-O5'-PA-O3A
34	I	501	ANP	C3'-C4'-C5'-O5'
34	I	501	ANP	O4'-C4'-C5'-O5'
34	I	501	ANP	PB-O3A-PA-O1A
36	M	501	ADP	PA-O3A-PB-O2B
34	H	501	ANP	C3'-C4'-C5'-O5'
34	K	501	ANP	O4'-C4'-C5'-O5'
34	H	501	ANP	C5'-O5'-PA-O2A
36	M	501	ADP	C5'-O5'-PA-O2A
34	H	501	ANP	O4'-C4'-C5'-O5'
34	H	501	ANP	C4'-C5'-O5'-PA
34	J	501	ANP	C4'-C5'-O5'-PA
36	M	501	ADP	C3'-C4'-C5'-O5'
36	M	501	ADP	PA-O3A-PB-O1B
34	I	501	ANP	PA-O3A-PB-O1B
34	L	501	ANP	PA-O3A-PB-O1B
36	M	501	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 29 short contacts:

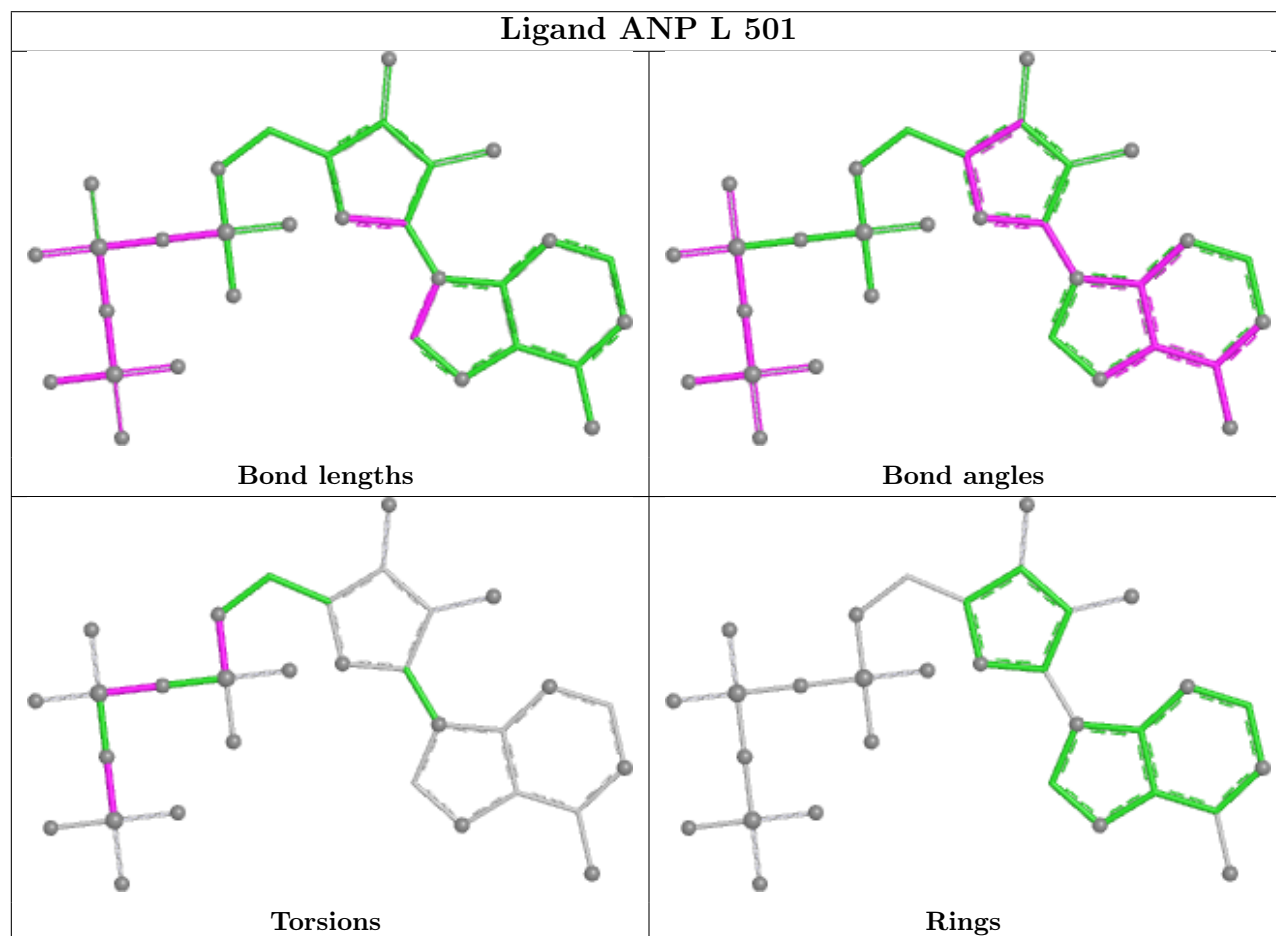
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	M	501	ADP	12	0
34	H	501	ANP	3	0
34	K	501	ANP	2	0
34	J	501	ANP	8	0

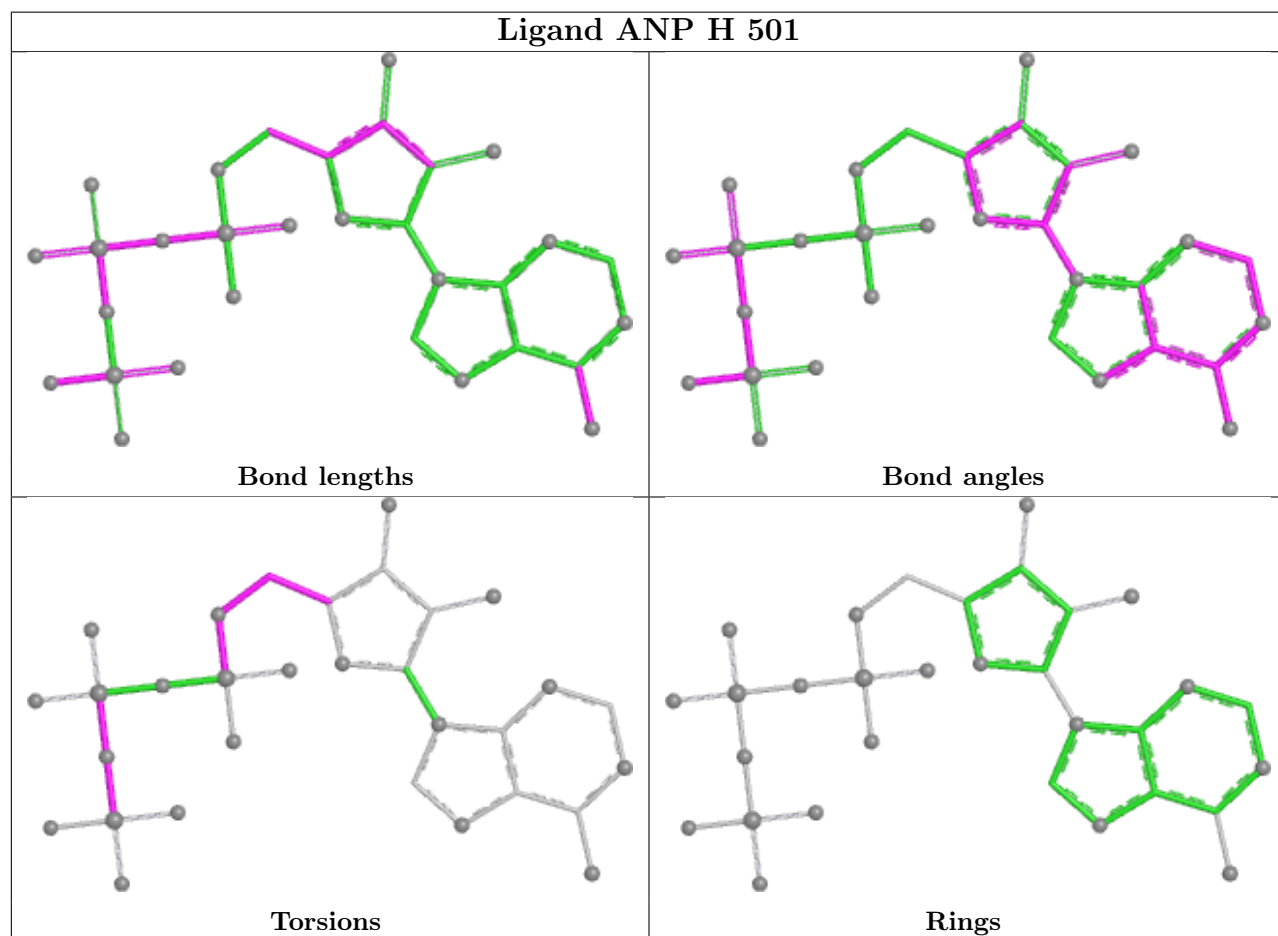
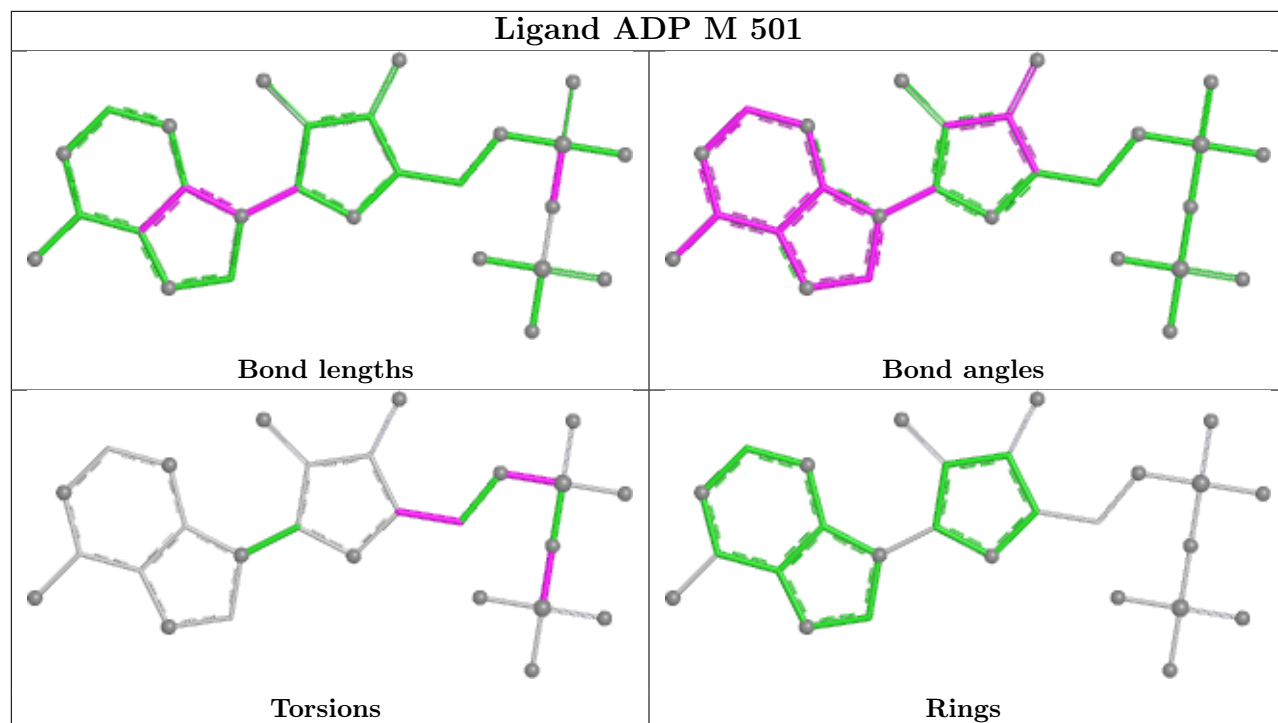
Continued on next page...

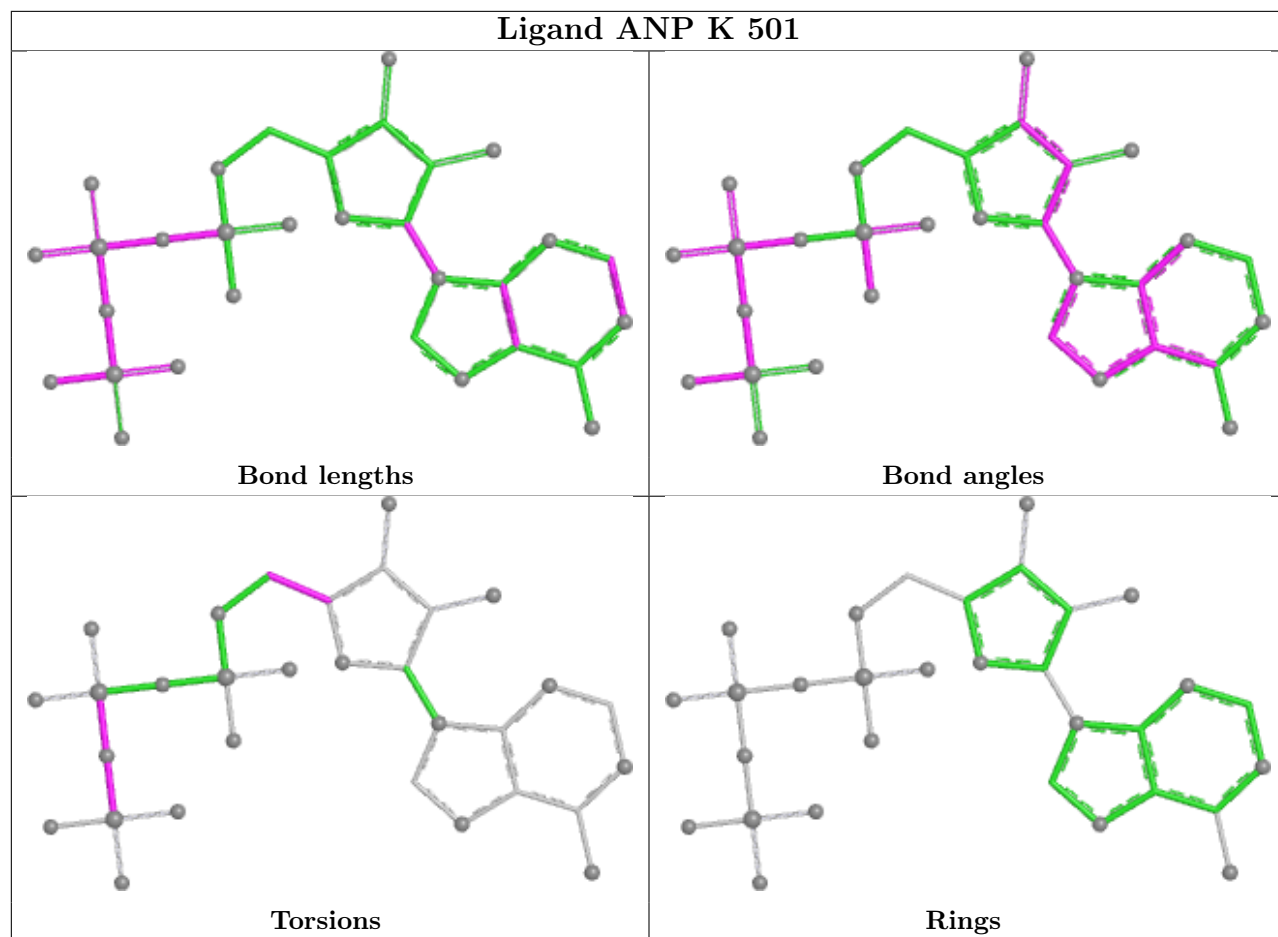
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	I	501	ANP	4	0

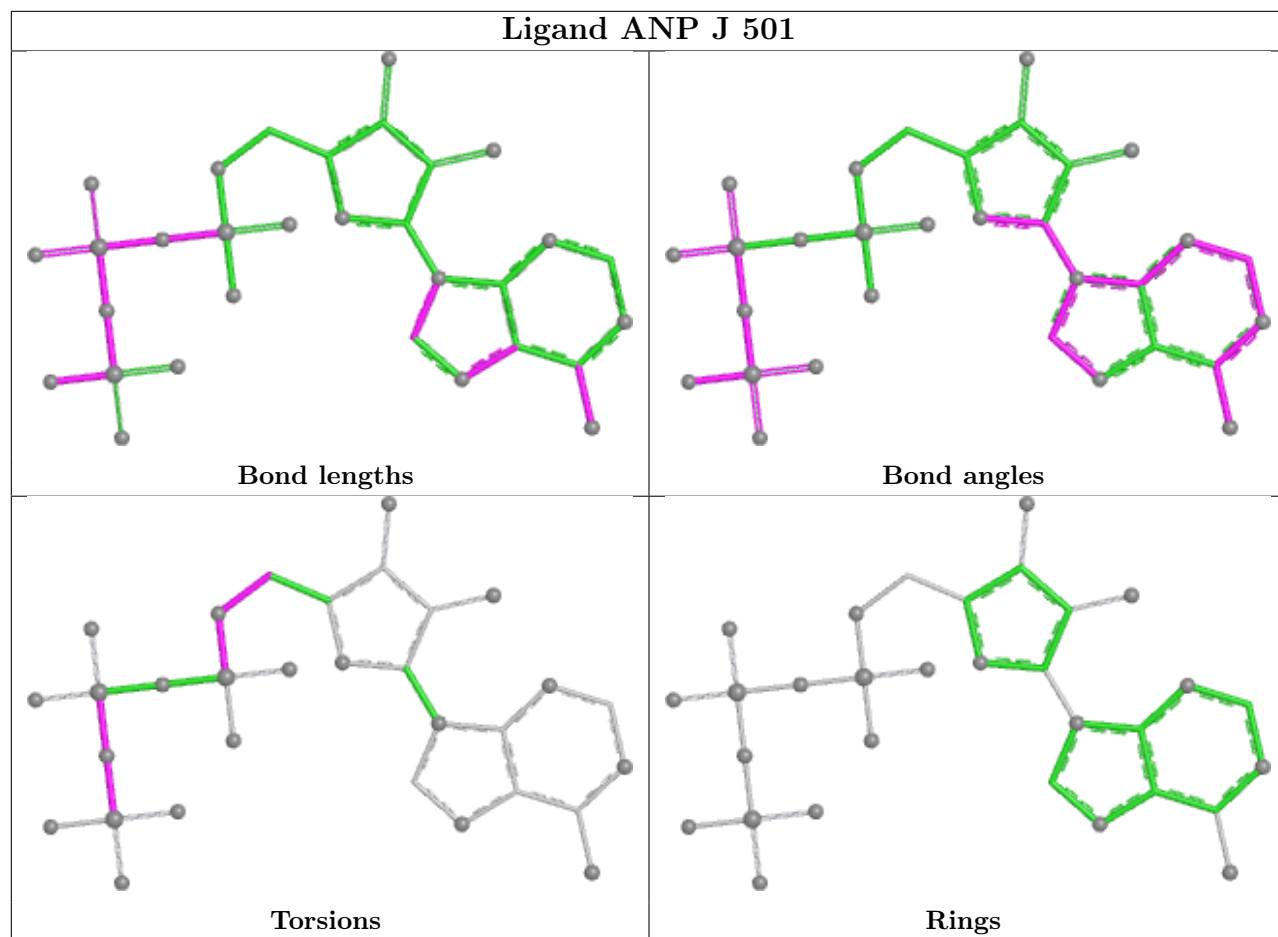
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

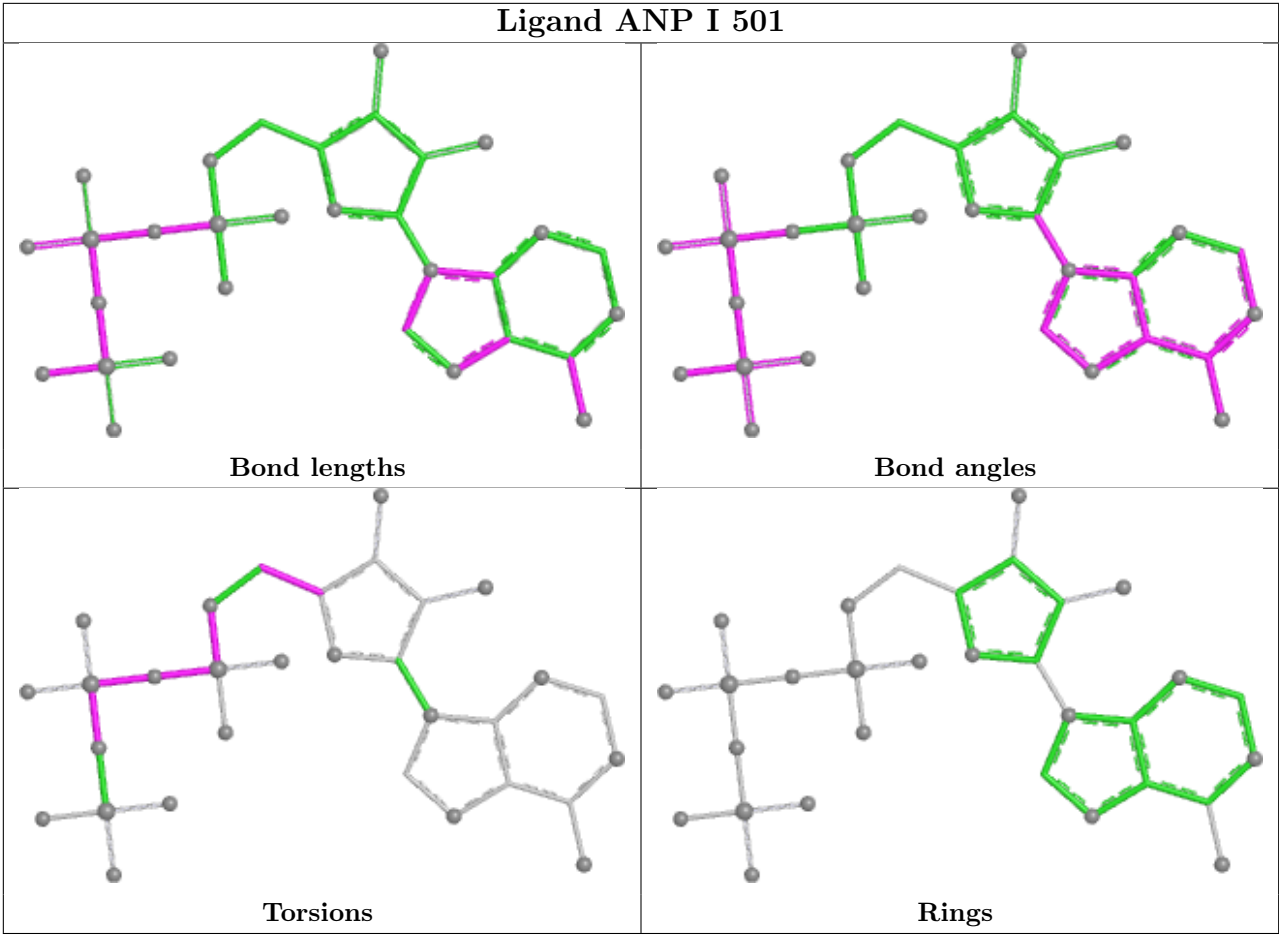






Ligand ANP J 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	186:GLN	C	187:ALA	N	1.19

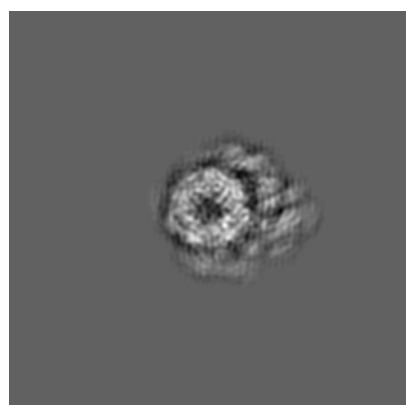
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3536. These allow visual inspection of the internal detail of the map and identification of artifacts.

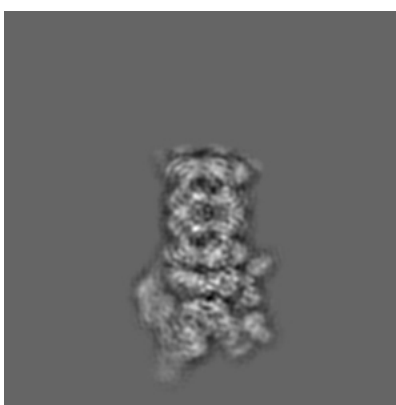
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

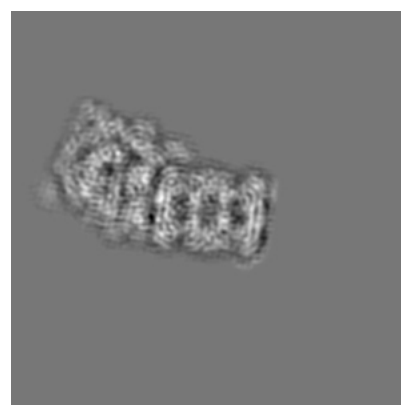
6.1.1 Primary map



X



Y

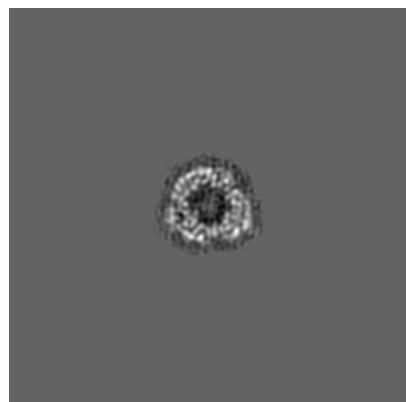


Z

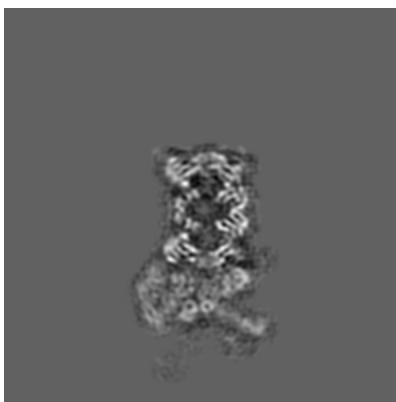
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

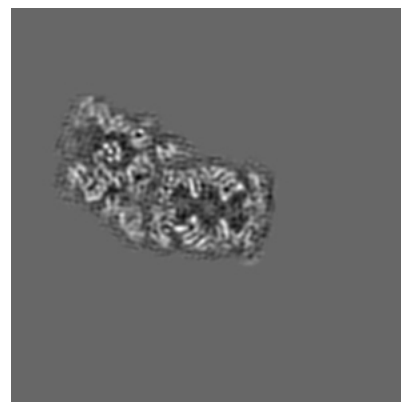
6.2.1 Primary map



X Index: 208



Y Index: 208

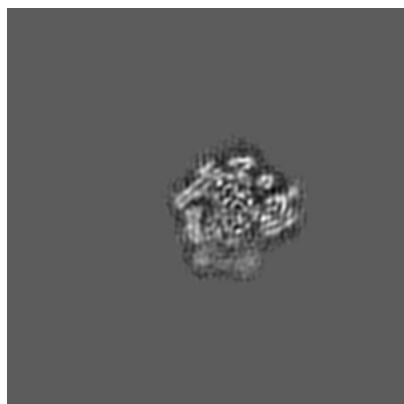


Z Index: 208

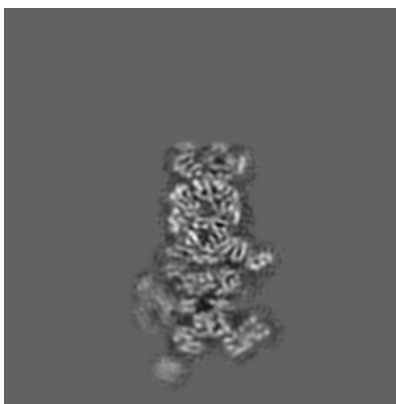
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

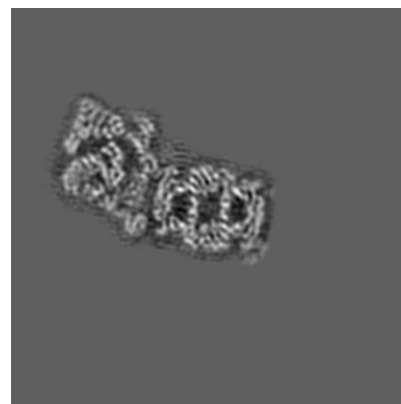
6.3.1 Primary map



X Index: 135



Y Index: 226

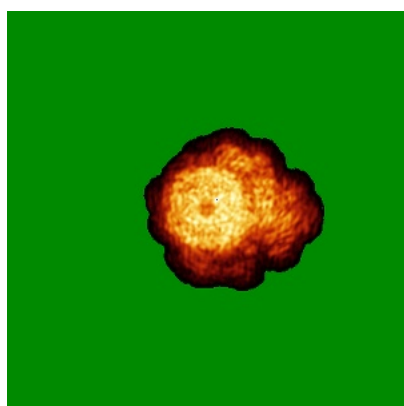


Z Index: 199

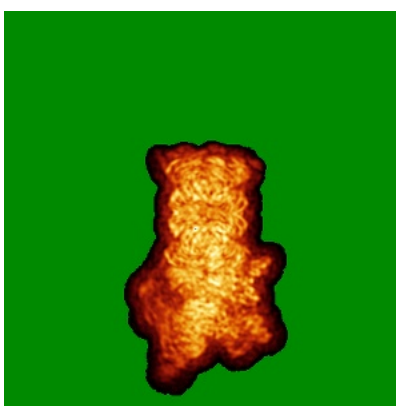
The images above show the largest variance slices of the map in three orthogonal directions.

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

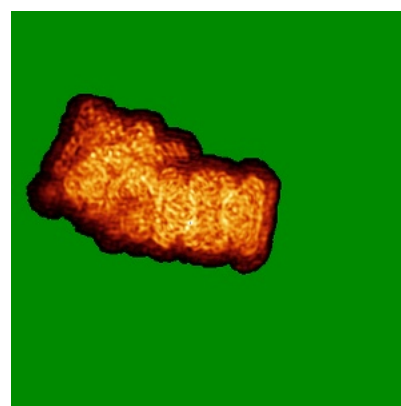
6.4.1 Primary map



X



Y

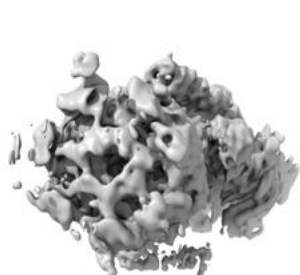


Z

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](#)

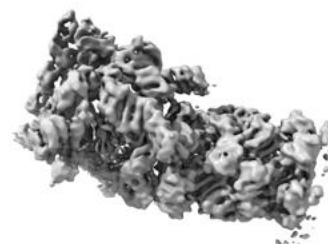
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

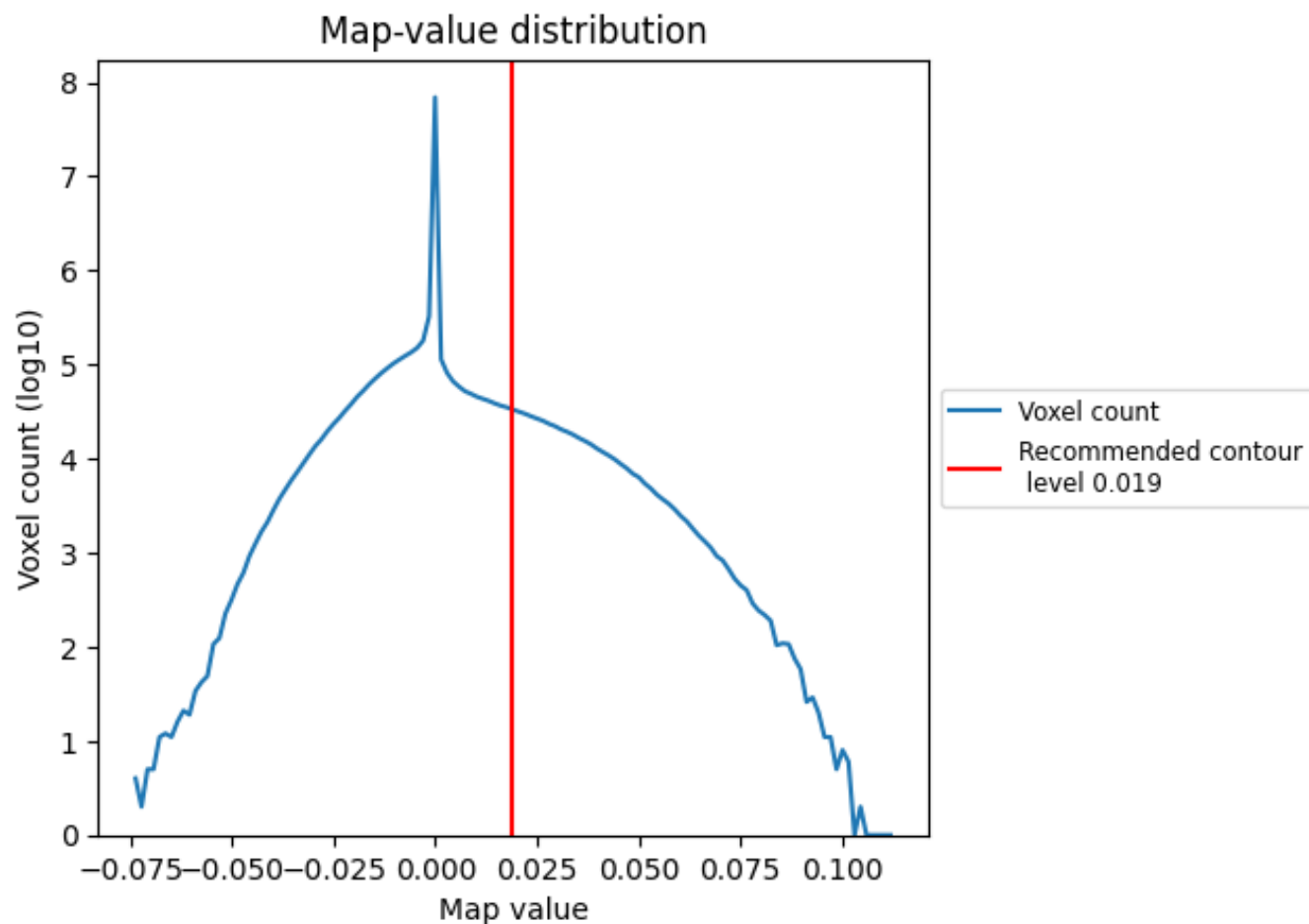
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

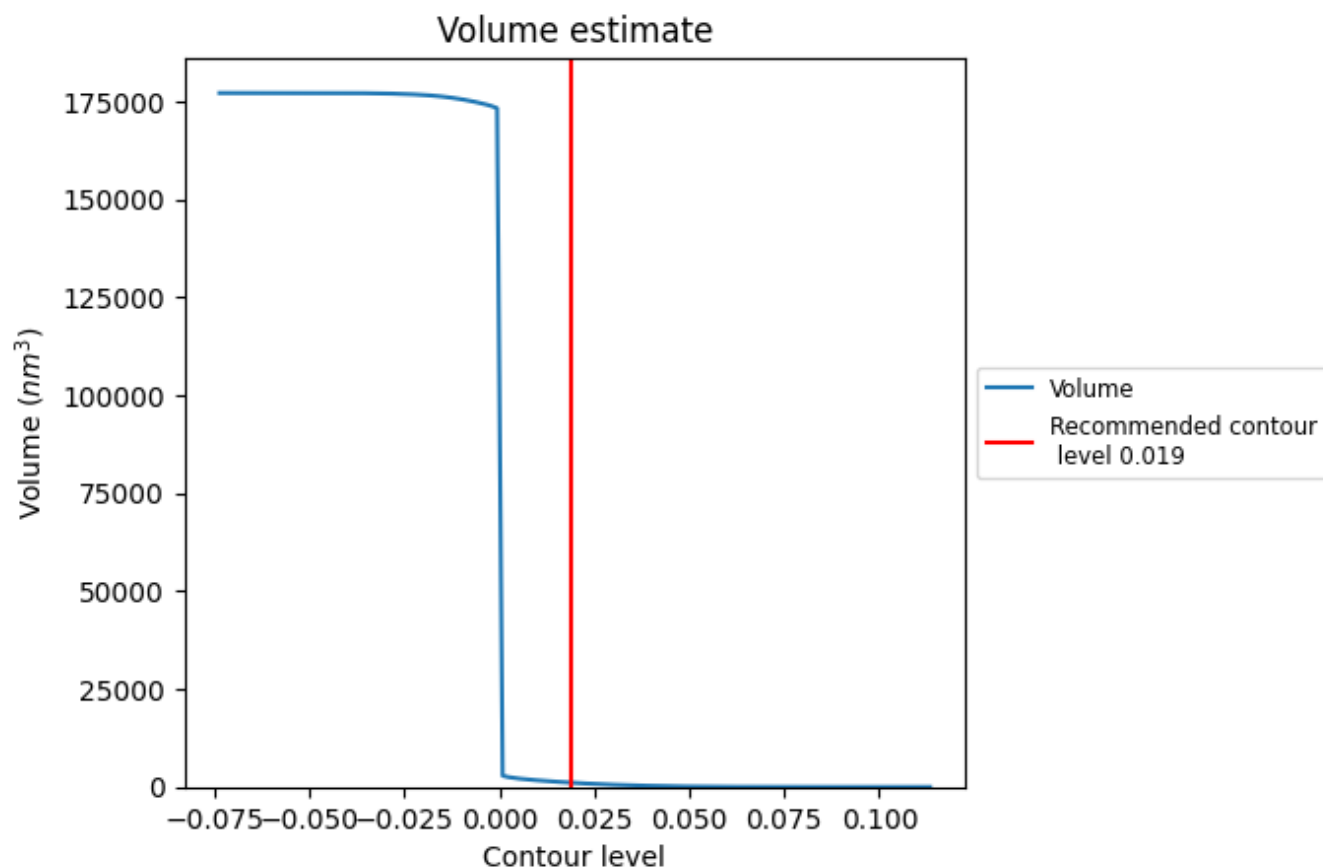
This section contains the results of statistical analysis of the map.

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.

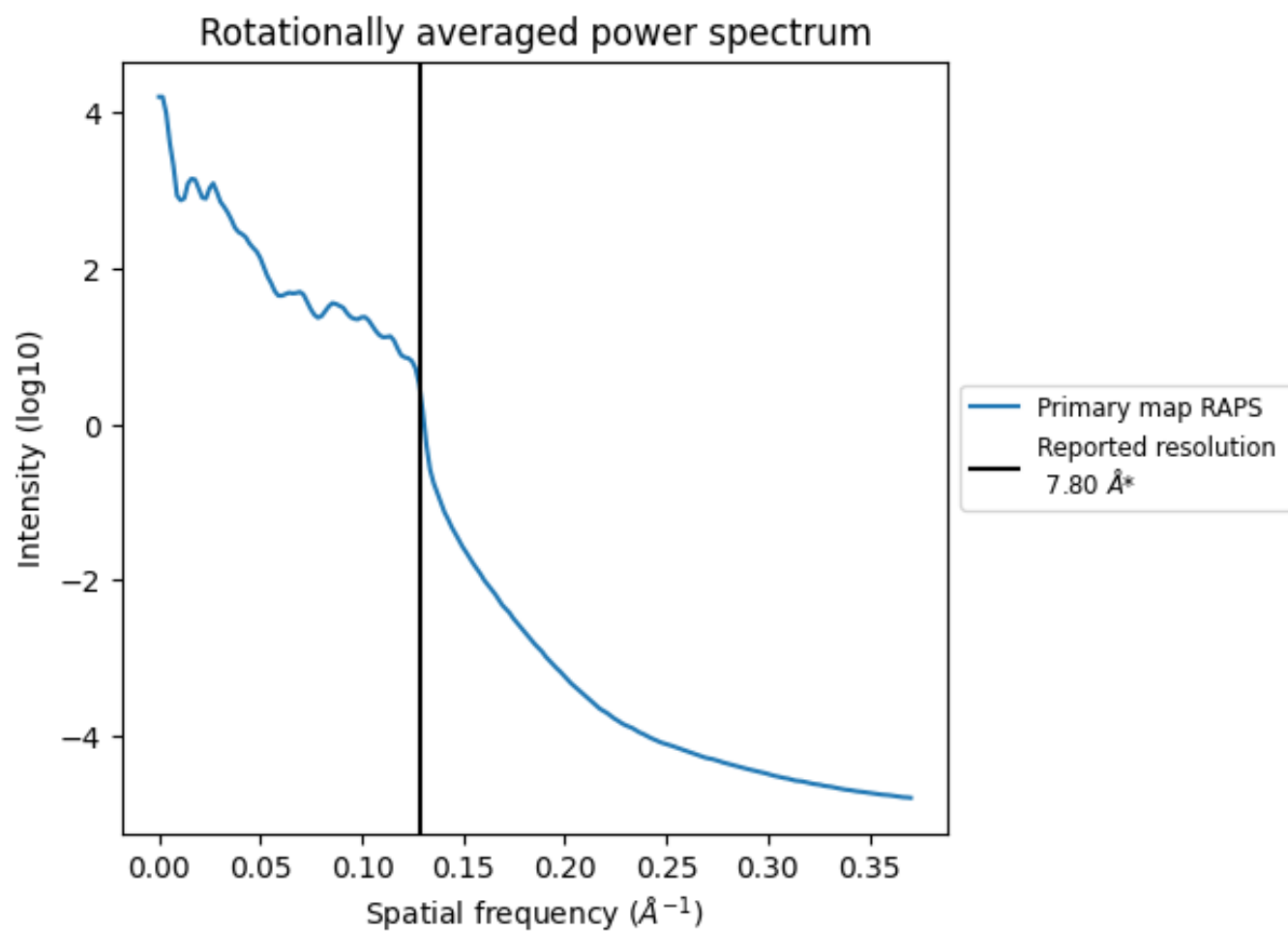
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1087 nm^3 ; this corresponds to an approximate mass of 982 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 0.128 $\text{\AA}^{-1}$

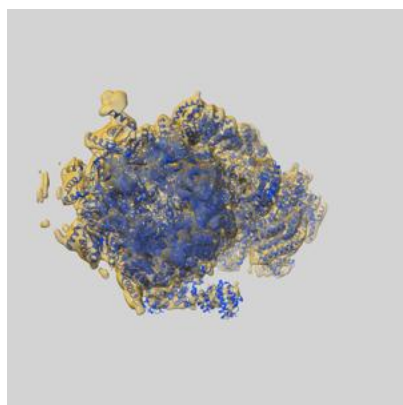
8 Fourier-Shell correlation

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

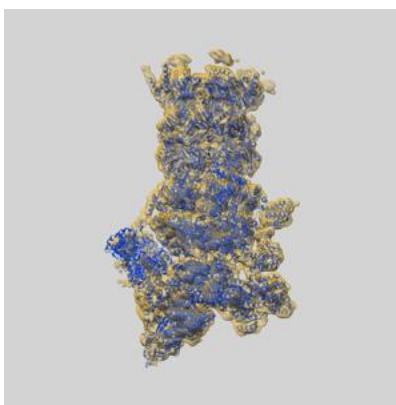
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3536 and PDB model 5MPB. Per-residue inclusion information can be found in section [3](#) on page [13](#).

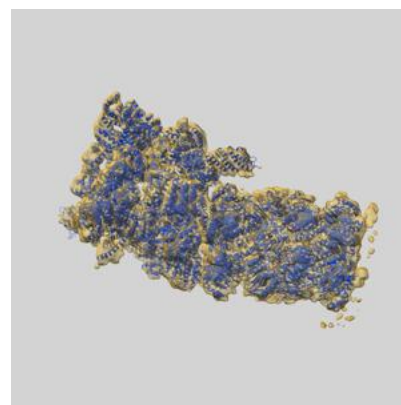
9.1 Map-model overlay [i](#)



X



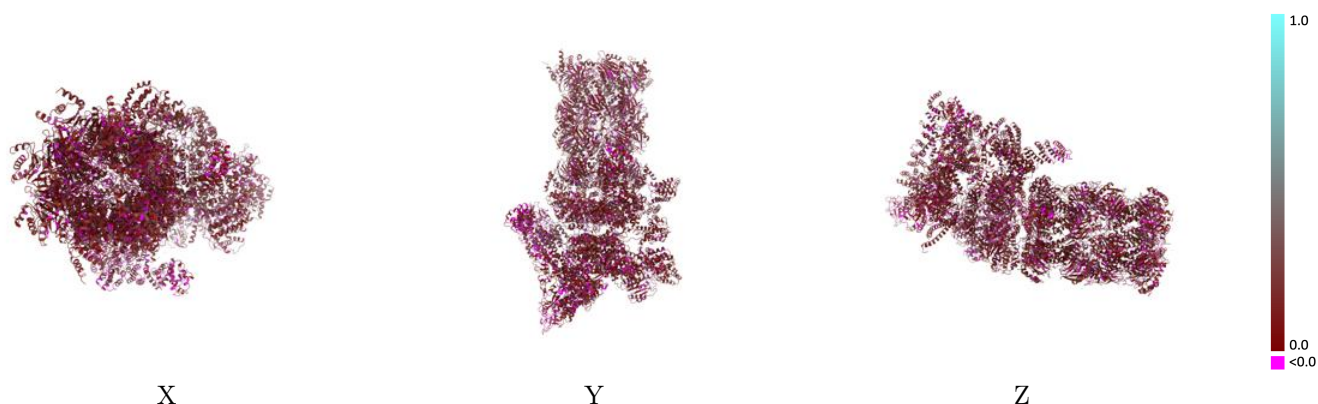
Y



Z

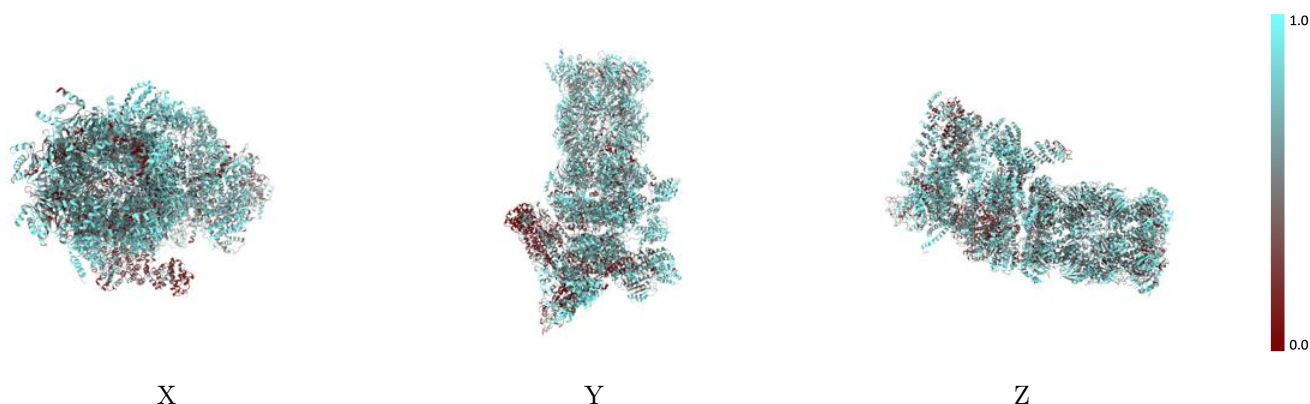
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



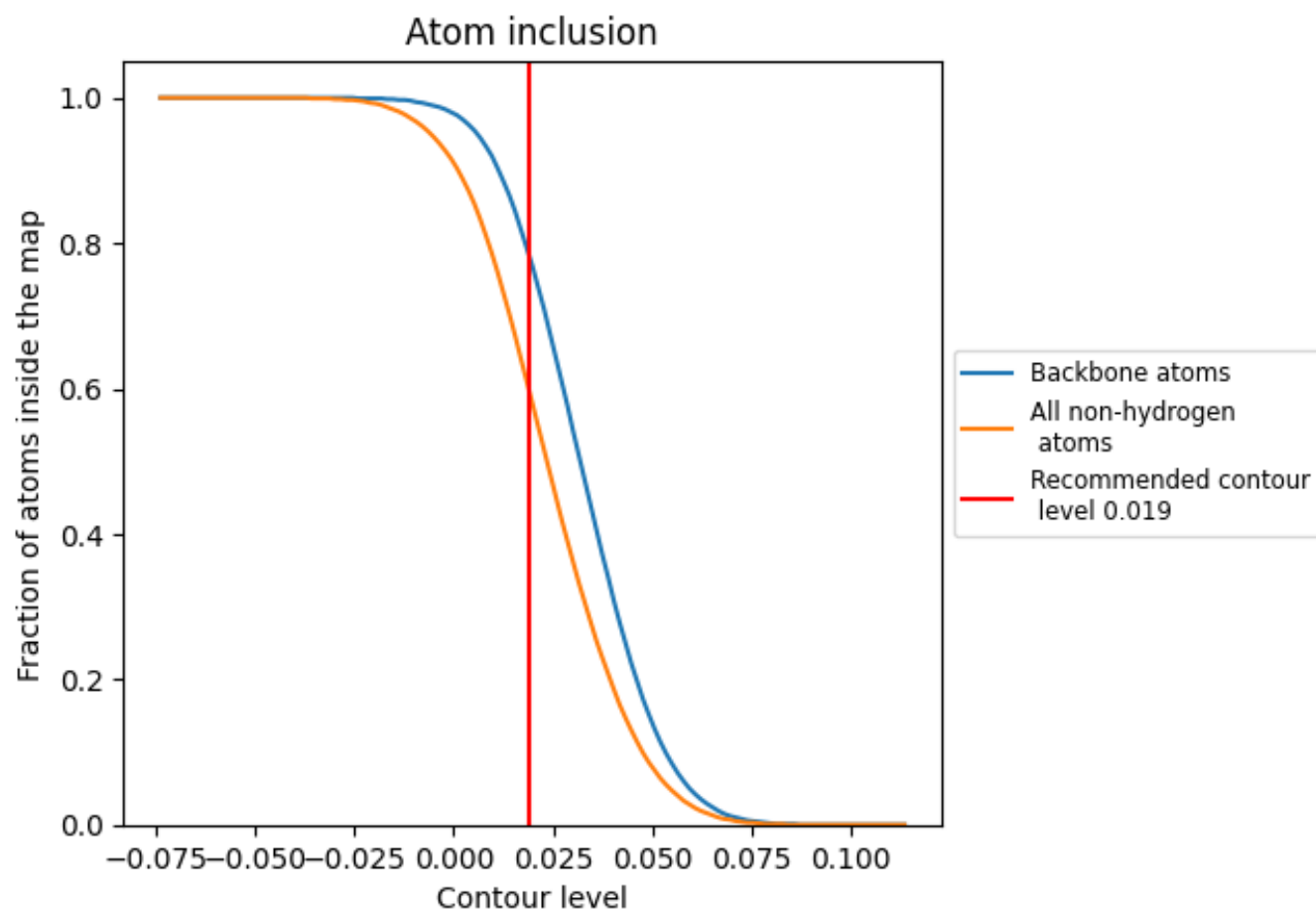
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5970	 0.1320
1	 0.6860	 0.1420
2	 0.6740	 0.1490
3	 0.6090	 0.1400
4	 0.6800	 0.1450
5	 0.7210	 0.1460
6	 0.6950	 0.1410
7	 0.6750	 0.1420
A	 0.6110	 0.1320
B	 0.5870	 0.1420
C	 0.6230	 0.1430
D	 0.6510	 0.1410
E	 0.6370	 0.1460
F	 0.6660	 0.1450
G	 0.6730	 0.1440
H	 0.5790	 0.1290
I	 0.4350	 0.1190
J	 0.5370	 0.1260
K	 0.5520	 0.1250
L	 0.5880	 0.1350
M	 0.5350	 0.1290
N	 0.5910	 0.1320
O	 0.6850	 0.1470
P	 0.7720	 0.1510
Q	 0.6960	 0.1370
R	 0.7160	 0.1460
S	 0.5750	 0.1300
T	 0.5040	 0.1260
U	 0.5900	 0.1380
V	 0.6060	 0.1380
W	 0.5940	 0.1200
X	 0.2580	 0.0610
Y	 0.4650	 0.1010
Z	 0.2840	 0.0710
a	 0.6220	 0.1400



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Chain	Atom inclusion	Q-score
b	 0.5670	 0.1360
c	 0.5880	 0.1410
d	 0.6470	 0.1360
e	 0.6200	 0.1450
f	 0.6480	 0.1460
g	 0.6540	 0.1440
h	 0.6740	 0.1410
i	 0.6270	 0.1350
j	 0.5930	 0.1320
k	 0.6850	 0.1430
l	 0.6910	 0.1370
m	 0.6700	 0.1330
n	 0.6420	 0.1350