Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID	:	6FVY / pdb_00006fvy
EMDB ID	:	EMD-4324
Title	:	26S proteasome, s6 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	6.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

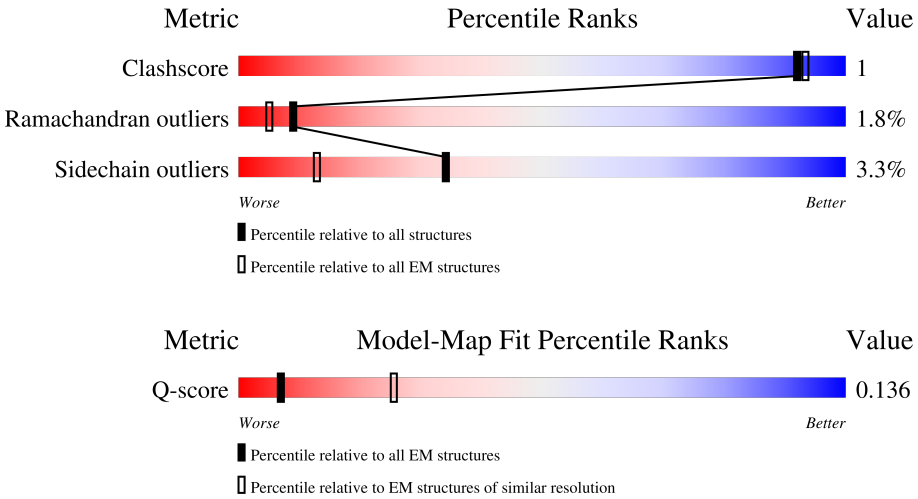
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (5.60 - 6.60)

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 <=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	244	41% 52% 6%
1	a	244	32% 48% 46% 5%
2	B	248	46% 47% 7%
2	b	248	38% 47% 48% 6%

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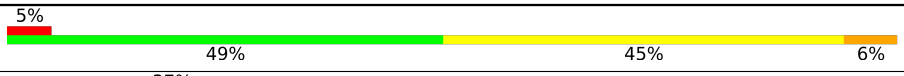
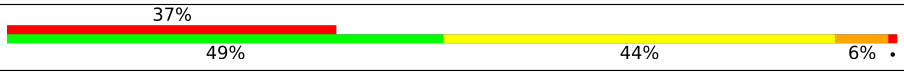
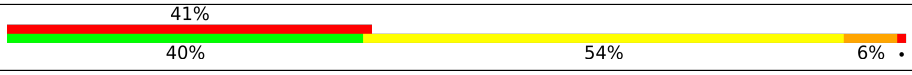
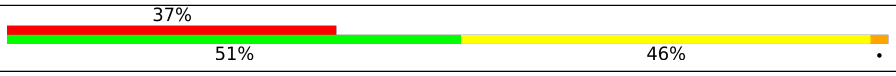
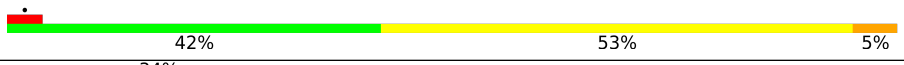
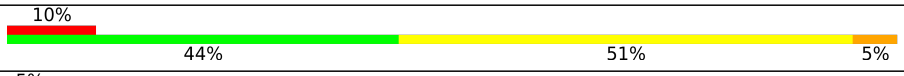
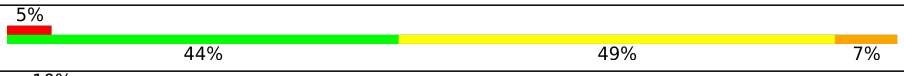
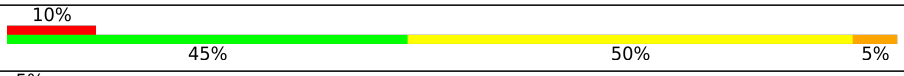
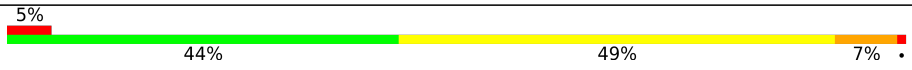
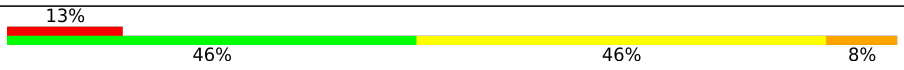
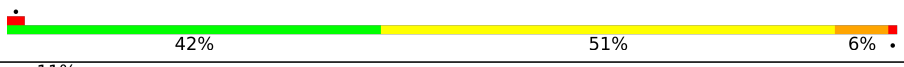
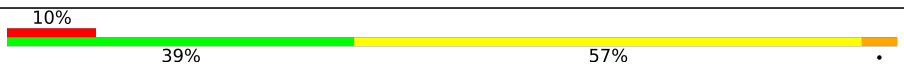
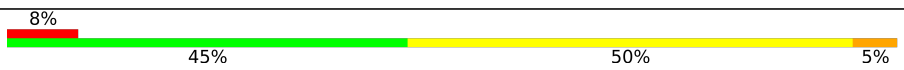
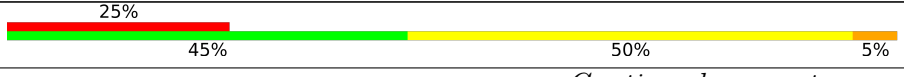
Mol	Chain	Length	Quality of chain
3	C	241	
3	c	241	
4	D	252	
4	d	252	
5	E	245	
5	e	245	
6	F	232	
6	f	232	
7	G	245	
7	g	245	
8	1	196	
8	h	196	
9	2	226	
9	i	226	
10	3	204	
10	j	204	
11	4	195	
11	k	195	
12	5	212	
12	l	212	
13	6	222	
13	m	222	
14	7	232	
14	n	232	
15	W	197	

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Mol	Chain	Length	Quality of chain
16	V	289	12% 39% 55%
17	T	266	16% 46% 48% 5%
18	X	127	80% 48% 46%
19	Y	89	46% 37% 58%
20	Z	970	42% 39% 48% 6% 7%
21	N	922	13% 46% 49% 5%
22	S	475	16% 41% 54% 5%
23	P	440	44% 53%
24	Q	434	6% 42% 52% 5%
25	R	405	6% 47% 48% 5%
26	U	304	13% 46% 50%
27	O	388	10% 43% 53%
28	H	426	30% 45% 48% 7%
29	I	385	21% 41% 53% 5%
30	K	394	14% 41% 52% 6%
31	L	388	13% 46% 47% 6%
32	M	421	26% 42% 51% 7%
33	J	405	19% 42% 48% 9%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 110555 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	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		
1	A	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		
2	B	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	241	Total	C	N	O	S	0	0
			1884	1190	315	376	3		
3	C	241	Total	C	N	O	S	0	0
			1884	1190	315	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	252	Total	C	N	O	S	0	0
			1986	1237	351	394	4		
4	D	238	Total	C	N	O	S	0	0
			1863	1166	326	367	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	245	Total	C	N	O	S	0	0
			1889	1179	317	386	7		
5	E	245	Total	C	N	O	S	0	0
			1889	1179	317	386	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	232	Total	C	N	O	S	0	0
			1784	1120	311	349	4		
6	F	232	Total	C	N	O	S	0	0
			1784	1120	311	349	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	245	Total	C	N	O	S	0	0
			1905	1211	331	359	4		
7	G	245	Total	C	N	O	S	0	0
			1905	1211	331	359	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

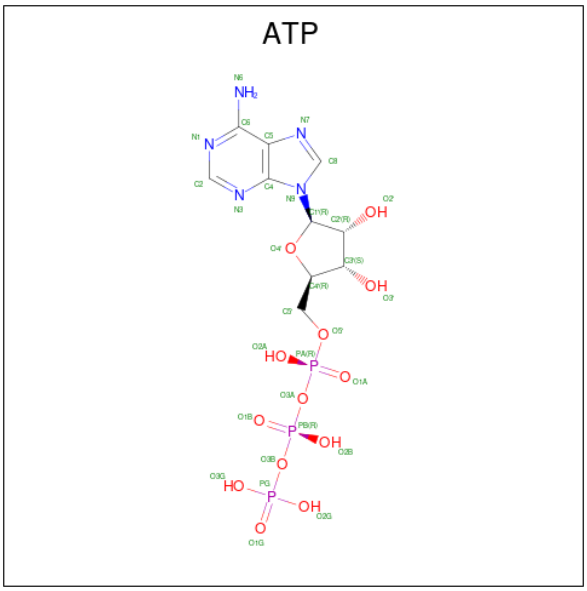
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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

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

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

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



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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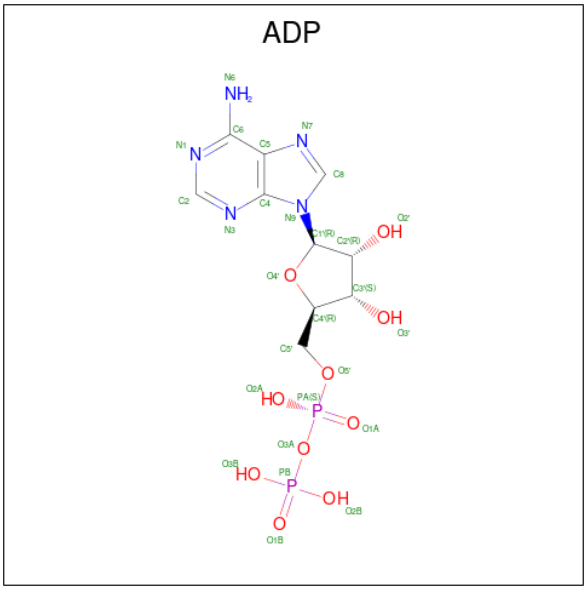
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



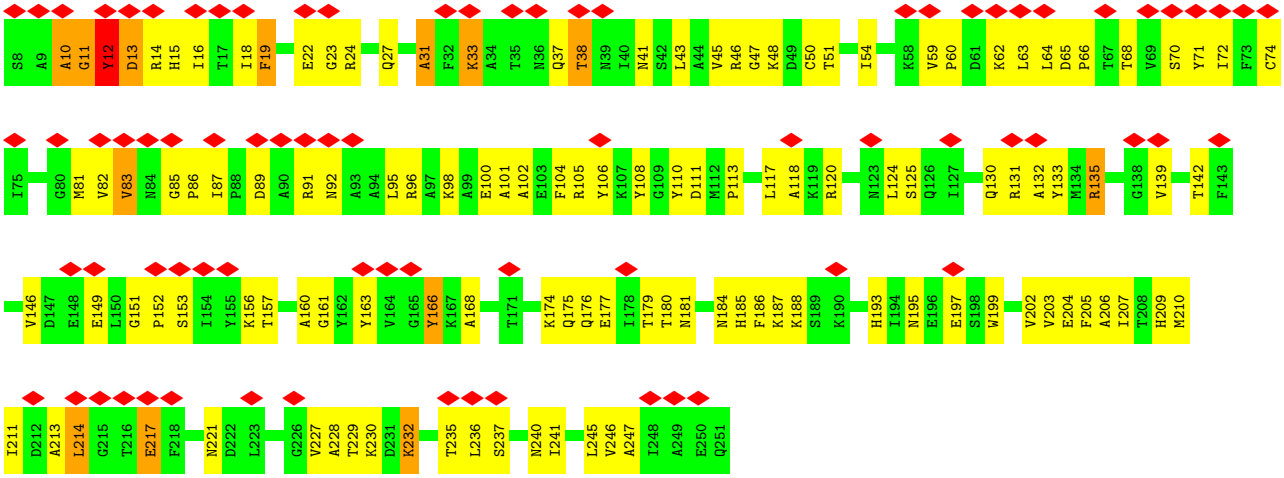
Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

Chain a:

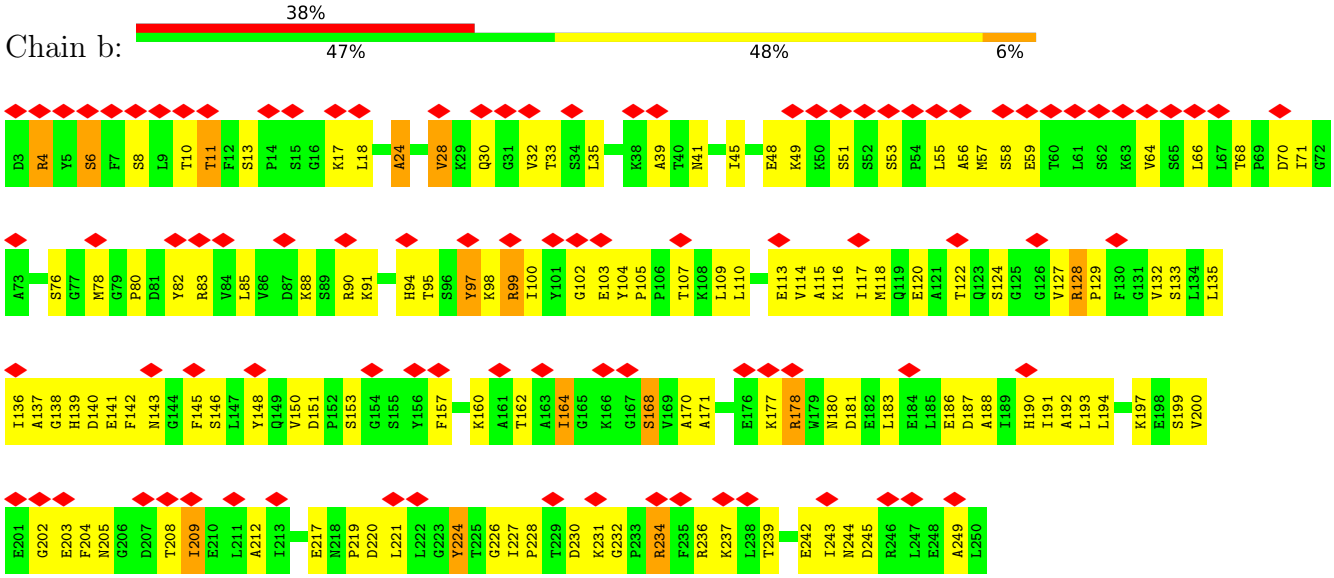


• Molecule 1: Proteasome subunit alpha type-1

Chain A:

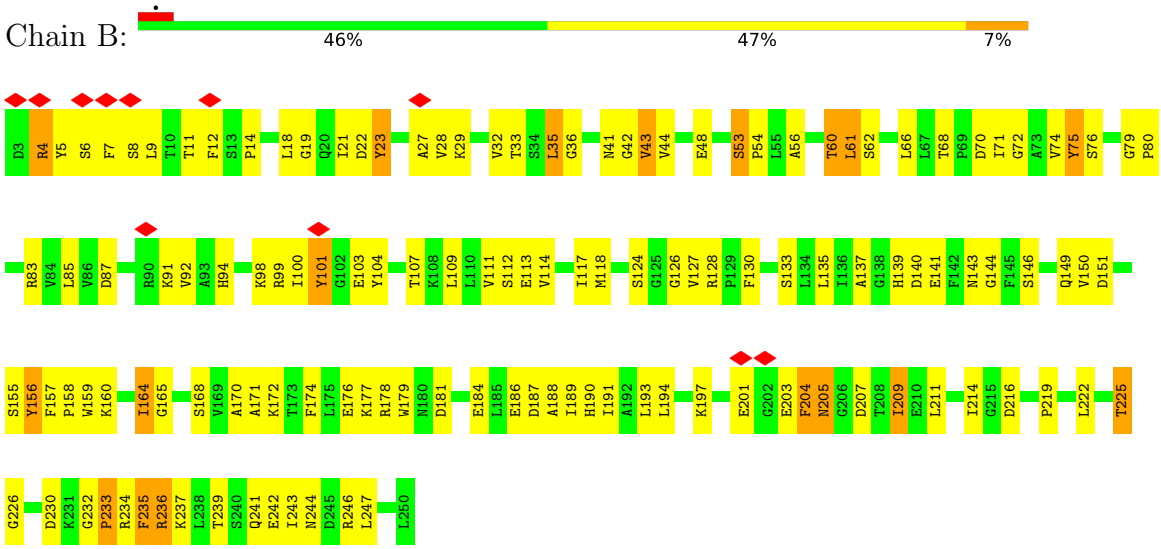
• Molecule 2: Proteasome subunit alpha type-2

Chain b:



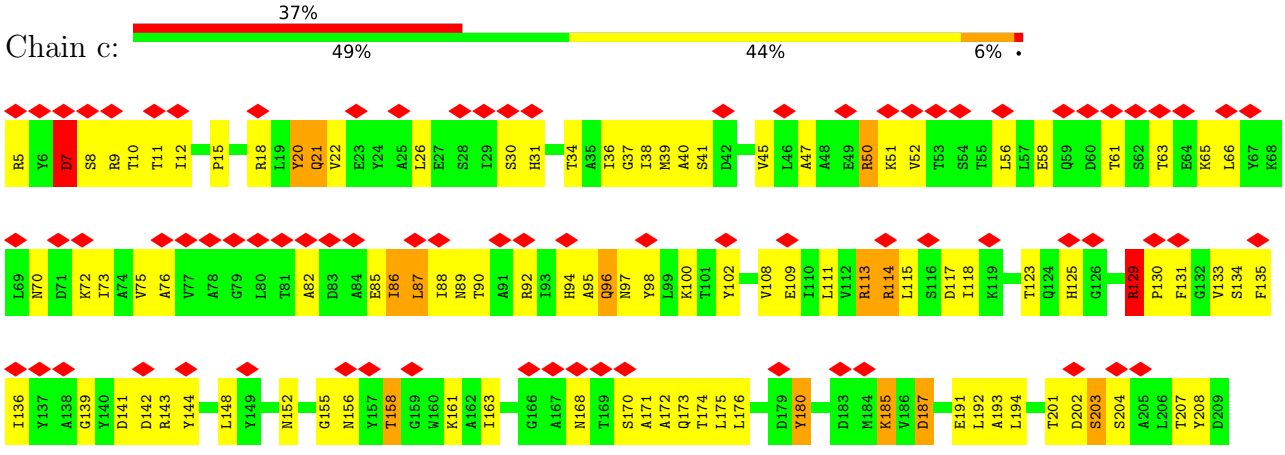
• Molecule 2: Proteasome subunit alpha type-2

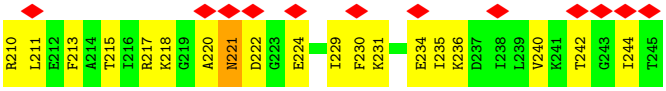
Chain B:



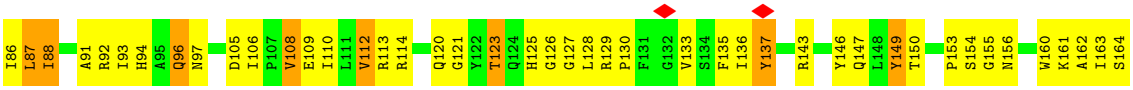
• Molecule 3: Proteasome subunit alpha type-3

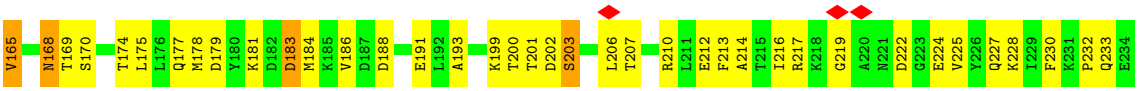
Chain c:

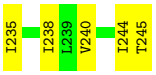




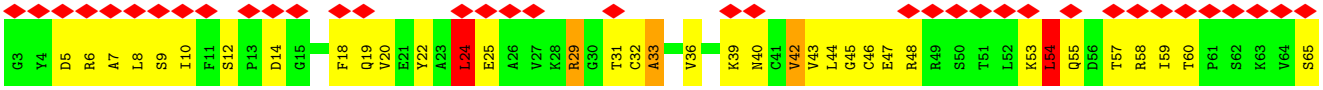
• Molecule 3: Proteasome subunit alpha type-3

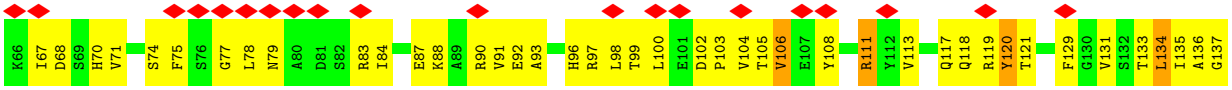


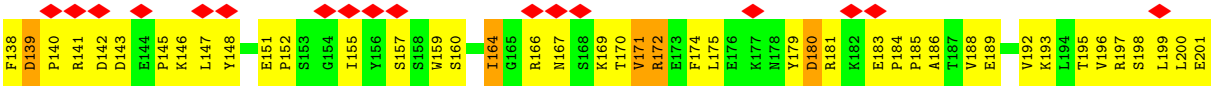


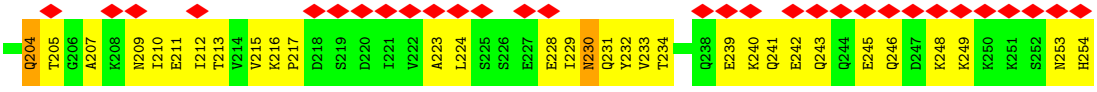


• Molecule 4: Proteasome subunit alpha type-4

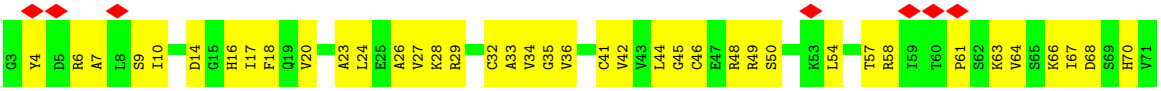


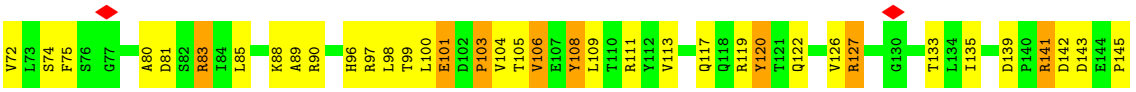


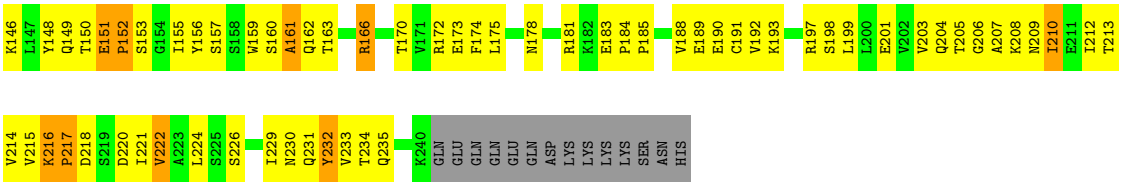




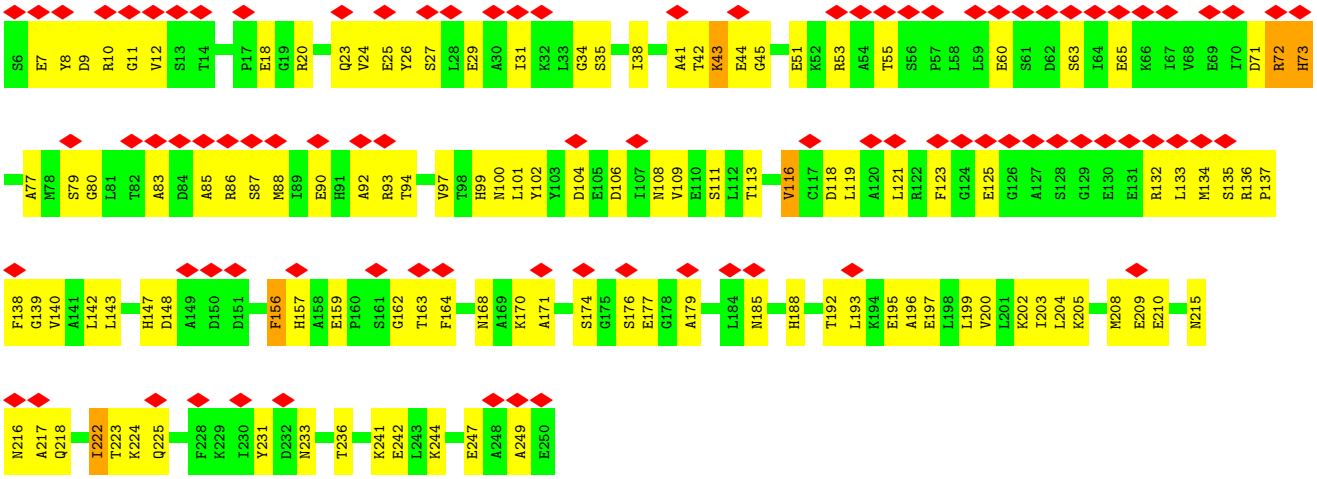
• Molecule 4: Proteasome subunit alpha type-4



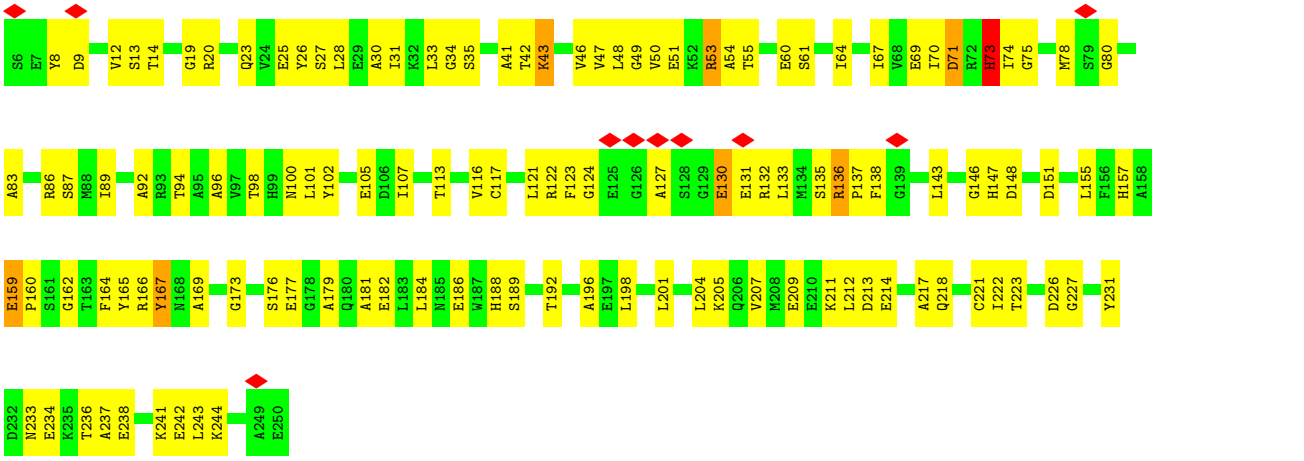




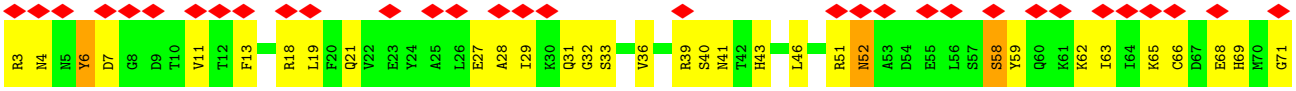
• Molecule 5: Proteasome subunit alpha type-5

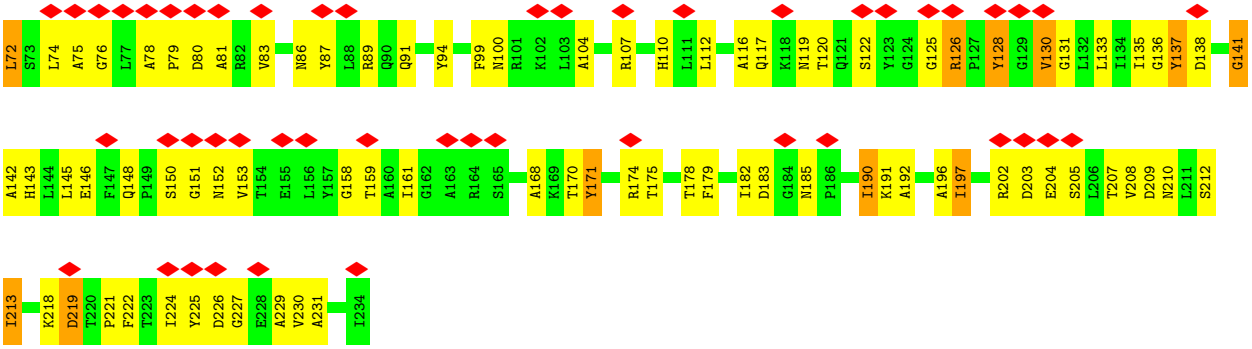


• Molecule 5: Proteasome subunit alpha type-5



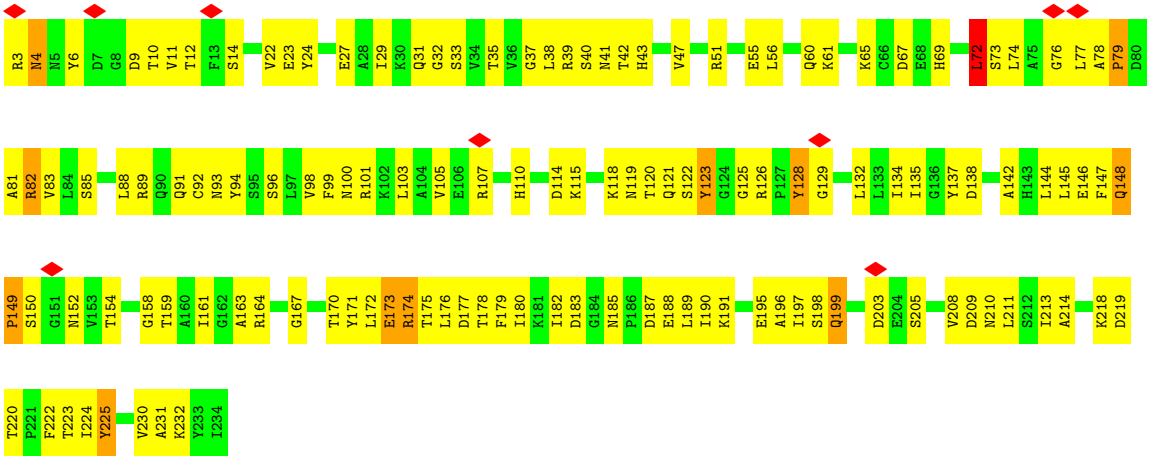
• Molecule 6: Proteasome subunit alpha type-6





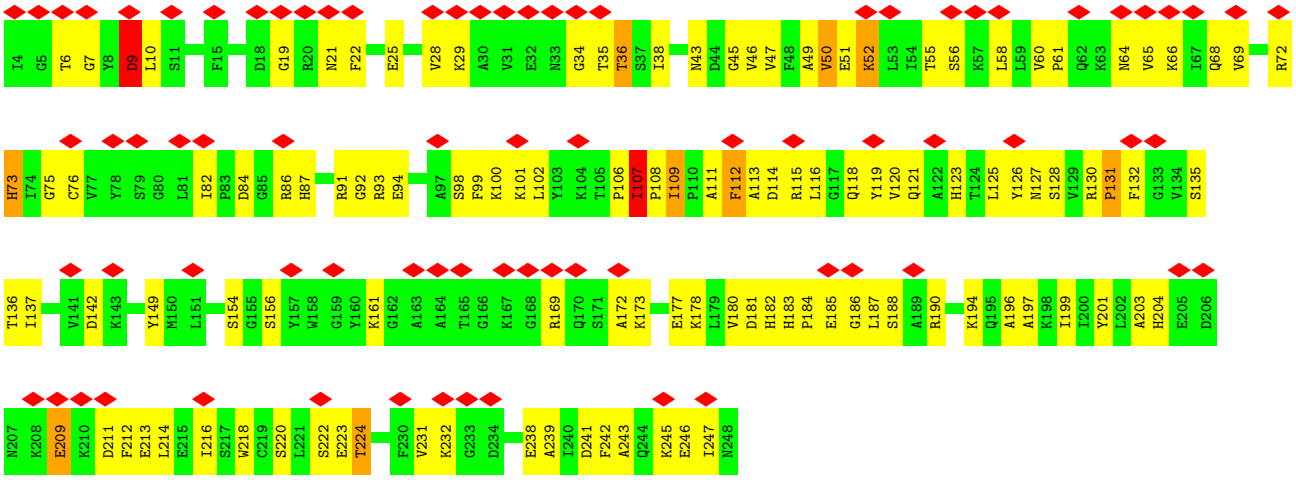
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



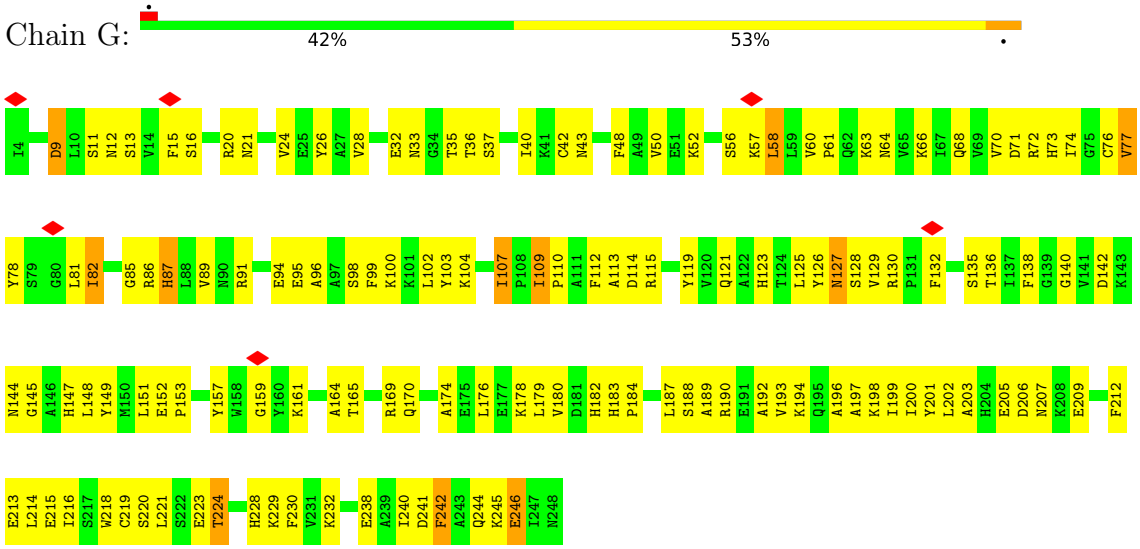
• Molecule 7: Probable proteasome subunit alpha type-7

Chain g:



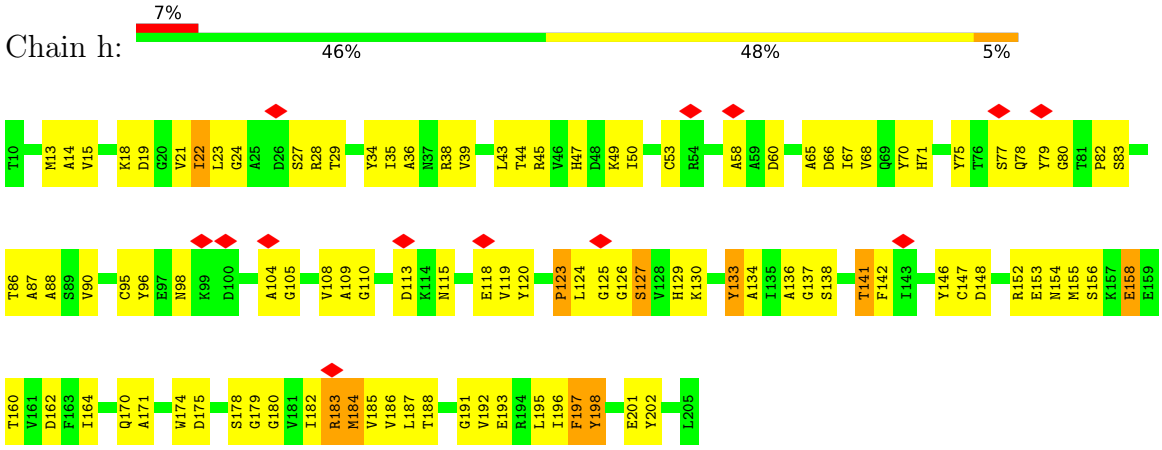
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



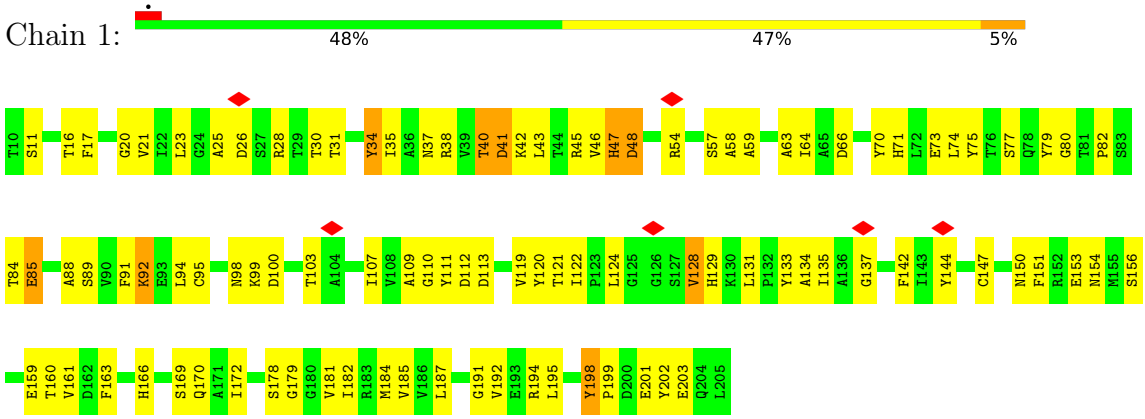
• Molecule 8: Proteasome subunit beta type-1

Chain h:



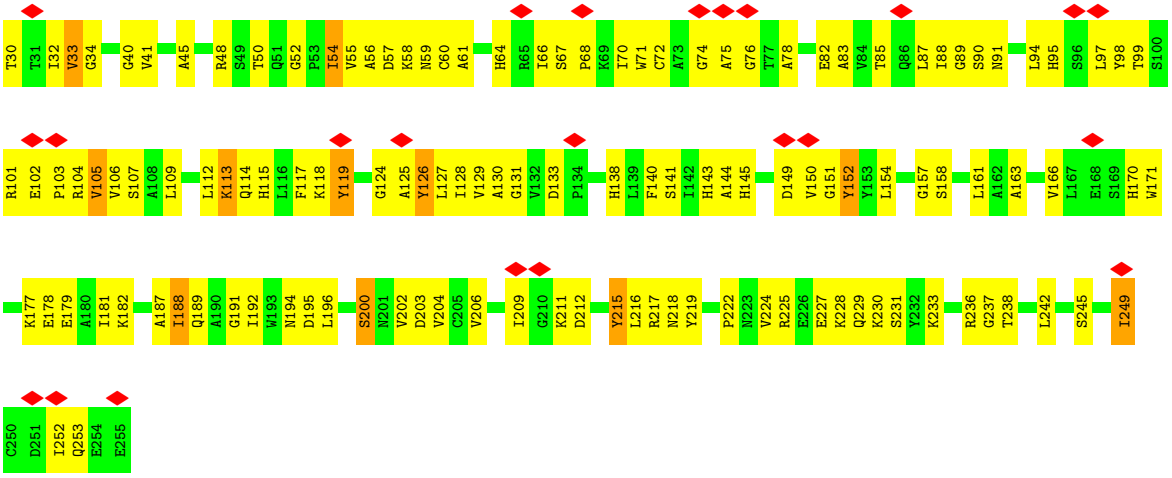
• Molecule 8: Proteasome subunit beta type-1

Chain 1:

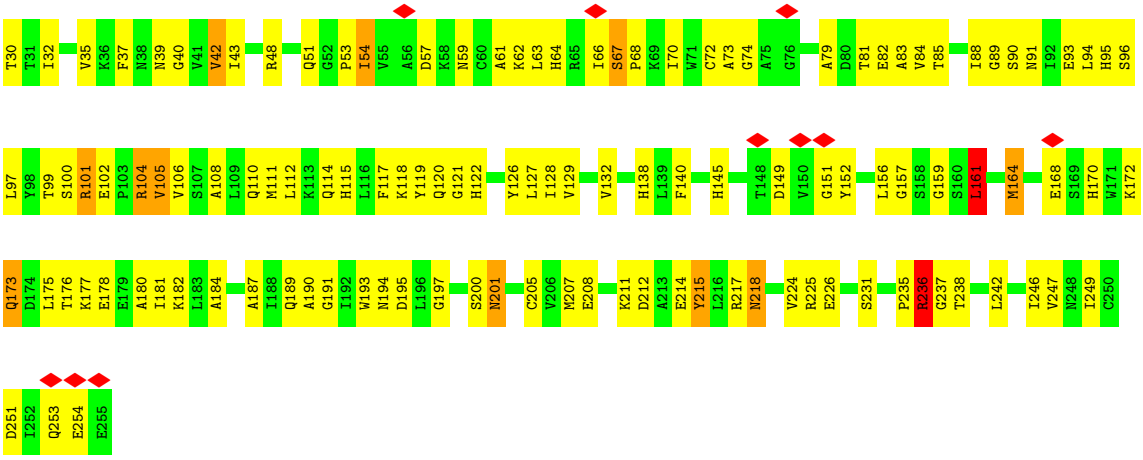


• Molecule 9: Proteasome subunit beta type-2

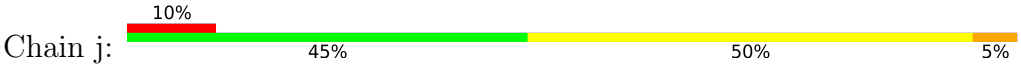
Chain i:

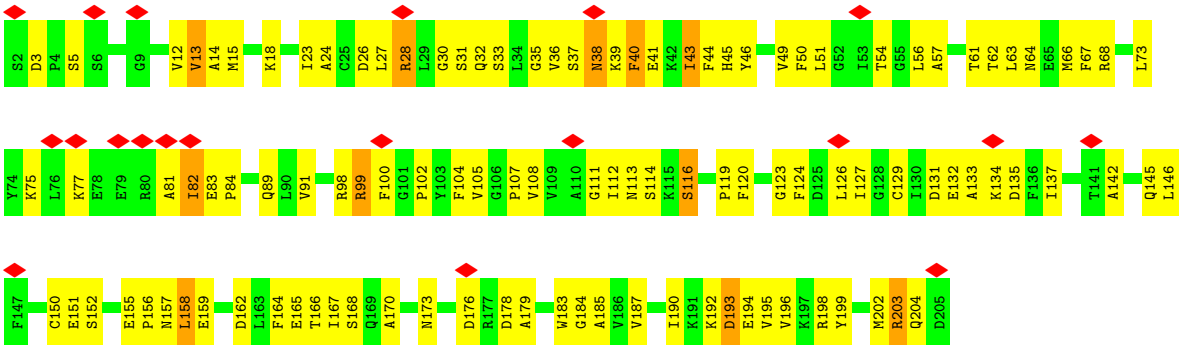


• Molecule 9: Proteasome subunit beta type-2



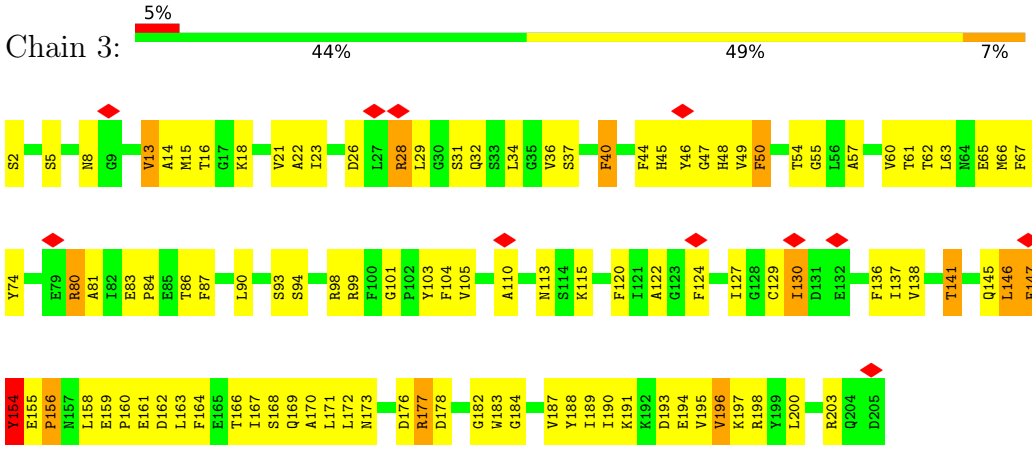
• Molecule 10: Proteasome subunit beta type-3





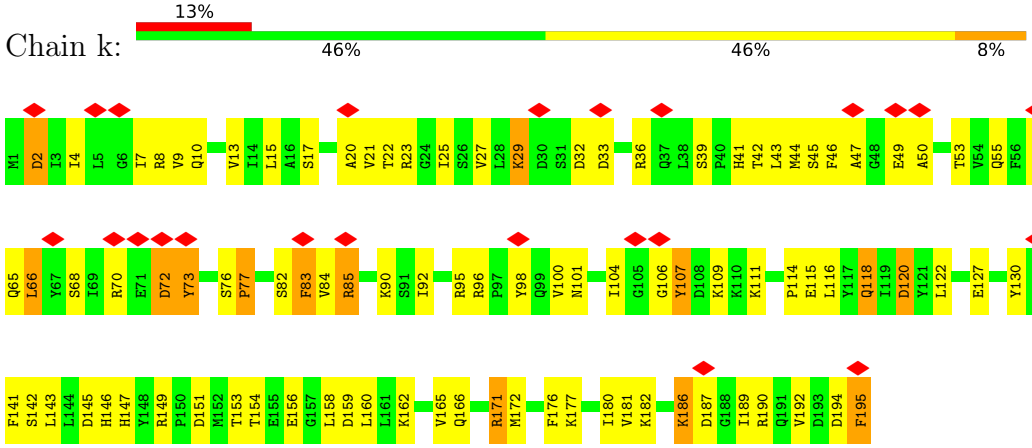
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



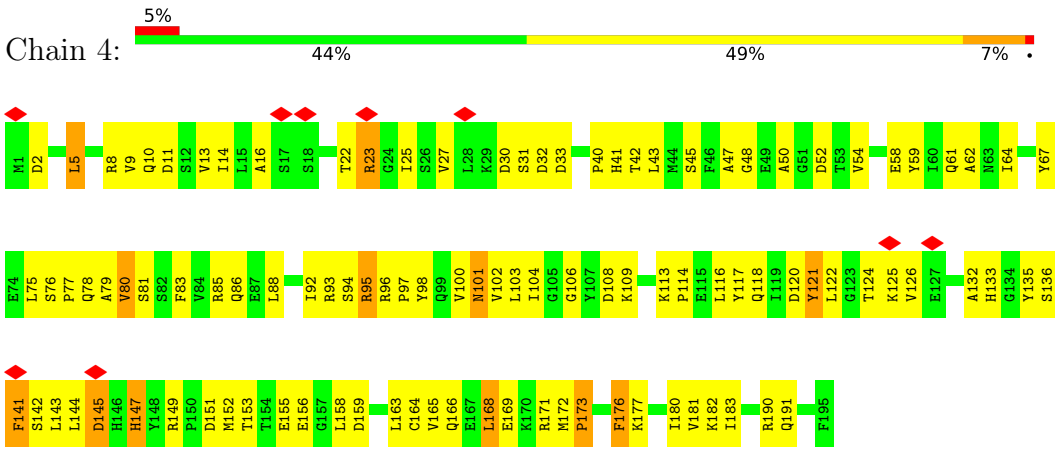
• Molecule 11: Proteasome subunit beta type-4

Chain k:



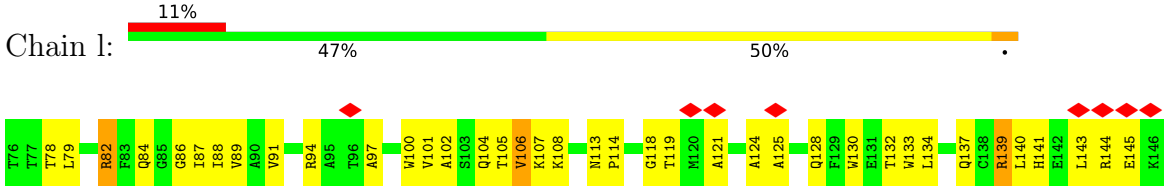
• Molecule 11: Proteasome subunit beta type-4

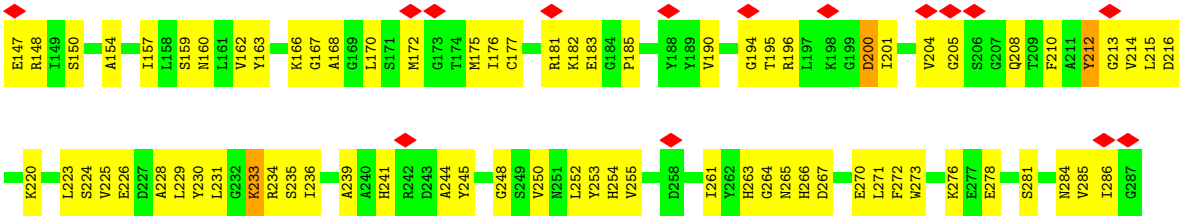
Chain 4:



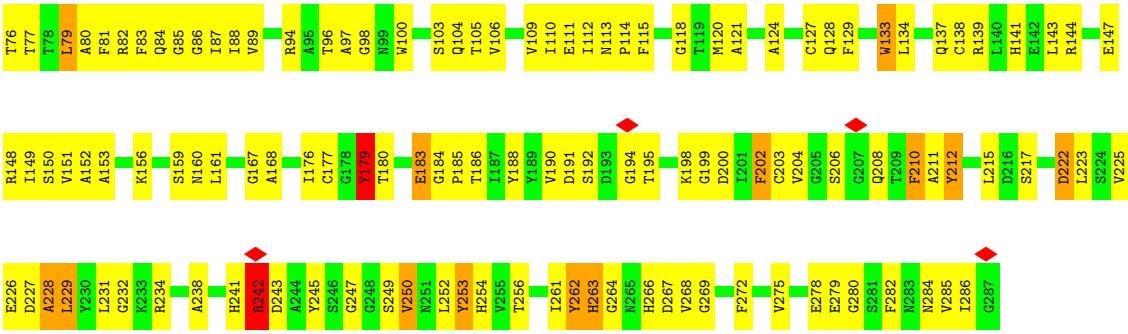
• Molecule 12: Proteasome subunit beta type-5

Chain l:

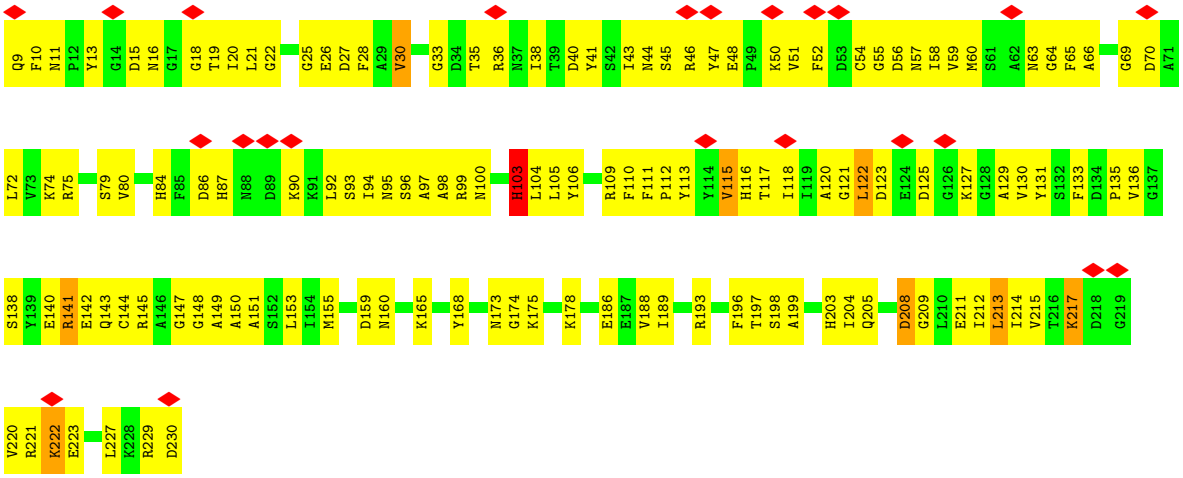




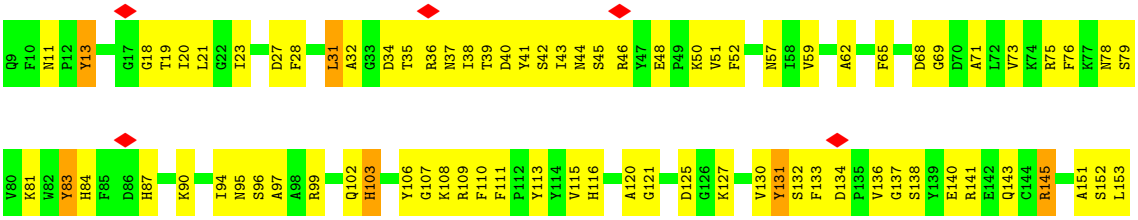
• Molecule 12: Proteasome subunit beta type-5

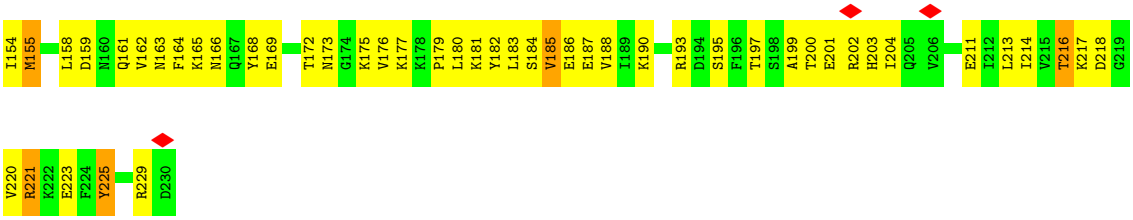


• Molecule 13: Proteasome subunit beta type-6

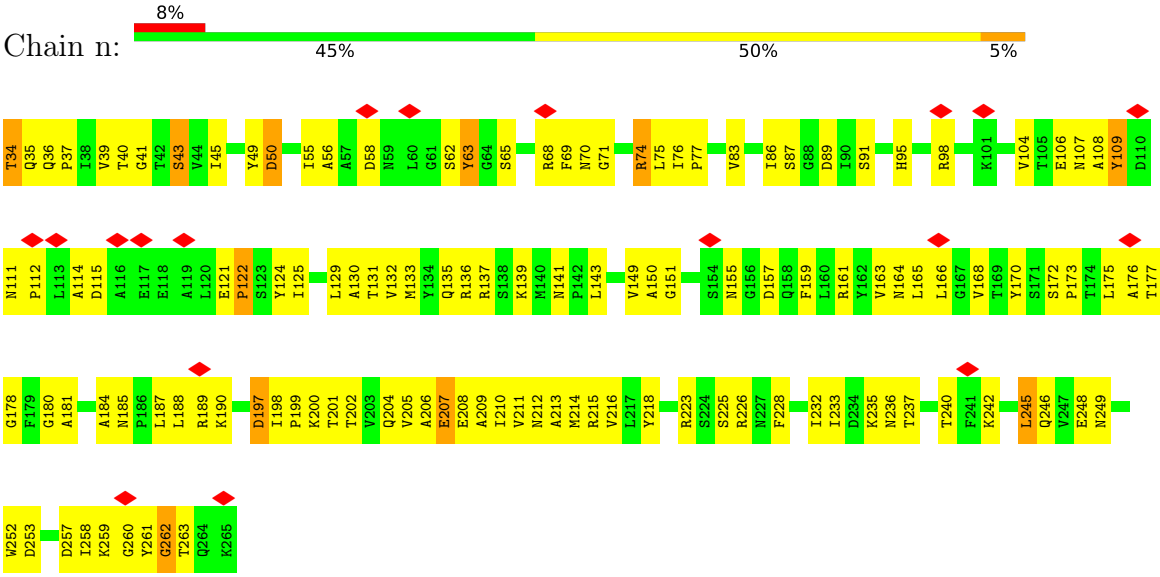


• Molecule 13: Proteasome subunit beta type-6

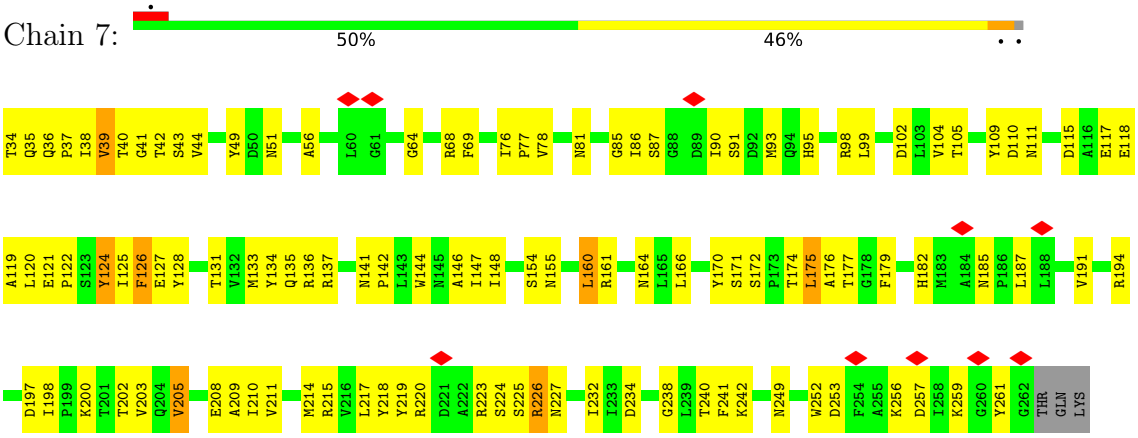




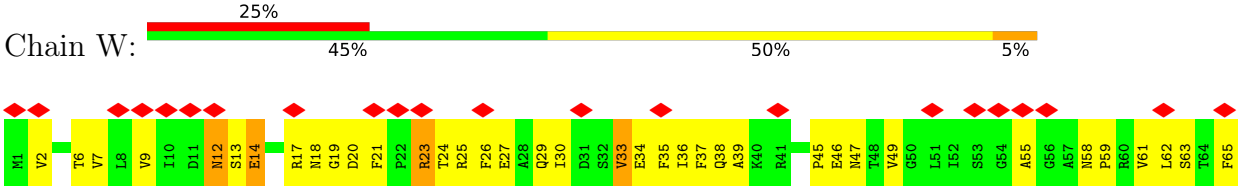
• Molecule 14: Proteasome subunit beta type-7

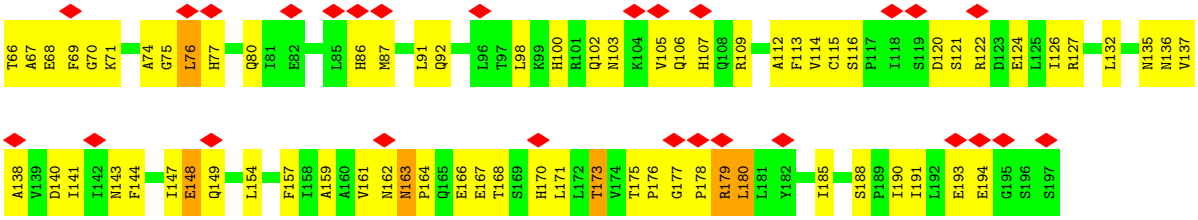


• Molecule 14: Proteasome subunit beta type-7



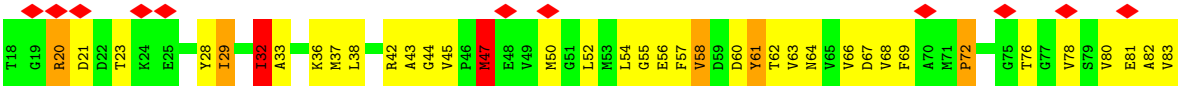
• Molecule 15: 26S proteasome regulatory subunit RPN10

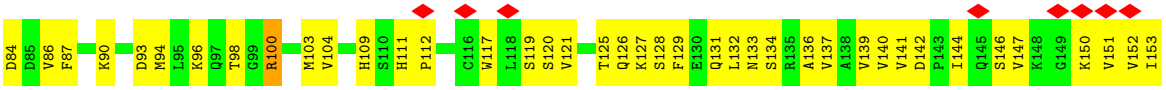


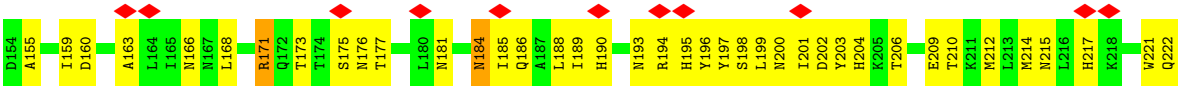


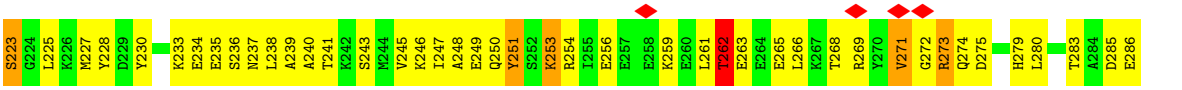
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

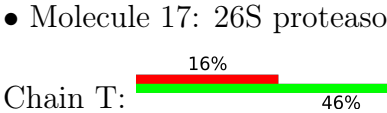
Chain V:





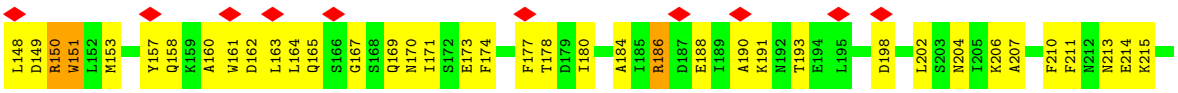






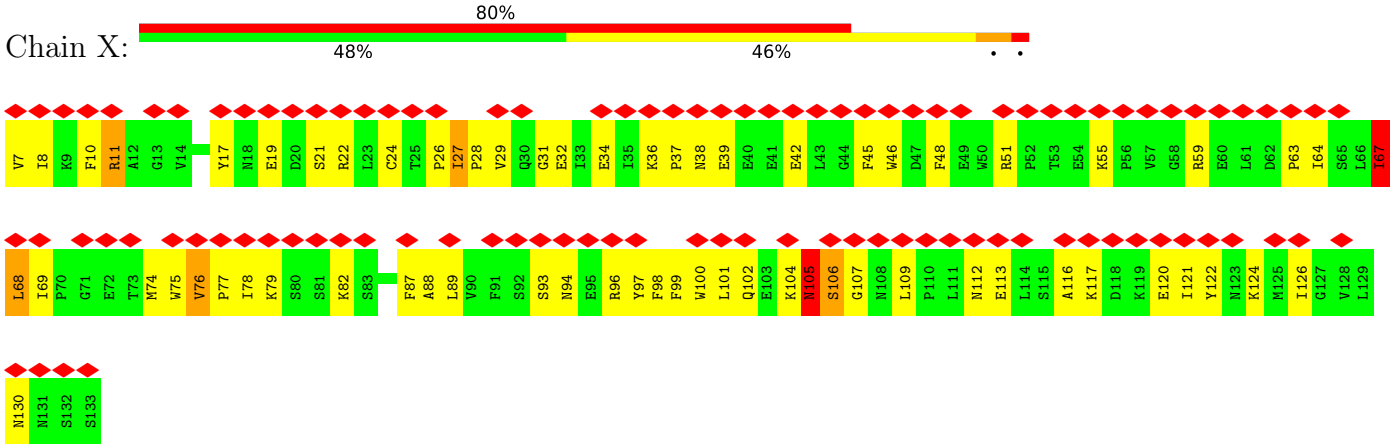
• Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:



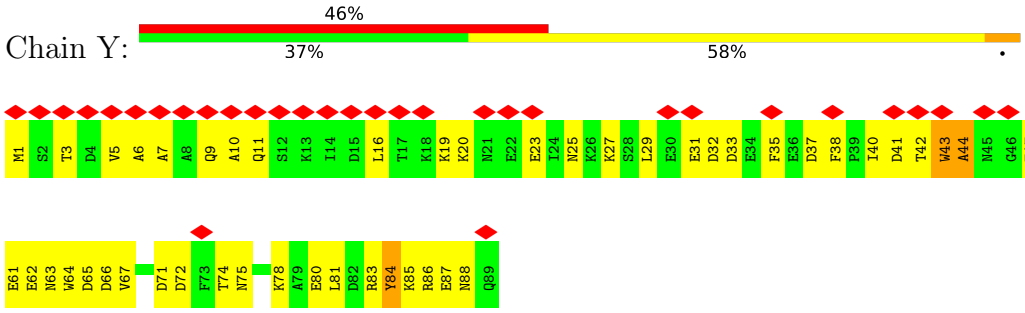
• Molecule 18: 26S proteasome regulatory subunit RPN13

Chain X:



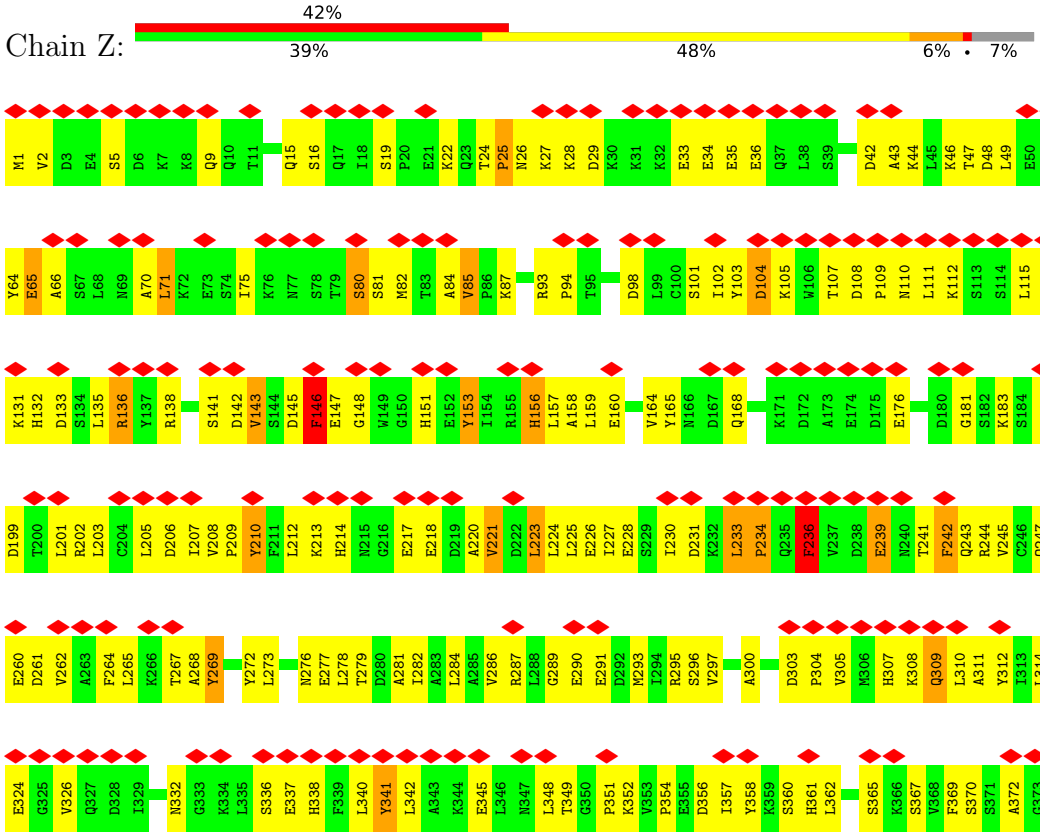
• Molecule 19: 26S proteasome complex subunit SEM1

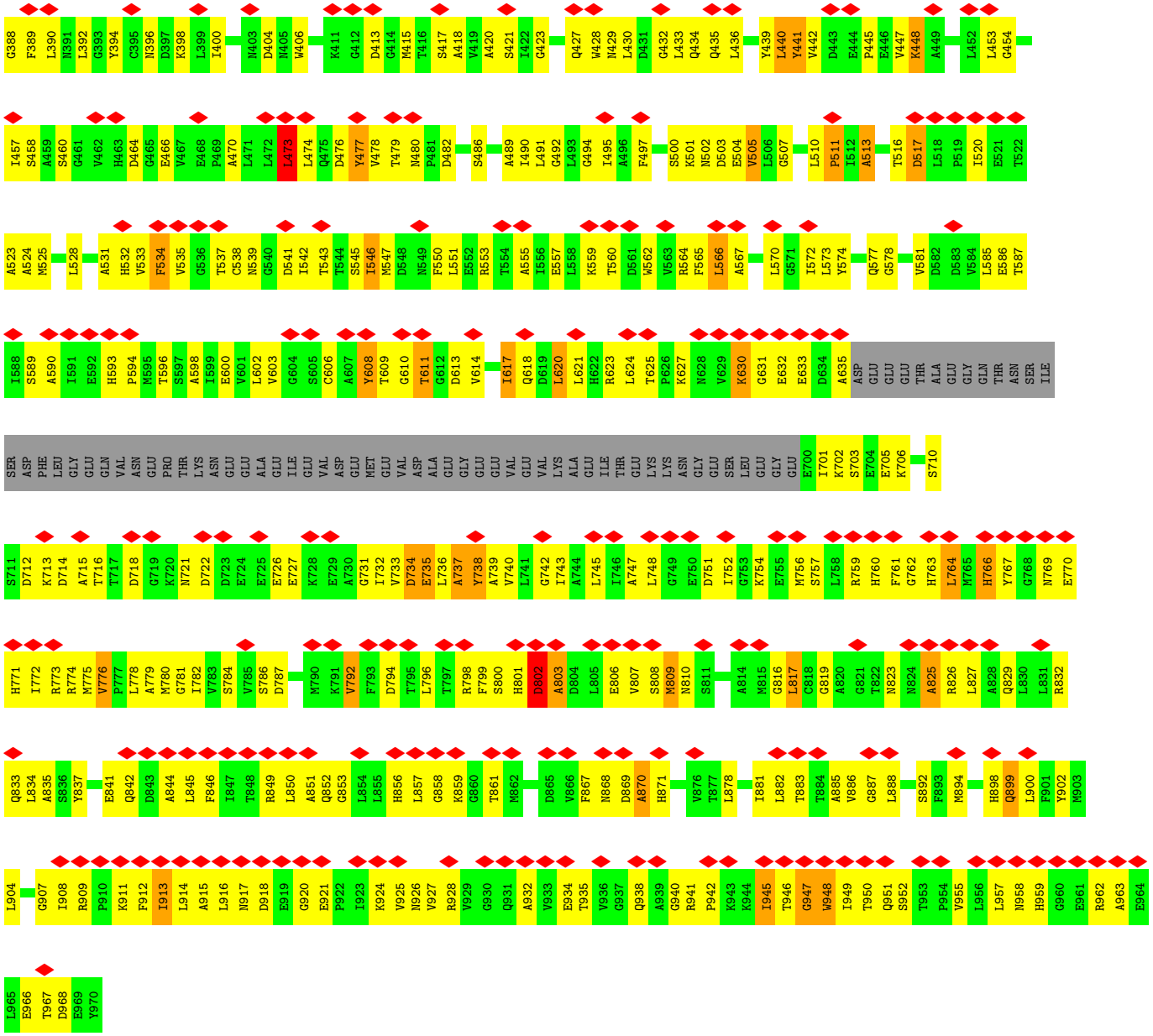
Chain Y:



• Molecule 20: 26S proteasome regulatory subunit RPN1

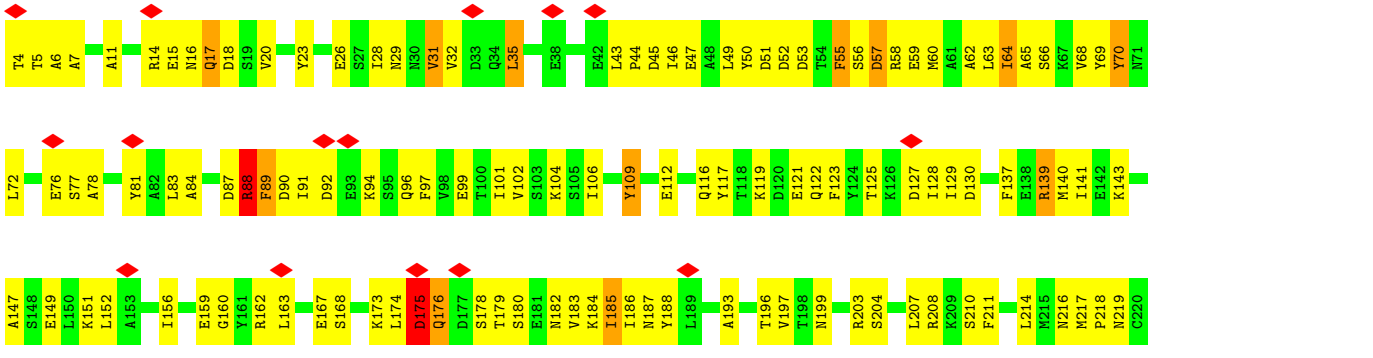
Chain Z:

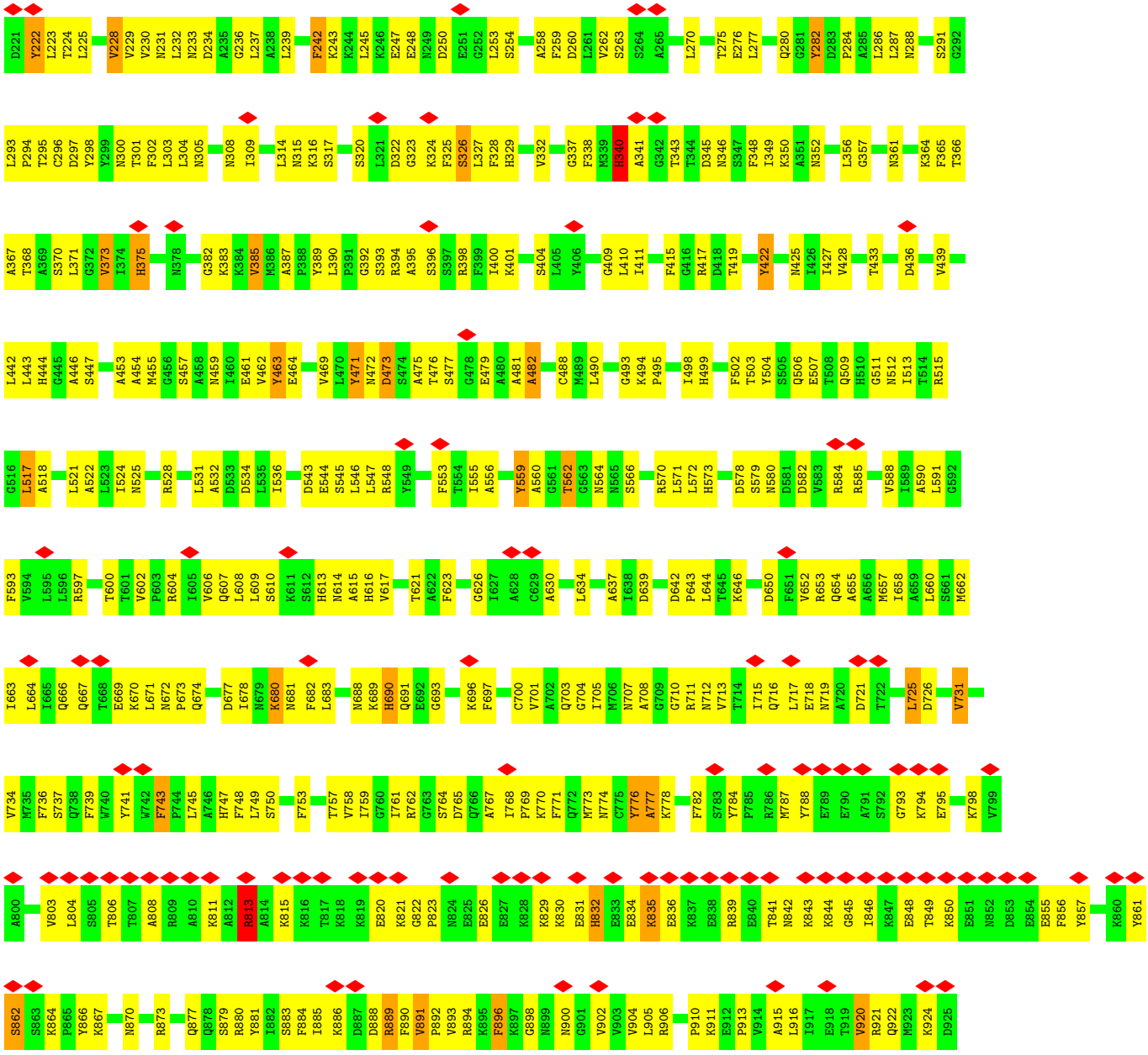




• Molecule 21: 26S proteasome regulatory subunit RPN2

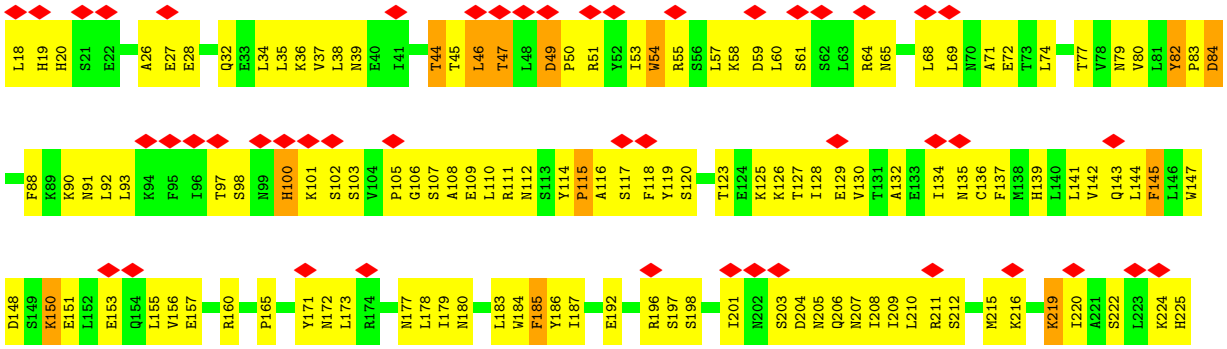
Chain N:

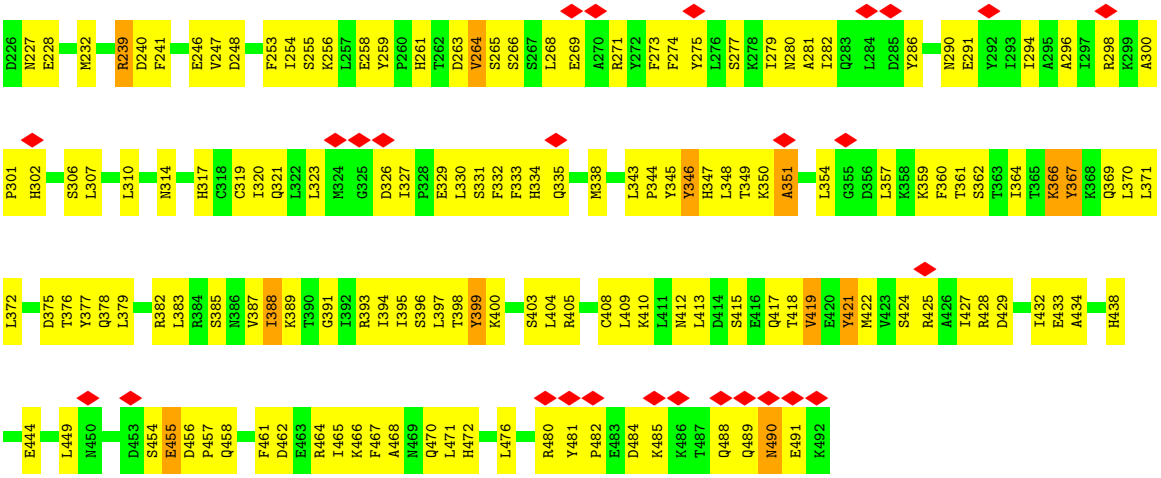




• Molecule 22: 26S proteasome regulatory subunit RPN3

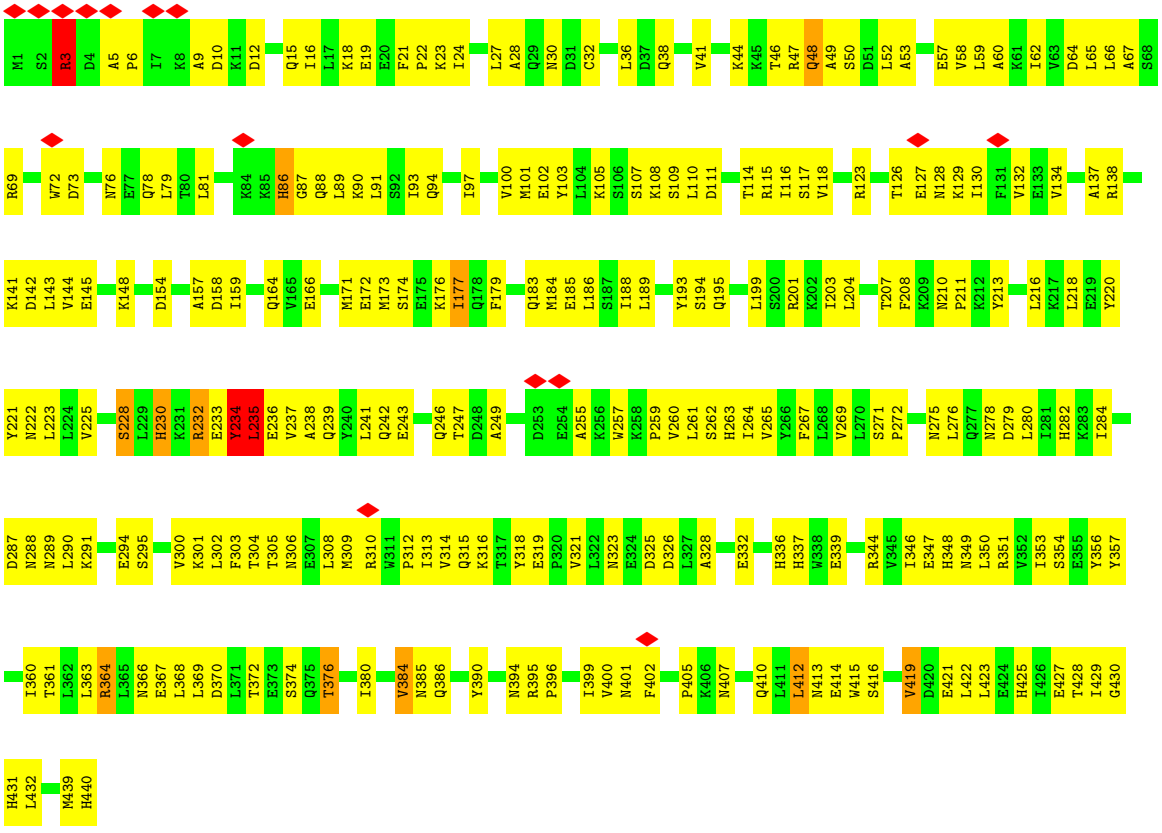
Chain S:





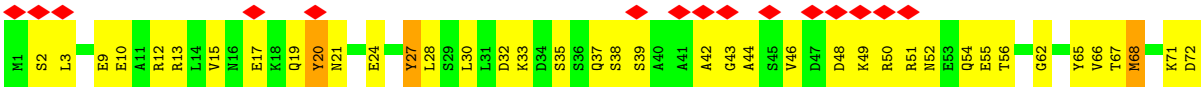
• Molecule 23: 26S proteasome regulatory subunit RPN5

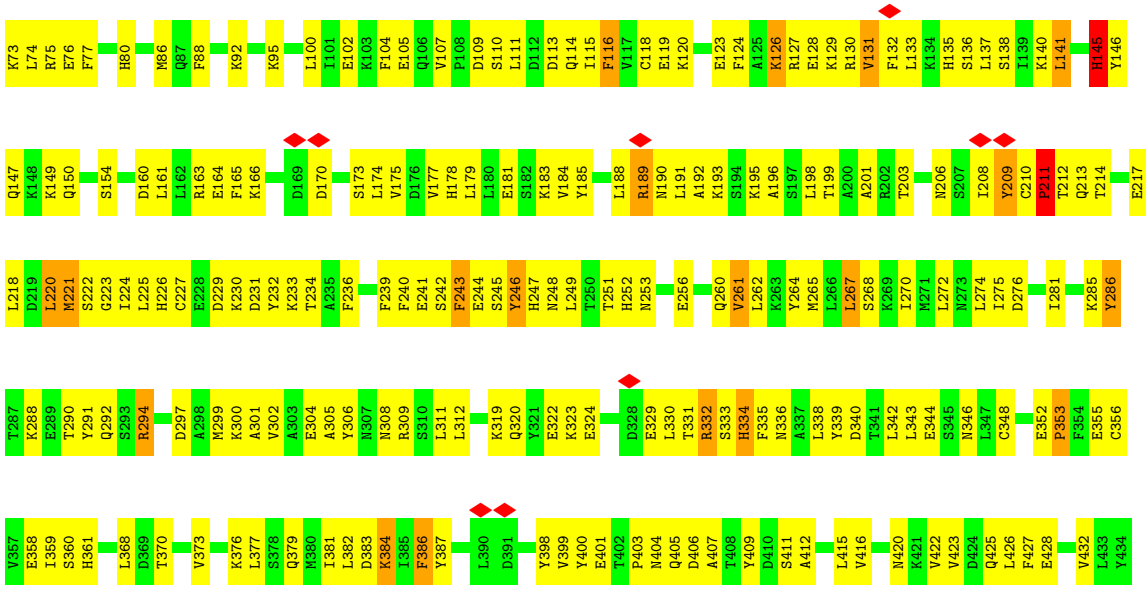
Chain P:



• Molecule 24: 26S proteasome regulatory subunit RPN6

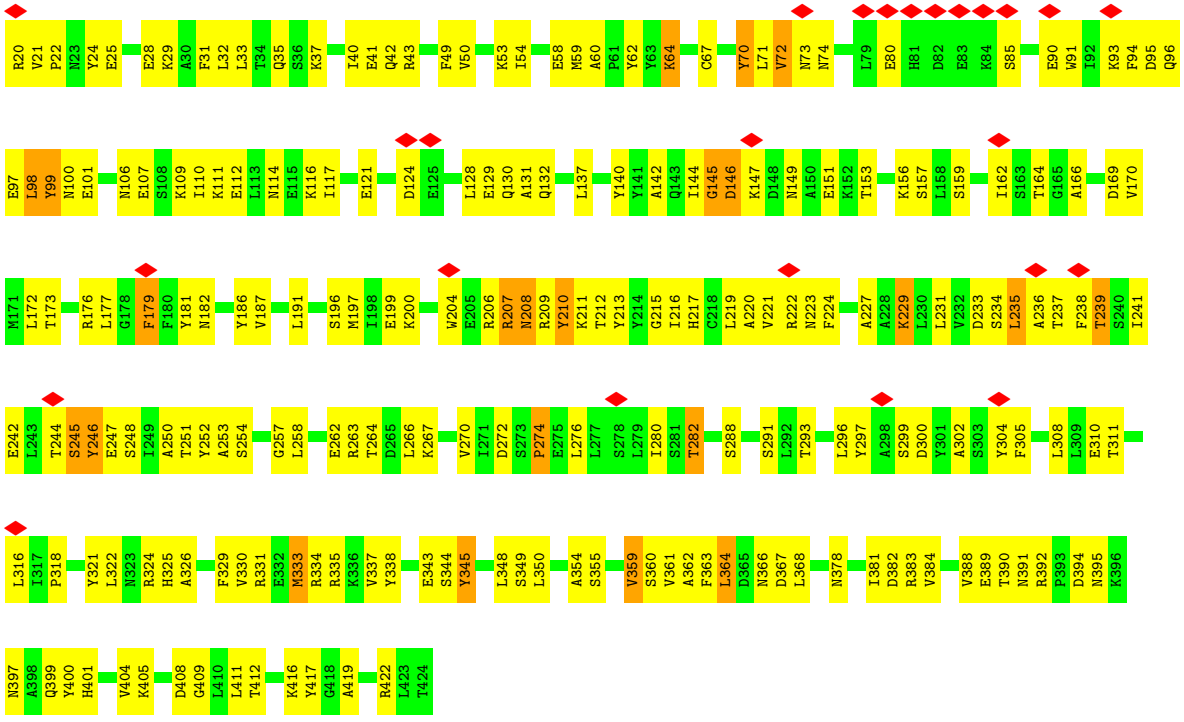
Chain Q:





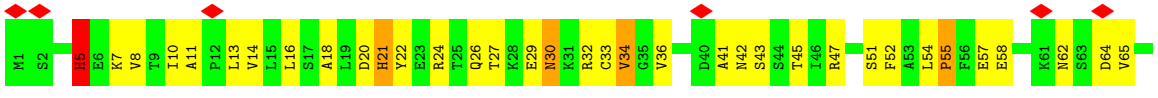
• Molecule 25: 26S proteasome regulatory subunit RPN7

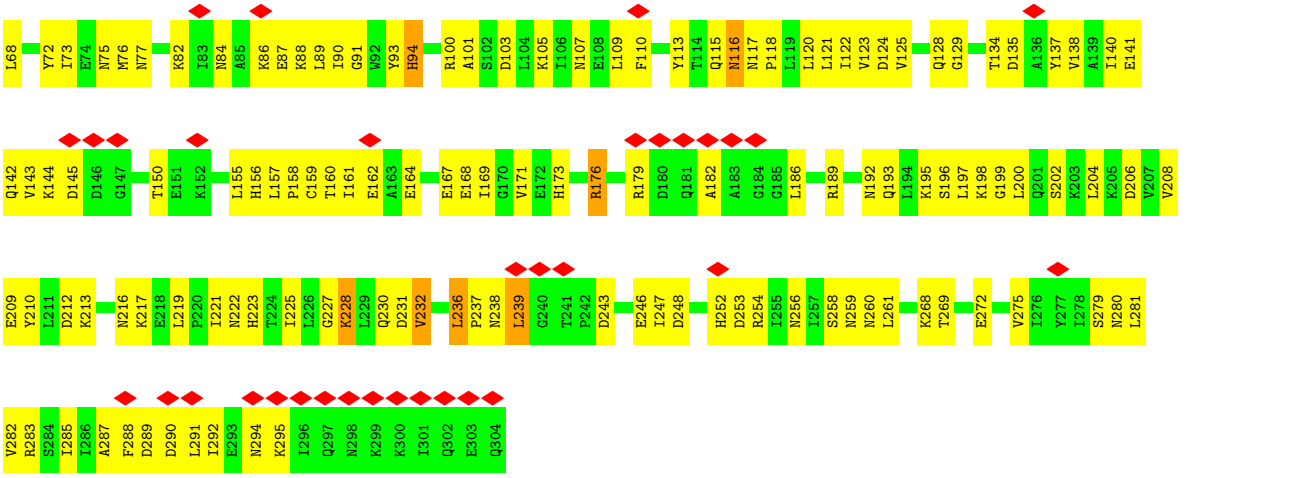
Chain R:



• Molecule 26: 26S proteasome regulatory subunit RPN8

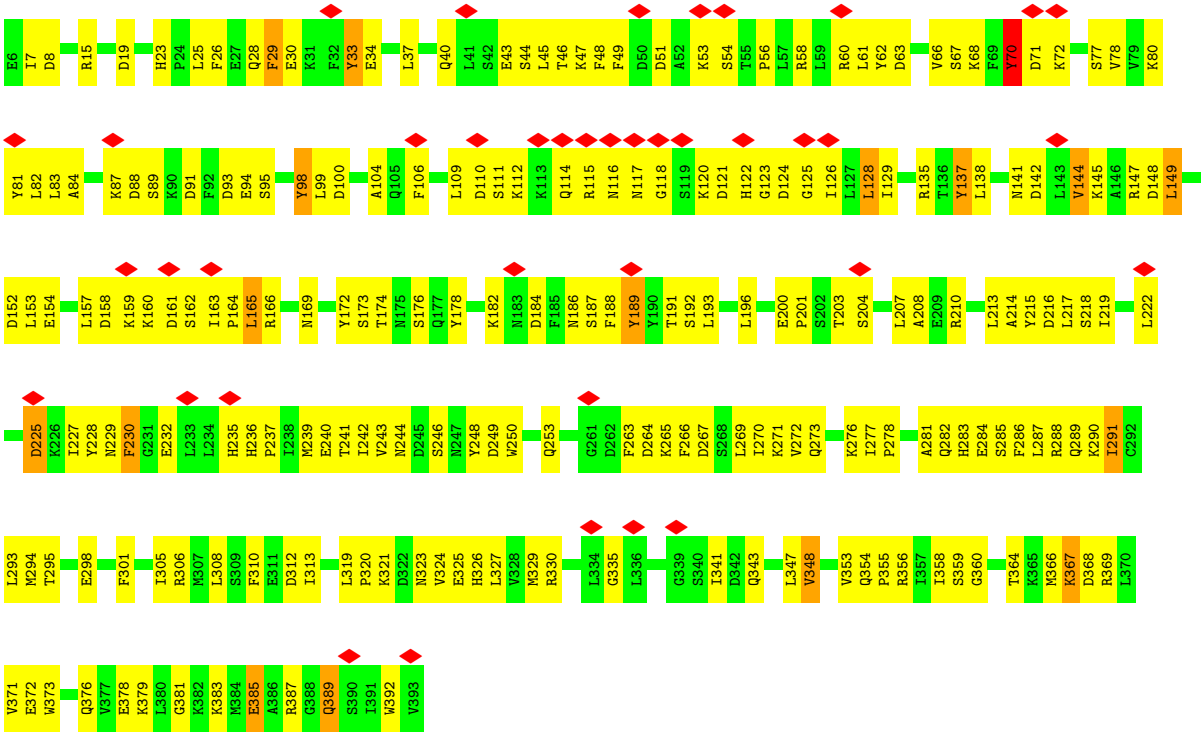
Chain U:





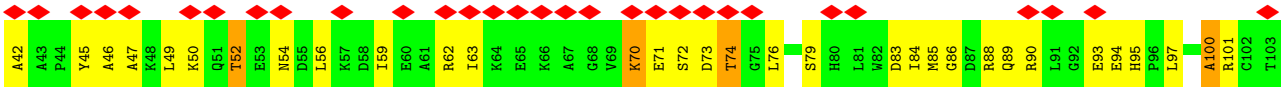
• Molecule 27: 26S proteasome regulatory subunit RPN9

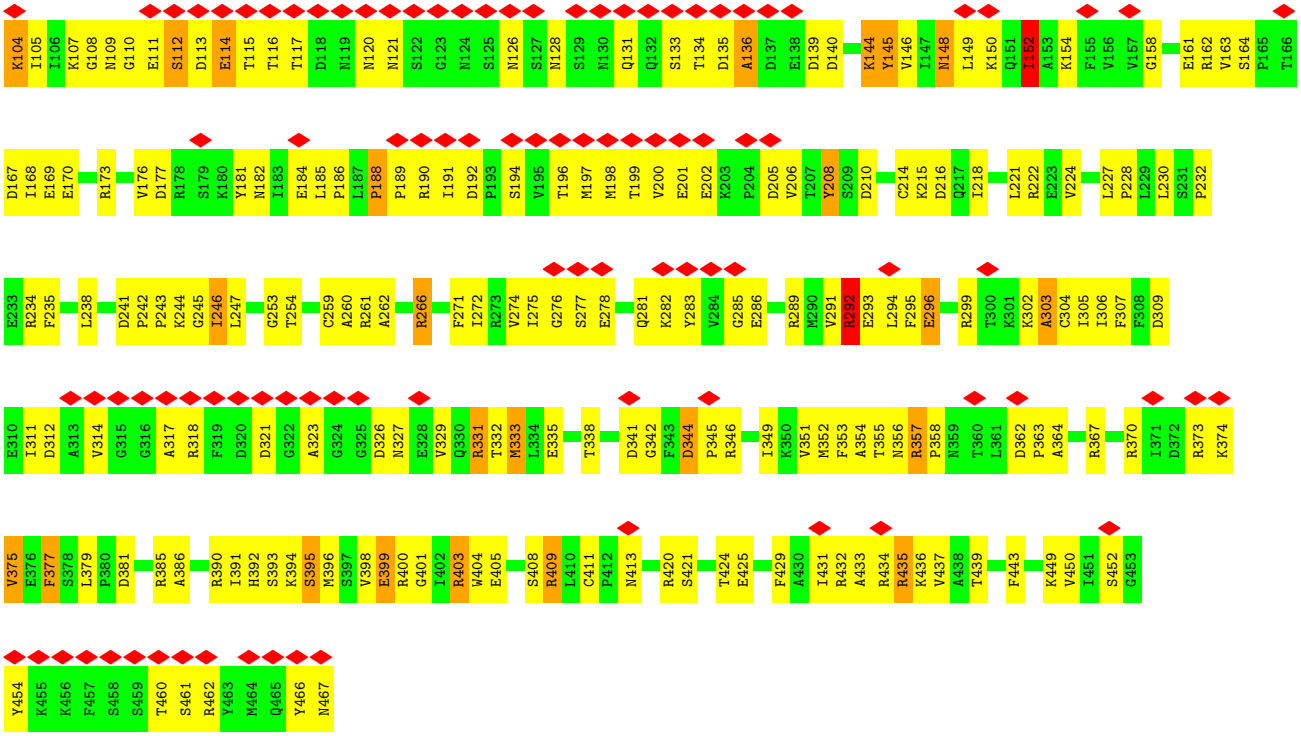
Chain O:



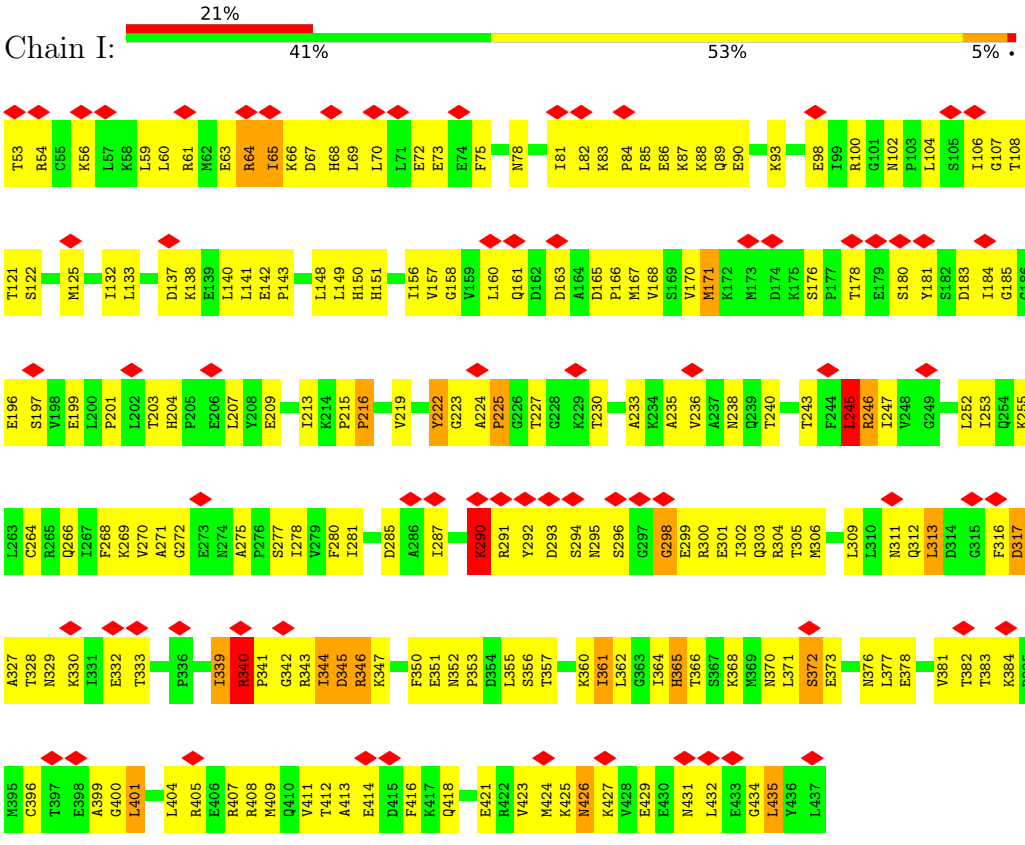
• Molecule 28: 26S proteasome regulatory subunit 7 homolog

Chain H:



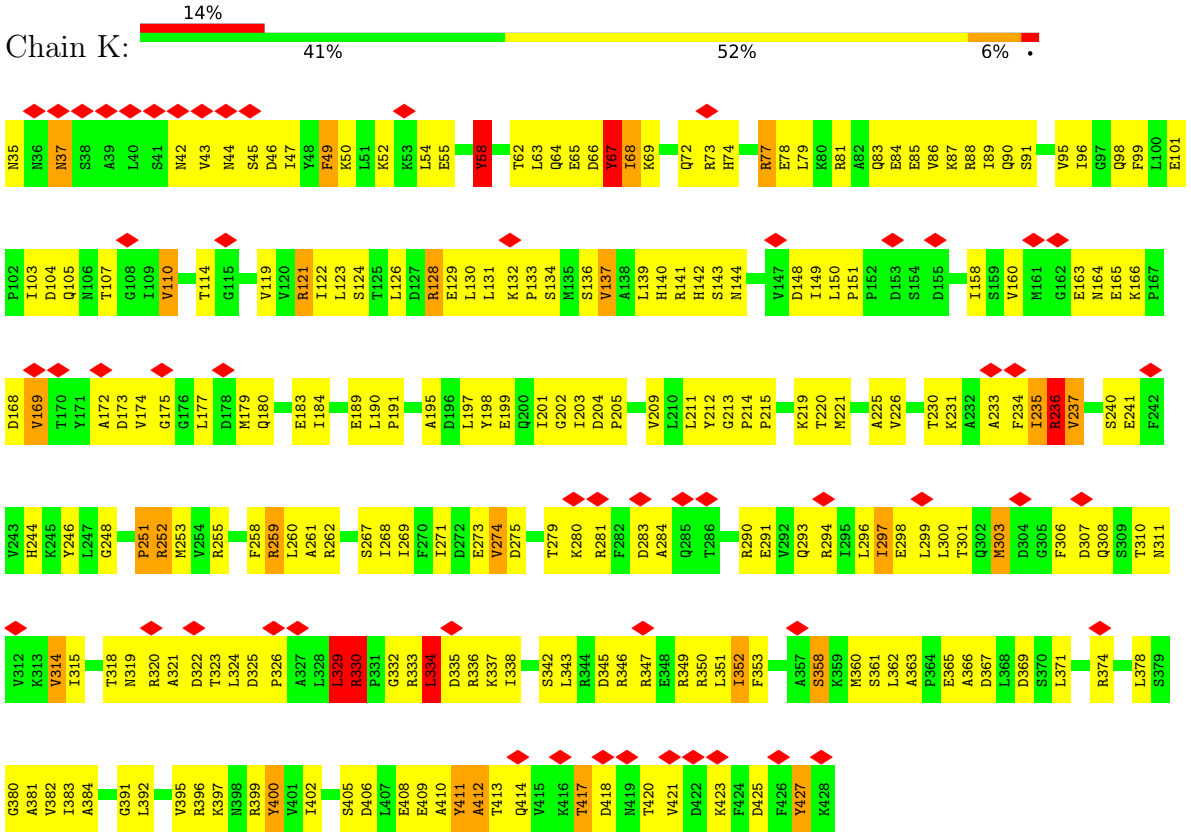


• Molecule 29: 26S proteasome regulatory subunit 4 homolog



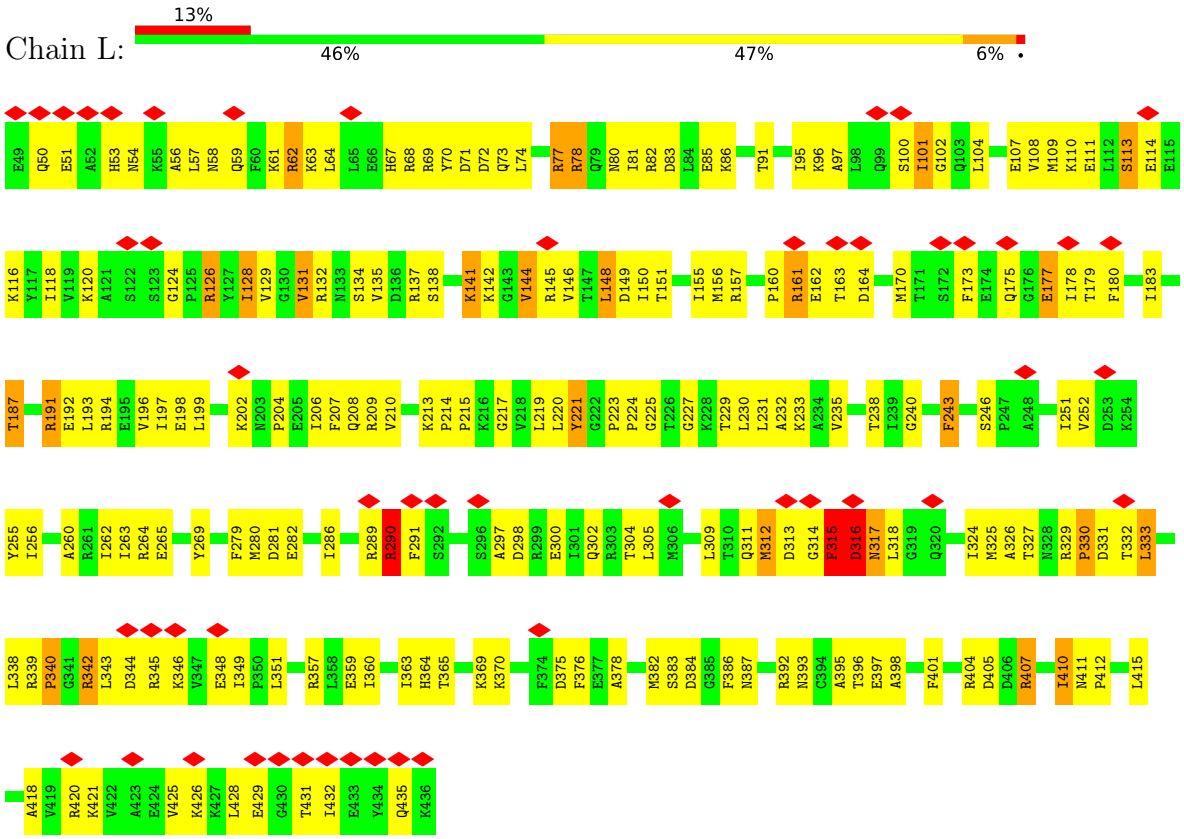
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

Chain K:



• Molecule 31: 26S proteasome subunit RPT4

Chain L:

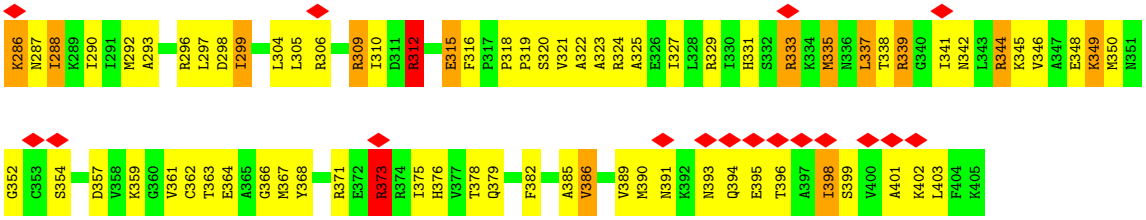


• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M:

• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:


K286 N287 I288 K289 I290 I291 M292 A293 R296 L297 D298 I299 L304 L305 R306 R309 I310 D311 R312 E315 F316 P317 P318 P319 S320 V321 A322 A323 R324 A325 E326 I327 L328 R329 I330 H331 S332 R333 K334 M335 N336 L337 T338 R339 G340 I341 N342 L343 R344 K345 V346 A347 E348 K349 M350 N351
G352 C353 S354 D357 W358 K359 G360 V361 C362 T363 E364 A365 G366 M367 Y368 R371 E372 R373 R374 I375 H376 V377 T378 Q379 F382 A385 V386 V389 M390 N391 K392 N393 Q394 E395 T396 A397 I398 S399 V400 A401 K402 L403 F404 K405

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184988	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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

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	2.31	81/1962 (4.1%)	2.48	136/2656 (5.1%)
1	a	2.23	66/1962 (3.4%)	2.49	134/2656 (5.0%)
2	B	2.26	78/1937 (4.0%)	2.45	132/2622 (5.0%)
2	b	2.26	73/1937 (3.8%)	2.41	121/2622 (4.6%)
3	C	2.27	71/1914 (3.7%)	2.36	107/2591 (4.1%)
3	c	2.20	58/1914 (3.0%)	2.42	125/2591 (4.8%)
4	D	2.45	98/1892 (5.2%)	2.49	119/2562 (4.6%)
4	d	2.35	87/2016 (4.3%)	2.51	146/2723 (5.4%)
5	E	2.23	62/1915 (3.2%)	2.44	126/2579 (4.9%)
5	e	2.26	73/1915 (3.8%)	2.47	125/2579 (4.8%)
6	F	2.38	80/1811 (4.4%)	2.37	101/2447 (4.1%)
6	f	2.26	64/1811 (3.5%)	2.39	107/2447 (4.4%)
7	G	2.36	93/1945 (4.8%)	2.44	122/2625 (4.6%)
7	g	2.25	77/1945 (4.0%)	2.44	110/2625 (4.2%)
8	1	2.35	59/1541 (3.8%)	2.45	102/2087 (4.9%)
8	h	2.20	47/1541 (3.0%)	2.33	92/2087 (4.4%)
9	2	2.29	68/1751 (3.9%)	2.48	114/2373 (4.8%)
9	i	2.30	68/1751 (3.9%)	2.51	128/2373 (5.4%)
10	3	2.30	76/1611 (4.7%)	2.42	103/2174 (4.7%)
10	j	2.36	71/1611 (4.4%)	2.48	118/2174 (5.4%)
11	4	2.38	67/1590 (4.2%)	2.38	105/2142 (4.9%)
11	k	2.33	64/1590 (4.0%)	2.38	89/2142 (4.2%)
12	5	2.29	62/1681 (3.7%)	2.45	116/2274 (5.1%)
12	l	2.35	72/1681 (4.3%)	2.42	98/2274 (4.3%)
13	6	2.34	81/1795 (4.5%)	2.40	105/2420 (4.3%)
13	m	2.37	78/1795 (4.3%)	2.43	124/2420 (5.1%)
14	7	2.33	71/1821 (3.9%)	2.42	107/2470 (4.3%)
14	n	2.28	74/1847 (4.0%)	2.44	115/2503 (4.6%)
15	W	2.27	61/1558 (3.9%)	2.42	97/2111 (4.6%)
16	V	2.29	85/2309 (3.7%)	2.48	166/3115 (5.3%)
17	T	2.21	72/2236 (3.2%)	2.49	155/3017 (5.1%)
18	X	2.17	34/1059 (3.2%)	2.33	50/1432 (3.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	2.25	27/741 (3.6%)	2.47	50/1000 (5.0%)
20	Z	2.39	252/7123 (3.5%)	2.62	638/9645 (6.6%)
21	N	2.26	265/7273 (3.6%)	2.49	497/9822 (5.1%)
22	S	2.30	162/3967 (4.1%)	2.56	308/5355 (5.8%)
23	P	2.22	127/3664 (3.5%)	2.46	280/4940 (5.7%)
24	Q	2.21	117/3556 (3.3%)	2.53	277/4787 (5.8%)
25	R	2.18	110/3314 (3.3%)	2.50	240/4469 (5.4%)
26	U	2.24	78/2461 (3.2%)	2.50	181/3327 (5.4%)
27	O	2.22	114/3247 (3.5%)	2.47	234/4380 (5.3%)
28	H	2.29	111/3363 (3.3%)	2.46	232/4532 (5.1%)
29	I	2.29	118/3061 (3.9%)	2.50	222/4121 (5.4%)
30	K	2.28	130/3156 (4.1%)	2.51	230/4261 (5.4%)
31	L	2.28	114/3129 (3.6%)	2.43	207/4204 (4.9%)
32	M	2.28	131/3323 (3.9%)	2.49	249/4478 (5.6%)
33	J	2.61	128/3212 (4.0%)	2.50	227/4316 (5.3%)
All	All	2.30	4255/112234 (3.8%)	2.47	7767/151550 (5.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	5
11	4	0	7
11	k	0	5
12	5	0	4
12	l	0	6
13	6	0	7
13	m	0	4
14	7	0	6
14	n	0	4
15	W	0	4
16	V	0	6
17	T	0	3
18	X	0	4
19	Y	0	1
20	Z	0	15
21	N	0	21
22	S	0	11
23	P	0	11
24	Q	0	14
25	R	0	13
26	U	0	5
27	O	0	5
28	H	0	13
29	I	0	11
30	K	0	18
31	L	0	21
32	M	0	7
33	J	0	17
All	All	0	353

All (4255) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	286	LYS	CD-CE	57.86	3.26	1.52
20	Z	738	TYR	CZ-OH	48.61	2.40	1.38
20	Z	948	TRP	CZ2-CH2	41.59	2.16	1.37
20	Z	948	TRP	CZ3-CH2	26.55	2.06	1.40
33	J	234	PHE	CG-CD2	20.28	1.81	1.38
33	J	234	PHE	CG-CD1	19.82	1.80	1.38
28	H	245	GLY	CA-C	-16.18	1.41	1.52
33	J	234	PHE	CD2-CE2	14.25	1.81	1.38
13	m	22	GLY	CA-C	-13.86	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	96	HIS	ND1-CE1	13.10	1.45	1.32
33	J	234	PHE	CE2-CZ	13.07	1.77	1.38
12	5	120	MET	CA-C	-12.97	1.37	1.52
33	J	234	PHE	CE1-CZ	12.74	1.76	1.38
14	7	198	ILE	CA-CB	12.28	1.60	1.54
9	i	45	ALA	CA-C	-11.67	1.38	1.52
17	T	186	ARG	CD-NE	11.67	1.62	1.46
14	n	175	LEU	CA-C	-11.57	1.38	1.52
13	m	141	ARG	CD-NE	11.47	1.62	1.46
15	W	138	ALA	CA-C	-11.46	1.38	1.52
7	G	183	HIS	CA-C	-11.45	1.43	1.52
2	B	41	ASN	N-CA	-11.04	1.37	1.47
20	Z	928	ARG	CA-C	-10.91	1.38	1.52
8	1	178	SER	C-N	10.82	1.43	1.33
29	I	382	THR	CA-C	-10.51	1.39	1.52
1	a	82	VAL	CA-CB	-10.50	1.41	1.54
13	6	45	SER	CA-C	-10.46	1.39	1.52
31	L	97	ALA	CA-C	-10.46	1.39	1.52
29	I	180	SER	CA-C	-10.38	1.40	1.52
20	Z	962	ARG	CD-NE	10.38	1.60	1.46
20	Z	776	VAL	CA-CB	-10.37	1.48	1.54
33	J	234	PHE	CD1-CE1	10.37	1.69	1.38
12	l	144	ARG	NE-CZ	10.31	1.44	1.33
16	V	86	VAL	CA-C	-10.28	1.40	1.52
12	l	102	ALA	CA-C	-10.27	1.39	1.52
28	H	396	MET	CA-C	-10.27	1.39	1.52
19	Y	42	THR	C-N	10.24	1.48	1.33
11	k	176	PHE	CA-C	-10.22	1.38	1.52
17	T	132	HIS	C-N	10.08	1.44	1.33
21	N	743	PHE	C-N	-9.98	1.24	1.34
6	F	60	GLN	N-CA	-9.94	1.33	1.46
32	M	345	ARG	NE-CZ	9.89	1.44	1.33
13	6	145	ARG	CA-C	-9.82	1.40	1.52
1	A	87	ILE	CA-CB	9.80	1.60	1.53
14	7	252	TRP	N-CA	-9.78	1.35	1.46
1	A	9	ALA	CA-C	-9.77	1.39	1.52
11	4	101	ASN	CA-C	-9.76	1.41	1.52
7	g	137	ILE	CA-C	-9.76	1.41	1.52
13	6	211	GLU	CA-C	-9.75	1.40	1.52
1	A	52	VAL	CA-C	-9.62	1.41	1.52
7	G	82	ILE	CA-CB	-9.61	1.49	1.54
2	B	48	GLU	CA-C	-9.60	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	409	ARG	NE-CZ	9.60	1.43	1.33
10	3	115	LYS	CA-CB	9.57	1.67	1.54
8	h	187	LEU	CA-C	-9.56	1.41	1.52
7	G	130	ARG	CD-NE	9.56	1.59	1.46
29	I	203	THR	C-N	9.56	1.40	1.33
21	N	101	ILE	C-N	9.55	1.46	1.33
31	L	407	ARG	NE-CZ	9.54	1.43	1.33
4	d	249	LYS	C-N	9.50	1.46	1.34
10	j	199	TYR	CA-C	-9.44	1.40	1.52
4	d	139	ASP	N-CA	-9.40	1.39	1.46
25	R	324	ARG	NE-CZ	9.38	1.43	1.33
14	n	70	ASN	CA-C	-9.37	1.41	1.52
13	6	79	SER	N-CA	-9.30	1.34	1.46
3	c	88	ILE	CA-C	-9.29	1.41	1.52
16	V	90	LYS	CA-C	-9.27	1.40	1.52
32	M	163	PHE	CA-C	-9.27	1.41	1.52
27	O	214	ALA	CA-C	-9.27	1.40	1.52
32	M	17	GLU	CA-C	-9.25	1.40	1.52
12	l	266	HIS	CA-C	-9.24	1.41	1.52
5	e	188	HIS	N-CA	-9.24	1.34	1.46
7	G	138	PHE	CA-C	-9.23	1.41	1.52
29	I	61	ARG	NE-CZ	9.20	1.43	1.33
14	7	120	LEU	CA-C	-9.18	1.39	1.52
20	Z	307	HIS	ND1-CE1	9.16	1.41	1.32
22	S	211	ARG	CD-NE	9.16	1.59	1.46
5	E	50	VAL	CA-C	-9.15	1.43	1.52
11	k	190	ARG	C-N	9.15	1.46	1.33
28	H	370	ARG	NE-CZ	9.11	1.43	1.33
1	A	146	VAL	CA-C	-9.10	1.41	1.52
26	U	253	ASP	CA-CB	9.09	1.67	1.53
14	n	136	ARG	CD-NE	9.09	1.58	1.46
5	E	186	GLU	CA-C	-9.07	1.42	1.52
6	F	51	ARG	CA-C	-9.04	1.41	1.52
31	L	192	GLU	CA-C	-9.04	1.41	1.52
1	a	45	VAL	CA-C	9.03	1.63	1.52
7	G	50	VAL	CA-C	-9.01	1.41	1.52
13	m	47	TYR	C-N	9.01	1.41	1.33
3	C	127	GLY	C-N	9.00	1.45	1.33
33	J	15	HIS	CA-C	-9.00	1.41	1.52
1	A	15	HIS	ND1-CE1	8.97	1.41	1.32
15	W	61	VAL	CA-CB	8.97	1.64	1.54
4	D	157	SER	CA-C	-8.97	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	213	ILE	CA-C	-8.96	1.41	1.52
10	3	167	ILE	N-CA	-8.96	1.35	1.46
11	k	60	ILE	CA-CB	-8.94	1.42	1.54
24	Q	407	ALA	CA-C	-8.93	1.41	1.52
32	M	248	ALA	N-CA	-8.93	1.37	1.46
19	Y	78	LYS	CA-CB	8.89	1.67	1.53
2	b	226	GLY	C-N	8.88	1.39	1.33
17	T	94	HIS	ND1-CE1	8.87	1.41	1.32
30	K	421	VAL	CA-CB	-8.86	1.44	1.54
1	A	58	LYS	CA-C	-8.85	1.41	1.52
33	J	38	THR	CA-C	-8.84	1.41	1.52
14	7	69	PHE	CA-C	-8.83	1.42	1.52
2	B	232	GLY	C-N	8.83	1.44	1.33
5	e	53	ARG	CD-NE	8.83	1.58	1.46
14	n	214	MET	C-N	8.82	1.45	1.33
24	Q	145	HIS	CA-C	-8.81	1.40	1.52
21	N	747	HIS	N-CA	-8.80	1.38	1.46
23	P	306	ASN	CA-CB	8.79	1.64	1.53
9	2	42	VAL	CA-CB	8.78	1.68	1.55
30	K	107	THR	CA-C	-8.77	1.41	1.52
4	D	10	ILE	CA-C	-8.74	1.41	1.52
6	f	99	PHE	C-N	8.74	1.44	1.33
33	J	339	ARG	NE-CZ	8.73	1.42	1.33
20	Z	336	SER	CA-C	-8.71	1.41	1.52
31	L	209	ARG	NE-CZ	8.71	1.42	1.33
11	4	43	LEU	CA-C	-8.67	1.42	1.52
8	1	23	LEU	C-N	8.67	1.43	1.33
6	F	51	ARG	NE-CZ	8.67	1.42	1.33
24	Q	292	GLN	CA-C	-8.66	1.42	1.52
13	6	169	GLU	CA-CB	8.66	1.67	1.52
18	X	10	PHE	CA-C	-8.66	1.42	1.52
20	Z	718	ASP	N-CA	8.64	1.56	1.46
9	2	205	CYS	N-CA	-8.63	1.36	1.46
7	g	75	GLY	CA-C	-8.61	1.43	1.52
5	E	53	ARG	CD-NE	8.61	1.58	1.46
21	N	671	LEU	C-N	8.61	1.41	1.33
20	Z	909	ARG	NE-CZ	8.61	1.42	1.33
2	B	61	LEU	CA-C	-8.59	1.42	1.52
12	5	266	HIS	ND1-CE1	8.57	1.41	1.32
13	6	153	LEU	CA-C	-8.57	1.42	1.52
20	Z	107	THR	CA-C	-8.55	1.42	1.53
4	D	141	ARG	NE-CZ	8.54	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	185	LEU	CA-C	-8.54	1.46	1.52
19	Y	27	LYS	CA-C	-8.53	1.41	1.52
27	O	162	SER	CA-C	-8.53	1.44	1.53
29	I	405	ARG	NE-CZ	8.53	1.42	1.33
32	M	197	ILE	CA-CB	-8.50	1.47	1.55
16	V	100	ARG	C-N	8.50	1.44	1.33
21	N	515	ARG	NE-CZ	8.50	1.42	1.33
13	6	32	ALA	CA-C	-8.48	1.42	1.52
21	N	616	HIS	ND1-CE1	8.47	1.41	1.32
25	R	392	ARG	CD-NE	8.46	1.58	1.46
27	O	15	ARG	NE-CZ	8.46	1.42	1.33
23	P	414	GLU	C-N	8.46	1.45	1.34
31	L	265	GLU	CA-CB	8.46	1.67	1.53
4	D	58	ARG	CA-C	-8.43	1.42	1.52
17	T	61	ILE	C-N	8.43	1.45	1.33
20	Z	189	ALA	CA-C	-8.43	1.40	1.52
26	U	10	ILE	CA-C	-8.43	1.41	1.52
5	E	75	GLY	CA-C	-8.42	1.44	1.52
16	V	292	ILE	C-N	8.42	1.44	1.33
20	Z	75	ILE	CA-C	-8.42	1.42	1.52
24	Q	294	ARG	NE-CZ	8.42	1.42	1.33
24	Q	72	ASP	CA-CB	8.41	1.66	1.53
4	D	139	ASP	C-N	8.40	1.43	1.34
5	e	63	SER	C-N	8.38	1.45	1.33
7	G	246	GLU	C-N	8.35	1.44	1.33
12	l	261	ILE	CA-C	-8.35	1.42	1.52
20	Z	157	LEU	C-N	8.34	1.46	1.33
4	d	137	GLY	CA-C	-8.34	1.42	1.51
22	S	351	ALA	C-N	8.34	1.44	1.33
32	M	74	GLN	CA-C	8.32	1.64	1.52
12	l	212	TYR	C-N	8.32	1.44	1.33
27	O	157	LEU	N-CA	-8.32	1.36	1.46
29	I	255	LYS	CA-C	-8.30	1.42	1.52
26	U	275	VAL	N-CA	8.30	1.57	1.46
8	1	166	HIS	ND1-CE1	8.29	1.40	1.32
14	7	202	THR	CA-C	-8.29	1.42	1.52
22	S	425	ARG	CD-NE	8.29	1.57	1.46
31	L	129	VAL	N-CA	-8.29	1.36	1.46
13	m	175	LYS	CA-C	8.27	1.64	1.52
20	Z	759	ARG	CD-NE	8.27	1.57	1.46
12	l	91	VAL	CA-C	-8.26	1.44	1.52
21	N	585	ARG	CD-NE	8.26	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	86	HIS	ND1-CE1	8.24	1.40	1.32
21	N	646	LYS	C-N	8.24	1.45	1.33
25	R	21	VAL	CA-C	-8.24	1.45	1.52
5	e	93	ARG	CA-C	8.23	1.63	1.52
7	G	169	ARG	CD-NE	8.23	1.57	1.46
16	V	109	HIS	CA-C	-8.23	1.42	1.52
28	H	408	SER	CA-C	8.22	1.64	1.52
31	L	69	ARG	CD-NE	8.22	1.57	1.46
11	k	111	LYS	CA-C	-8.22	1.43	1.52
30	K	236	ARG	CD-NE	8.21	1.57	1.46
15	W	109	ARG	CZ-NH2	8.20	1.44	1.33
23	P	94	GLN	C-N	8.20	1.45	1.33
30	K	346	ARG	CD-NE	8.20	1.57	1.46
5	E	211	LYS	CA-C	-8.20	1.43	1.52
33	J	399	SER	C-N	8.19	1.43	1.33
24	Q	127	ARG	NE-CZ	8.18	1.42	1.33
16	V	94	MET	C-N	8.18	1.44	1.33
22	S	263	ASP	C-N	-8.17	1.26	1.33
9	i	217	ARG	NE-CZ	8.17	1.42	1.33
29	I	150	HIS	ND1-CE1	8.16	1.40	1.32
21	N	643	PRO	N-CD	-8.15	1.36	1.47
1	A	120	ARG	NE-CZ	8.15	1.42	1.33
13	6	116	HIS	CG-CD2	8.15	1.44	1.35
27	O	229	ASN	N-CA	-8.15	1.36	1.46
11	4	14	ILE	C-N	8.15	1.45	1.33
21	N	453	ALA	CA-C	-8.14	1.42	1.52
20	Z	909	ARG	CD-NE	8.13	1.57	1.46
29	I	412	THR	C-N	8.13	1.44	1.33
1	a	105	ARG	N-CA	-8.12	1.36	1.46
3	C	50	ARG	NE-CZ	8.11	1.42	1.33
12	l	223	LEU	N-CA	-8.11	1.36	1.46
3	C	64	GLU	CA-C	8.11	1.64	1.52
9	2	173	GLN	C-N	8.11	1.44	1.33
3	C	147	GLN	CA-C	-8.10	1.42	1.52
1	A	55	SER	N-CA	-8.10	1.35	1.45
1	A	23	GLY	CA-C	-8.09	1.40	1.51
20	Z	555	ALA	C-N	8.09	1.41	1.33
33	J	258	VAL	CA-C	-8.08	1.43	1.52
26	U	36	VAL	CA-C	-8.08	1.43	1.52
3	C	161	LYS	C-N	8.07	1.43	1.33
9	i	224	VAL	N-CA	-8.06	1.36	1.46
9	2	57	ASP	CA-C	-8.06	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	574	TYR	C-N	8.06	1.44	1.33
32	M	117	ALA	CA-C	-8.06	1.42	1.52
4	D	181	ARG	CD-NE	8.04	1.57	1.46
29	I	171	MET	CA-C	-8.05	1.42	1.52
26	U	58	GLU	CA-C	-8.04	1.43	1.52
7	G	132	PHE	CA-C	-8.03	1.42	1.53
6	F	135	ILE	CA-C	-8.02	1.43	1.52
7	g	106	PRO	CA-C	-8.02	1.42	1.52
21	N	258	ALA	CA-C	-8.02	1.42	1.52
25	R	391	ASN	C-N	8.01	1.41	1.33
20	Z	525	MET	N-CA	-8.01	1.35	1.46
16	V	236	SER	CA-C	-8.01	1.42	1.52
32	M	198	VAL	CA-CB	-8.00	1.44	1.54
26	U	253	ASP	N-CA	-8.00	1.36	1.46
27	O	63	ASP	CA-C	-8.00	1.42	1.52
21	N	55	PHE	CA-C	-8.00	1.43	1.52
21	N	20	VAL	CA-CB	8.00	1.63	1.54
9	i	140	PHE	CA-C	-7.99	1.42	1.52
11	k	76	SER	CA-CB	7.99	1.65	1.53
22	S	418	THR	N-CA	-7.99	1.36	1.46
13	m	121	GLY	N-CA	-7.98	1.37	1.45
21	N	700	CYS	N-CA	-7.98	1.36	1.46
33	J	271	THR	CA-C	-7.98	1.42	1.52
22	S	177	ASN	C-N	7.97	1.44	1.33
21	N	315	ASN	N-CA	-7.96	1.35	1.46
2	b	227	ILE	CA-C	7.95	1.58	1.52
21	N	902	VAL	CA-CB	-7.95	1.44	1.54
7	g	131	PRO	CA-CB	7.95	1.65	1.53
28	H	235	PHE	CA-C	-7.95	1.42	1.52
11	4	108	ASP	N-CA	-7.95	1.36	1.46
22	S	36	LYS	CA-CB	7.95	1.65	1.53
24	Q	124	PHE	CA-CB	7.94	1.63	1.52
5	E	67	ILE	CA-CB	-7.94	1.44	1.54
26	U	34	VAL	CA-CB	-7.94	1.44	1.54
10	3	45	HIS	ND1-CE1	7.93	1.40	1.32
10	3	147	PHE	N-CA	-7.93	1.36	1.46
7	G	228	HIS	CB-CG	7.92	1.61	1.50
33	J	325	ALA	N-CA	-7.92	1.36	1.46
7	G	94	GLU	N-CA	-7.91	1.36	1.46
6	f	209	ASP	C-N	7.89	1.45	1.33
32	M	432	PHE	CA-C	-7.88	1.46	1.52
21	N	693	GLY	N-CA	-7.88	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	113	TYR	CA-C	-7.88	1.43	1.52
1	a	120	ARG	N-CA	-7.88	1.36	1.46
23	P	9	ALA	CA-CB	7.88	1.65	1.53
27	O	201	PRO	N-CA	-7.87	1.36	1.47
21	N	417	ARG	NE-CZ	7.87	1.41	1.33
1	a	59	VAL	CA-C	-7.86	1.46	1.53
6	F	144	LEU	CA-C	-7.86	1.43	1.52
14	7	176	ALA	CA-C	-7.86	1.43	1.52
15	W	17	ARG	NE-CZ	7.86	1.41	1.33
14	n	232	ILE	C-N	7.86	1.43	1.33
4	D	166	ARG	CD-NE	7.86	1.57	1.46
19	Y	31	GLU	CA-C	-7.86	1.45	1.53
30	K	201	ILE	CA-C	-7.86	1.43	1.52
32	M	400	MET	CA-C	-7.85	1.42	1.52
2	B	160	LYS	N-CA	-7.85	1.36	1.46
13	m	84	HIS	ND1-CE1	7.85	1.40	1.32
2	b	17	LYS	C-N	7.84	1.44	1.33
7	g	204	HIS	ND1-CE1	7.84	1.40	1.32
23	P	412	LEU	N-CA	-7.84	1.36	1.46
5	e	60	GLU	CA-CB	7.84	1.63	1.53
30	K	320	ARG	N-CA	-7.84	1.36	1.46
6	F	11	VAL	C-N	7.83	1.44	1.33
21	N	394	ARG	CD-NE	7.83	1.57	1.46
27	O	125	GLY	N-CA	-7.83	1.35	1.45
23	P	288	ASN	CA-C	-7.83	1.43	1.53
21	N	532	ALA	CA-C	-7.83	1.42	1.52
26	U	121	LEU	CA-C	-7.82	1.43	1.52
8	1	103	THR	CA-C	7.81	1.61	1.52
4	d	172	ARG	C-N	7.81	1.44	1.33
7	G	40	ILE	CA-CB	-7.81	1.44	1.54
27	O	265	LYS	C-N	7.81	1.44	1.33
25	R	360	SER	CA-C	-7.80	1.42	1.53
27	O	389	GLN	CA-C	-7.80	1.43	1.52
12	l	214	VAL	CA-CB	-7.79	1.45	1.54
12	5	112	ILE	CA-C	-7.79	1.43	1.52
21	N	447	SER	C-O	-7.79	1.15	1.24
13	m	147	GLY	N-CA	-7.79	1.38	1.44
2	B	178	ARG	CZ-NH1	7.78	1.43	1.32
23	P	309	MET	CA-C	-7.78	1.43	1.52
10	3	152	SER	CA-C	-7.77	1.43	1.52
20	Z	480	ASN	CA-CB	7.77	1.65	1.53
33	J	391	ASN	CA-CB	7.76	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	178	THR	C-N	7.76	1.44	1.33
29	I	387	LEU	C-N	7.76	1.44	1.33
22	S	100	HIS	ND1-CE1	7.75	1.40	1.32
3	c	222	ASP	CA-C	-7.75	1.42	1.53
11	k	194	ASP	CA-C	-7.75	1.43	1.52
22	S	19	HIS	ND1-CE1	7.74	1.40	1.32
32	M	398	ALA	C-N	7.74	1.43	1.33
23	P	203	ILE	CA-C	-7.74	1.42	1.52
6	F	37	GLY	N-CA	7.73	1.54	1.45
4	d	131	VAL	CA-C	-7.73	1.43	1.52
13	6	229	ARG	NE-CZ	7.73	1.41	1.33
29	I	411	VAL	N-CA	-7.72	1.37	1.46
4	d	42	VAL	N-CA	-7.72	1.37	1.46
12	5	204	VAL	CA-C	-7.72	1.44	1.52
28	H	176	VAL	CA-C	-7.72	1.43	1.52
22	S	160	ARG	CD-NE	7.71	1.57	1.46
6	F	144	LEU	CA-CB	7.71	1.65	1.53
4	D	198	SER	N-CA	-7.71	1.37	1.46
20	Z	436	LEU	N-CA	-7.71	1.37	1.46
21	N	602	VAL	CA-CB	7.70	1.59	1.53
29	I	306	MET	CA-C	-7.70	1.43	1.52
10	j	57	ALA	CA-C	-7.70	1.42	1.52
21	N	382	GLY	CA-C	-7.70	1.43	1.52
12	l	175	MET	CA-C	-7.70	1.43	1.52
9	2	126	TYR	CA-C	-7.69	1.43	1.52
29	I	168	VAL	CA-CB	-7.69	1.44	1.54
14	n	223	ARG	NE-CZ	7.69	1.41	1.33
19	Y	86	ARG	CZ-NH1	7.69	1.43	1.32
4	d	96	HIS	ND1-CE1	7.68	1.40	1.32
22	S	264	VAL	CA-CB	-7.68	1.47	1.55
30	K	399	ARG	CA-C	-7.68	1.42	1.53
18	X	69	ILE	CA-CB	7.68	1.62	1.53
14	7	95	HIS	ND1-CE1	7.68	1.40	1.32
5	e	249	ALA	C-N	7.67	1.44	1.33
28	H	140	ASP	CA-CB	7.66	1.59	1.53
8	1	184	MET	CA-C	-7.66	1.43	1.52
3	C	120	GLN	CA-C	-7.65	1.43	1.52
8	h	15	VAL	N-CA	-7.64	1.36	1.46
21	N	889	ARG	CD-NE	7.64	1.56	1.46
16	V	171	ARG	CD-NE	7.64	1.56	1.46
4	d	48	ARG	CA-C	-7.64	1.43	1.52
6	f	182	ILE	CA-C	-7.64	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ARG	N-CA	-7.64	1.39	1.46
12	l	254	HIS	ND1-CE1	7.63	1.40	1.32
30	K	173	ASP	C-N	7.63	1.43	1.33
10	j	43	ILE	CA-CB	7.62	1.63	1.54
30	K	378	LEU	C-N	7.62	1.44	1.33
32	M	329	ARG	NE-CZ	7.62	1.41	1.33
22	S	139	HIS	C-N	7.62	1.43	1.33
21	N	813	ARG	C-N	7.62	1.44	1.34
1	a	153	SER	C-N	7.62	1.43	1.33
9	2	226	GLU	CA-C	-7.61	1.43	1.52
21	N	915	ALA	N-CA	-7.61	1.36	1.46
20	Z	517	ASP	CA-C	-7.60	1.43	1.52
22	S	110	LEU	N-CA	-7.60	1.36	1.45
32	M	341	GLY	C-N	7.60	1.44	1.33
1	A	74	CYS	C-N	7.59	1.43	1.33
31	L	120	LYS	C-N	7.59	1.43	1.33
30	K	89	ILE	CA-C	-7.59	1.43	1.52
8	h	96	TYR	CA-C	-7.59	1.43	1.52
32	M	243	PHE	CA-C	-7.59	1.43	1.53
22	S	68	LEU	C-N	7.59	1.41	1.32
6	f	183	ASP	CA-C	-7.58	1.43	1.52
24	Q	50	ARG	CD-NE	7.58	1.56	1.46
4	d	215	VAL	C-N	7.58	1.42	1.32
8	1	98	ASN	CA-CB	7.58	1.63	1.53
1	A	90	ALA	CA-C	-7.57	1.43	1.52
21	N	332	VAL	CA-C	-7.57	1.43	1.52
25	R	221	VAL	C-N	7.57	1.43	1.33
9	i	113	LYS	N-CA	-7.57	1.37	1.46
21	N	447	SER	N-CA	-7.57	1.37	1.46
12	l	145	GLU	CA-CB	7.56	1.64	1.54
2	b	142	PHE	CA-C	-7.55	1.42	1.52
28	H	238	LEU	C-N	7.55	1.43	1.32
10	3	190	ILE	CA-C	-7.55	1.43	1.52
22	S	301	PRO	CA-C	-7.55	1.43	1.52
4	D	45	GLY	CA-C	-7.54	1.45	1.51
27	O	219	ILE	CA-C	-7.54	1.43	1.52
24	Q	55	GLU	CA-CB	7.54	1.65	1.53
10	j	30	GLY	N-CA	-7.54	1.37	1.45
1	A	231	ASP	CA-CB	7.54	1.63	1.53
22	S	298	ARG	NE-CZ	7.54	1.41	1.33
7	g	121	GLN	N-CA	-7.53	1.37	1.46
21	N	741	TYR	CA-C	-7.53	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	122	HIS	ND1-CE1	7.53	1.40	1.32
3	C	114	ARG	CZ-NH2	7.53	1.43	1.33
21	N	617	VAL	CA-CB	-7.52	1.44	1.54
14	7	86	ILE	CA-C	-7.51	1.43	1.52
4	d	60	THR	CA-C	-7.51	1.45	1.53
4	d	119	ARG	CD-NE	7.51	1.56	1.46
9	i	253	GLN	CA-C	-7.50	1.42	1.52
11	4	190	ARG	CD-NE	7.50	1.56	1.46
31	L	118	ILE	CA-CB	-7.50	1.45	1.54
20	Z	56	LEU	CA-C	-7.49	1.45	1.53
11	4	173	PRO	CA-CB	-7.49	1.43	1.53
21	N	387	ALA	CA-C	-7.48	1.43	1.52
23	P	237	VAL	CA-C	-7.47	1.43	1.52
12	l	234	ARG	CD-NE	7.47	1.56	1.46
1	A	218	PHE	CA-C	-7.47	1.43	1.52
1	A	240	ASN	C-N	7.47	1.43	1.33
17	T	70	ILE	CA-C	-7.47	1.43	1.52
8	h	136	ALA	N-CA	-7.46	1.36	1.46
2	b	100	ILE	C-O	-7.46	1.16	1.24
21	N	778	LYS	CA-C	-7.46	1.42	1.52
9	i	236	ARG	CD-NE	7.46	1.56	1.46
4	d	213	THR	N-CA	-7.46	1.36	1.45
3	C	217	ARG	NE-CZ	7.46	1.41	1.33
6	F	161	ILE	CA-C	-7.46	1.44	1.52
22	S	46	LEU	C-N	7.45	1.44	1.33
14	7	176	ALA	N-CA	-7.45	1.36	1.46
22	S	114	TYR	N-CA	-7.45	1.36	1.45
1	a	135	ARG	CA-CB	7.44	1.64	1.54
7	g	87	HIS	CA-CB	7.44	1.65	1.53
13	m	122	LEU	CA-C	-7.44	1.43	1.52
22	S	261	HIS	CA-C	-7.44	1.43	1.52
10	j	187	VAL	CA-C	-7.44	1.43	1.52
31	L	177	GLU	CA-C	-7.44	1.42	1.52
32	M	154	LEU	CA-C	7.44	1.61	1.52
23	P	304	THR	CA-C	-7.43	1.43	1.53
5	e	188	HIS	ND1-CE1	7.43	1.40	1.32
8	h	110	GLY	CA-C	-7.43	1.43	1.51
23	P	189	LEU	CA-C	-7.43	1.42	1.52
5	e	249	ALA	N-CA	-7.42	1.36	1.46
10	j	91	VAL	CA-C	-7.42	1.43	1.52
4	D	215	VAL	CA-CB	-7.42	1.45	1.54
14	7	93	MET	CA-CB	7.42	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	702	LYS	N-CA	-7.42	1.37	1.46
22	S	332	PHE	CA-CB	7.42	1.64	1.53
33	J	337	LEU	C-N	7.42	1.43	1.33
4	D	172	ARG	CA-C	-7.42	1.43	1.52
10	3	190	ILE	CA-CB	-7.42	1.45	1.54
14	n	223	ARG	CA-CB	7.41	1.63	1.53
33	J	16	GLU	N-CA	-7.41	1.37	1.46
31	L	224	PRO	CA-CB	7.41	1.64	1.53
21	N	808	ALA	C-N	7.40	1.43	1.33
1	A	121	MET	N-CA	-7.40	1.37	1.46
29	I	394	ALA	C-N	7.40	1.43	1.33
33	J	371	ARG	CD-NE	7.39	1.56	1.46
10	j	199	TYR	CA-CB	7.39	1.64	1.53
16	V	20	ARG	NE-CZ	7.39	1.41	1.33
16	V	121	VAL	CA-CB	-7.39	1.44	1.54
7	G	151	LEU	CA-C	-7.38	1.43	1.52
21	N	890	PHE	CA-C	-7.38	1.43	1.52
14	n	111	ASN	N-CA	-7.38	1.38	1.46
10	3	70	LYS	CA-C	-7.38	1.43	1.52
26	U	87	GLU	N-CA	-7.38	1.37	1.46
29	I	133	LEU	CA-CB	7.37	1.66	1.53
31	L	357	ARG	NE-CZ	7.37	1.41	1.33
12	l	170	LEU	CA-C	-7.37	1.43	1.52
23	P	366	ASN	N-CA	7.37	1.55	1.46
20	Z	116	ALA	C-N	7.36	1.43	1.33
33	J	51	LEU	CA-C	7.36	1.62	1.52
6	f	51	ARG	NE-CZ	7.36	1.41	1.33
6	F	231	ALA	CA-C	-7.36	1.42	1.52
13	6	75	ARG	NE-CZ	7.36	1.41	1.33
25	R	72	VAL	N-CA	-7.35	1.37	1.46
2	b	97	TYR	N-CA	-7.35	1.38	1.46
24	Q	184	VAL	CA-CB	-7.35	1.45	1.54
33	J	195	LYS	CA-C	-7.35	1.43	1.52
33	J	200	ARG	NE-CZ	7.34	1.41	1.33
13	m	150	ALA	C-N	7.34	1.43	1.33
31	L	315	PHE	C-N	7.34	1.43	1.33
15	W	121	SER	C-N	7.34	1.43	1.33
15	W	170	HIS	CE1-NE2	7.34	1.39	1.32
21	N	463	TYR	CA-C	-7.34	1.43	1.52
31	L	264	ARG	NE-CZ	7.32	1.41	1.33
7	g	209	GLU	C-N	7.32	1.42	1.33
20	Z	727	GLU	CA-CB	7.32	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	513	ILE	CA-C	-7.32	1.43	1.52
24	Q	251	THR	N-CA	-7.31	1.37	1.46
13	m	120	ALA	N-CA	-7.31	1.36	1.45
1	A	80	GLY	N-CA	7.31	1.52	1.44
14	n	213	ALA	CA-C	-7.30	1.43	1.52
33	J	57	PHE	CA-C	-7.30	1.43	1.52
23	P	337	HIS	ND1-CE1	7.30	1.39	1.32
11	4	96	ARG	NE-CZ	7.30	1.41	1.33
21	N	130	ASP	CA-C	-7.30	1.45	1.53
21	N	477	SER	C-N	7.29	1.42	1.34
1	a	23	GLY	CA-C	-7.29	1.41	1.51
4	D	122	GLN	N-CA	-7.29	1.37	1.46
27	O	165	LEU	CA-C	-7.28	1.43	1.52
22	S	26	ALA	CA-C	7.28	1.62	1.52
22	S	271	ARG	NE-CZ	7.27	1.41	1.33
32	M	192	GLU	CA-CB	7.27	1.64	1.53
20	Z	156	HIS	ND1-CE1	7.27	1.39	1.32
32	M	336	ALA	CA-C	-7.27	1.43	1.52
4	d	90	ARG	CZ-NH2	7.26	1.42	1.33
13	6	99	ARG	NE-CZ	7.26	1.41	1.33
3	c	203	SER	N-CA	-7.26	1.37	1.45
21	N	769	PRO	CA-C	-7.26	1.46	1.53
10	3	13	VAL	CA-CB	-7.26	1.45	1.54
14	7	226	ARG	CD-NE	7.26	1.56	1.46
25	R	33	LEU	CA-C	-7.26	1.43	1.52
8	1	54	ARG	NE-CZ	7.26	1.41	1.33
32	M	41	ILE	CA-C	7.25	1.61	1.52
3	C	174	THR	CA-CB	-7.25	1.41	1.53
13	6	37	ASN	N-CA	-7.25	1.36	1.46
10	3	83	GLU	CA-C	-7.25	1.43	1.52
21	N	300	ASN	CA-CB	7.25	1.65	1.53
11	4	59	TYR	C-N	7.24	1.42	1.34
27	O	124	ASP	N-CA	-7.24	1.37	1.46
17	T	43	ASP	CA-C	-7.24	1.44	1.53
22	S	79	ASN	C-N	7.23	1.40	1.33
13	6	28	PHE	CA-CB	7.23	1.67	1.54
23	P	287	ASP	CA-CB	7.23	1.64	1.53
12	5	212	TYR	C-O	-7.23	1.15	1.24
24	Q	249	LEU	CA-C	-7.23	1.43	1.53
29	I	183	ASP	CA-C	-7.23	1.43	1.52
10	j	142	ALA	N-CA	-7.22	1.37	1.46
12	l	278	GLU	CA-C	-7.22	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	247	LEU	CA-CB	7.22	1.65	1.53
26	U	216	ASN	CA-CB	7.22	1.65	1.53
23	P	201	ARG	N-CA	-7.22	1.36	1.46
25	R	207	ARG	CD-NE	7.22	1.56	1.46
3	c	61	THR	CA-C	-7.21	1.44	1.52
26	U	212	ASP	CA-C	-7.21	1.43	1.52
2	b	55	LEU	N-CA	-7.21	1.36	1.46
5	E	136	ARG	N-CA	-7.21	1.39	1.45
6	F	205	SER	CA-C	-7.21	1.43	1.52
21	N	571	LEU	CA-CB	7.21	1.64	1.53
24	Q	368	LEU	C-N	7.20	1.43	1.33
33	J	180	ALA	N-CA	-7.20	1.36	1.46
20	Z	947	GLY	CA-C	-7.20	1.41	1.51
7	G	164	ALA	CA-C	-7.20	1.43	1.52
30	K	128	ARG	CZ-NH1	7.20	1.42	1.32
7	G	135	SER	CA-C	-7.20	1.43	1.52
17	T	167	GLY	N-CA	-7.20	1.34	1.45
4	D	58	ARG	CD-NE	7.19	1.56	1.46
28	H	162	ARG	CA-CB	7.19	1.65	1.54
29	I	291	ARG	CD-NE	7.19	1.56	1.46
14	7	133	MET	C-N	7.19	1.43	1.33
3	C	53	THR	CA-C	-7.18	1.43	1.52
32	M	344	ASP	CA-CB	7.17	1.65	1.53
28	H	107	LYS	CA-C	-7.17	1.44	1.52
10	3	99	ARG	CD-NE	7.17	1.56	1.46
21	N	597	ARG	N-CA	-7.17	1.36	1.46
23	P	223	LEU	CA-C	-7.17	1.43	1.52
22	S	490	ASN	CA-C	-7.17	1.43	1.52
17	T	97	SER	CA-C	-7.17	1.43	1.52
4	d	67	ILE	C-N	7.17	1.40	1.33
22	S	462	ASP	N-CA	-7.17	1.37	1.46
23	P	308	LEU	CA-C	-7.16	1.44	1.52
28	H	435	ARG	CD-NE	7.16	1.56	1.46
1	A	207	ILE	N-CA	-7.16	1.38	1.46
14	7	136	ARG	CD-NE	7.16	1.56	1.46
21	N	203	ARG	CD-NE	7.16	1.56	1.46
22	S	93	LEU	CA-CB	7.16	1.64	1.53
5	E	201	LEU	CA-C	-7.16	1.43	1.52
3	C	114	ARG	CD-NE	7.15	1.56	1.46
14	n	143	LEU	CA-CB	7.15	1.62	1.53
1	a	68	THR	CA-C	-7.15	1.43	1.52
10	3	18	LYS	CA-C	-7.15	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	80	ARG	CD-NE	7.15	1.56	1.46
12	5	133	TRP	N-CA	-7.14	1.37	1.46
32	M	45	ARG	CD-NE	7.14	1.56	1.46
27	O	164	PRO	N-CA	-7.14	1.38	1.47
4	D	64	VAL	CA-C	-7.13	1.44	1.52
7	g	35	THR	C-N	7.13	1.43	1.33
20	Z	574	TYR	N-CA	-7.13	1.36	1.46
30	K	121	ARG	NE-CZ	7.13	1.40	1.33
12	5	148	ARG	C-N	7.13	1.43	1.33
21	N	867	LYS	N-CA	-7.13	1.37	1.46
33	J	205	HIS	CB-CG	7.12	1.60	1.50
20	Z	261	ASP	CA-C	-7.12	1.43	1.52
9	2	106	VAL	C-N	7.12	1.43	1.33
17	T	144	TYR	CA-CB	7.12	1.63	1.53
8	h	86	THR	N-CA	-7.12	1.37	1.46
12	l	84	GLN	CA-CB	7.11	1.64	1.53
30	K	179	MET	CA-C	-7.11	1.43	1.52
21	N	17	GLN	N-CA	-7.10	1.37	1.46
28	H	409	ARG	CD-NE	7.10	1.56	1.46
7	g	7	GLY	CA-C	-7.10	1.45	1.52
15	W	170	HIS	ND1-CE1	7.10	1.39	1.32
21	N	896	PHE	C-N	7.10	1.44	1.33
3	c	18	ARG	CZ-NH2	7.10	1.42	1.33
3	c	5	ARG	NE-CZ	7.10	1.40	1.33
21	N	906	ARG	NE-CZ	7.10	1.40	1.33
32	M	277	ILE	CA-C	-7.10	1.43	1.52
20	Z	826	ARG	NE-CZ	7.10	1.40	1.33
12	l	143	LEU	N-CA	-7.09	1.37	1.46
21	N	606	VAL	CA-CB	7.09	1.62	1.54
6	f	66	CYS	CA-CB	7.09	1.64	1.53
4	D	85	LEU	N-CA	-7.09	1.37	1.46
6	F	220	THR	CA-C	7.09	1.60	1.52
5	E	49	GLY	N-CA	-7.09	1.37	1.45
20	Z	913	ILE	CB-CG1	7.09	1.67	1.53
2	B	209	ILE	N-CA	-7.09	1.38	1.46
27	O	213	LEU	CA-C	-7.09	1.43	1.52
19	Y	43	TRP	NE1-CE2	7.09	1.45	1.37
14	n	76	ILE	N-CA	-7.09	1.40	1.46
7	G	190	ARG	CD-NE	7.09	1.56	1.46
11	4	9	VAL	CA-CB	-7.09	1.44	1.54
27	O	308	LEU	CA-C	-7.09	1.43	1.52
31	L	54	ASN	CA-CB	7.09	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	112	ILE	CA-C	7.08	1.61	1.52
22	S	227	ASN	N-CA	-7.08	1.37	1.46
3	c	51	LYS	CA-C	-7.08	1.43	1.52
20	Z	551	LEU	CA-C	-7.08	1.43	1.52
12	l	104	GLN	CA-CB	7.08	1.64	1.53
32	M	281	ASP	C-N	7.08	1.42	1.33
13	m	215	VAL	CA-C	-7.07	1.43	1.52
7	G	123	HIS	CB-CG	-7.07	1.40	1.50
30	K	343	LEU	C-N	7.07	1.43	1.33
33	J	296	ARG	NE-CZ	7.07	1.40	1.33
15	W	162	ASN	CA-CB	7.06	1.61	1.53
33	J	38	THR	C-N	7.06	1.43	1.33
23	P	405	PRO	N-CA	-7.06	1.38	1.47
1	A	135	ARG	NE-CZ	7.05	1.40	1.33
33	J	6	THR	CA-C	-7.05	1.46	1.53
27	O	305	ILE	CA-CB	-7.05	1.46	1.54
23	P	127	GLU	CA-C	-7.04	1.42	1.52
27	O	276	LYS	C-N	7.04	1.41	1.33
6	f	100	ASN	CA-C	-7.04	1.44	1.53
21	N	56	SER	C-N	7.04	1.43	1.33
13	m	21	LEU	C-N	7.04	1.41	1.33
11	k	60	ILE	C-N	7.04	1.43	1.33
14	n	130	ALA	N-CA	-7.04	1.38	1.46
24	Q	50	ARG	NE-CZ	7.04	1.40	1.33
20	Z	312	TYR	CA-C	-7.04	1.43	1.52
30	K	65	GLU	C-N	7.04	1.43	1.33
5	E	60	GLU	CA-CB	7.03	1.61	1.53
16	V	103	MET	CA-C	-7.03	1.44	1.52
24	Q	136	SER	C-N	7.03	1.44	1.33
4	d	254	HIS	CE1-NE2	-7.03	1.25	1.32
1	a	71	TYR	C-N	7.03	1.42	1.33
7	G	170	GLN	CA-C	-7.03	1.43	1.52
7	G	87	HIS	ND1-CE1	7.03	1.39	1.32
32	M	45	ARG	CA-C	-7.03	1.43	1.52
27	O	60	ARG	NE-CZ	7.03	1.40	1.33
32	M	423	GLN	N-CA	-7.03	1.37	1.45
7	G	20	ARG	NE-CZ	7.02	1.40	1.33
7	g	188	SER	CA-C	-7.02	1.43	1.53
4	D	18	PHE	CA-C	-7.02	1.43	1.52
19	Y	3	THR	C-N	7.02	1.41	1.33
22	S	224	LYS	N-CA	-7.02	1.36	1.46
18	X	51	ARG	NE-CZ	7.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	241	ASP	CA-CB	7.01	1.64	1.53
20	Z	593	HIS	N-CA	7.01	1.53	1.46
10	j	37	SER	CA-C	-7.01	1.43	1.52
6	F	40	SER	CA-C	-7.01	1.43	1.52
25	R	239	THR	CA-C	-7.01	1.44	1.52
7	g	135	SER	CA-C	-7.01	1.44	1.52
21	N	253	LEU	N-CA	-7.01	1.38	1.46
21	N	462	VAL	N-CA	-7.01	1.38	1.46
20	Z	598	ALA	CA-C	-7.00	1.43	1.52
11	k	181	VAL	CA-C	-7.00	1.43	1.52
24	Q	409	TYR	CA-C	7.00	1.61	1.52
25	R	384	VAL	N-CA	-7.00	1.38	1.46
29	I	364	ILE	C-N	7.00	1.43	1.33
31	L	420	ARG	NE-CZ	7.00	1.40	1.33
32	M	90	GLU	C-N	7.00	1.43	1.33
5	e	208	MET	CA-CB	7.00	1.64	1.53
9	2	101	ARG	CD-NE	7.00	1.56	1.46
25	R	267	LYS	CA-C	-7.00	1.44	1.52
6	f	72	LEU	CA-CB	7.00	1.66	1.53
22	S	90	LYS	CA-C	-7.00	1.43	1.52
4	D	155	ILE	CA-CB	-6.99	1.45	1.54
28	H	131	GLN	CA-C	-6.99	1.43	1.52
7	g	55	THR	C-N	6.99	1.42	1.33
12	l	216	ASP	CA-C	-6.99	1.43	1.52
2	B	21	ILE	CA-CB	-6.99	1.46	1.54
22	S	206	GLN	CA-C	-6.99	1.42	1.52
8	1	124	LEU	C-N	6.99	1.42	1.33
13	6	132	SER	N-CA	-6.99	1.37	1.46
2	b	137	ALA	CA-C	-6.98	1.44	1.52
21	N	845	GLY	C-O	6.98	1.30	1.23
25	R	173	THR	N-CA	-6.98	1.38	1.46
21	N	839	ARG	NE-CZ	6.97	1.40	1.33
21	N	913	PRO	CA-C	-6.97	1.44	1.52
33	J	309	ARG	CZ-NH2	6.96	1.42	1.33
4	d	211	GLU	CA-C	-6.96	1.44	1.52
14	7	187	LEU	CA-C	-6.96	1.44	1.52
21	N	208	ARG	NE-CZ	6.96	1.40	1.33
28	H	206	VAL	CA-CB	-6.96	1.45	1.54
32	M	53	HIS	CE1-NE2	6.96	1.39	1.32
9	2	214	GLU	CA-C	-6.96	1.44	1.53
14	n	55	ILE	CA-C	-6.95	1.44	1.52
33	J	354	SER	N-CA	-6.95	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	25	GLU	CA-C	-6.95	1.44	1.52
11	k	95	ARG	N-CA	-6.95	1.36	1.46
15	W	68	GLU	C-N	6.95	1.44	1.33
21	N	58	ARG	CD-NE	6.95	1.55	1.46
23	P	401	ASN	CA-CB	6.95	1.61	1.53
29	I	296	SER	CA-CB	6.95	1.66	1.53
21	N	352	ASN	CA-CB	6.94	1.62	1.53
23	P	143	LEU	C-N	6.94	1.42	1.33
23	P	166	GLU	CA-C	-6.94	1.44	1.52
24	Q	383	ASP	CA-CB	6.94	1.64	1.53
10	j	105	VAL	CA-CB	6.94	1.63	1.55
13	m	213	LEU	CA-C	-6.93	1.44	1.52
8	1	73	GLU	CA-C	-6.93	1.44	1.52
10	j	165	GLU	N-CA	-6.93	1.38	1.46
4	D	50	SER	C-N	6.93	1.42	1.33
8	1	45	ARG	NE-CZ	6.93	1.40	1.33
25	R	331	ARG	CA-C	-6.93	1.44	1.52
30	K	399	ARG	NE-CZ	6.93	1.40	1.33
9	i	61	ALA	CA-C	-6.93	1.44	1.52
22	S	220	ILE	N-CA	-6.93	1.38	1.46
30	K	319	ASN	CA-CB	-6.93	1.43	1.53
9	i	216	LEU	CA-C	-6.92	1.44	1.53
12	l	167	GLY	C-N	6.92	1.42	1.33
5	E	205	LYS	CA-C	-6.92	1.43	1.52
2	B	155	SER	CA-C	-6.92	1.44	1.52
2	B	172	LYS	C-N	6.92	1.43	1.33
7	g	52	LYS	CA-CB	6.92	1.63	1.53
22	S	208	ILE	N-CA	6.92	1.54	1.46
29	I	384	LYS	C-N	6.92	1.42	1.33
9	i	141	SER	C-N	6.92	1.43	1.33
3	C	110	ILE	CA-CB	-6.92	1.45	1.54
9	2	242	LEU	N-CA	-6.92	1.38	1.46
25	R	128	LEU	CA-CB	6.92	1.64	1.53
12	l	182	LYS	C-N	6.92	1.43	1.33
4	D	75	PHE	CA-C	-6.91	1.44	1.52
27	O	269	LEU	C-N	6.91	1.42	1.34
21	N	798	LYS	C-N	6.91	1.43	1.34
9	i	231	SER	CA-C	-6.91	1.43	1.53
20	Z	511	PRO	C-N	6.91	1.39	1.33
16	V	37	MET	N-CA	-6.91	1.38	1.46
21	N	888	ASP	CA-C	6.91	1.61	1.52
11	k	140	THR	C-N	6.91	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	61	SER	CA-CB	6.91	1.65	1.53
27	O	56	PRO	N-CA	6.90	1.52	1.47
21	N	700	CYS	CA-C	-6.90	1.44	1.52
3	c	155	GLY	C-N	6.89	1.42	1.33
32	M	412	HIS	ND1-CE1	6.89	1.39	1.32
11	k	21	VAL	CA-CB	-6.89	1.45	1.54
13	m	33	GLY	C-N	6.89	1.42	1.33
30	K	151	PRO	CA-C	6.89	1.58	1.52
25	R	43	ARG	NE-CZ	6.89	1.40	1.33
13	m	142	GLU	CA-C	-6.88	1.44	1.52
31	L	193	LEU	CA-C	-6.88	1.43	1.52
22	S	130	VAL	N-CA	-6.88	1.39	1.46
33	J	89	GLN	CA-C	-6.88	1.44	1.52
13	6	11	ASN	C-N	6.88	1.40	1.33
15	W	137	VAL	N-CA	-6.88	1.38	1.46
7	g	99	PHE	C-N	6.88	1.43	1.33
33	J	85	LEU	CA-C	-6.87	1.44	1.52
26	U	176	ARG	CA-C	-6.87	1.43	1.52
3	c	40	ALA	CA-C	-6.87	1.44	1.52
8	h	39	VAL	N-CA	-6.87	1.37	1.46
10	j	39	LYS	CA-C	-6.87	1.44	1.52
11	k	96	ARG	CZ-NH1	6.87	1.42	1.32
14	7	124	TYR	CA-CB	6.87	1.64	1.53
21	N	711	ARG	NE-CZ	6.87	1.40	1.33
29	I	245	LEU	CA-C	-6.87	1.44	1.53
10	3	150	CYS	C-N	6.87	1.43	1.33
21	N	444	HIS	ND1-CE1	6.87	1.39	1.32
26	U	123	VAL	CA-CB	-6.87	1.45	1.53
29	I	160	LEU	CA-C	-6.87	1.44	1.53
30	K	205	PRO	CA-C	-6.87	1.48	1.51
7	G	194	LYS	N-CA	-6.86	1.38	1.46
6	F	189	LEU	CA-C	-6.86	1.43	1.52
21	N	185	ILE	CA-CB	-6.86	1.46	1.54
9	2	170	HIS	ND1-CE1	6.86	1.39	1.32
16	V	235	GLU	N-CA	-6.86	1.38	1.46
5	e	125	GLU	CA-C	-6.86	1.44	1.52
9	i	30	THR	C-N	6.86	1.43	1.33
2	B	184	GLU	CA-CB	6.86	1.64	1.53
13	6	44	ASN	C-N	6.85	1.43	1.33
3	c	220	ALA	CA-C	-6.85	1.44	1.52
13	6	71	ALA	N-CA	-6.85	1.38	1.46
18	X	28	PRO	N-CD	-6.85	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	240	ILE	CA-C	-6.85	1.44	1.52
7	g	51	GLU	N-CA	-6.85	1.37	1.46
2	b	234	ARG	C-N	6.84	1.42	1.33
11	k	101	ASN	CA-C	-6.84	1.44	1.52
12	5	242	ARG	CD-NE	6.84	1.55	1.46
21	N	345	ASP	CA-C	-6.84	1.44	1.52
20	Z	132	HIS	CG-ND1	-6.84	1.30	1.38
27	O	135	ARG	NE-CZ	6.84	1.40	1.33
30	K	251	PRO	C-N	6.84	1.43	1.33
6	F	129	GLY	CA-C	-6.84	1.42	1.51
32	M	213	ARG	NE-CZ	6.84	1.40	1.33
2	b	99	ARG	NE-CZ	6.84	1.40	1.33
11	4	67	TYR	CA-C	-6.84	1.43	1.52
14	7	182	HIS	ND1-CE1	6.83	1.39	1.32
21	N	889	ARG	CA-C	6.83	1.61	1.52
2	b	234	ARG	N-CA	-6.83	1.38	1.46
9	i	106	VAL	CA-C	-6.83	1.44	1.52
20	Z	110	ASN	CA-C	-6.83	1.44	1.52
12	5	127	CYS	C-N	6.83	1.42	1.33
28	H	100	ALA	C-N	6.83	1.42	1.33
7	G	70	VAL	CA-C	-6.82	1.44	1.52
31	L	180	PHE	CA-C	-6.82	1.44	1.52
13	m	150	ALA	CA-C	-6.82	1.43	1.52
10	3	65	GLU	C-N	6.82	1.43	1.33
14	7	147	ILE	CA-CB	-6.82	1.44	1.54
30	K	367	ASP	N-CA	-6.82	1.37	1.46
3	c	40	ALA	C-N	6.82	1.43	1.33
15	W	170	HIS	CA-C	-6.82	1.43	1.52
14	n	131	THR	CA-C	-6.81	1.44	1.52
8	1	194	ARG	CZ-NH1	6.81	1.42	1.32
7	g	190	ARG	NE-CZ	6.81	1.40	1.33
5	E	181	ALA	CA-C	-6.81	1.44	1.52
27	O	387	ARG	CA-CB	6.81	1.63	1.53
31	L	132	ARG	NE-CZ	6.81	1.40	1.33
31	L	332	THR	N-CA	-6.81	1.38	1.46
10	j	36	VAL	CA-C	-6.81	1.46	1.52
20	Z	951	GLN	CA-CB	6.81	1.64	1.53
6	f	143	HIS	ND1-CE1	6.80	1.39	1.32
9	i	154	LEU	CA-CB	6.80	1.65	1.53
4	D	66	LYS	CA-C	-6.80	1.44	1.52
24	Q	214	THR	C-N	6.80	1.42	1.33
6	F	138	ASP	C-N	6.80	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	202	MET	C-O	6.80	1.32	1.23
17	T	202	LEU	CA-CB	6.80	1.64	1.53
6	F	23	GLU	N-CA	-6.80	1.38	1.46
21	N	225	LEU	N-CA	-6.80	1.38	1.46
21	N	921	ARG	CD-NE	6.80	1.55	1.46
24	Q	213	GLN	CA-C	-6.80	1.44	1.52
31	L	342	ARG	NE-CZ	6.80	1.40	1.33
23	P	328	ALA	N-CA	-6.79	1.37	1.46
25	R	110	ILE	CA-C	-6.79	1.44	1.52
4	D	191	CYS	CA-C	-6.79	1.44	1.52
15	W	154	LEU	CA-CB	6.79	1.64	1.53
21	N	747	HIS	ND1-CE1	6.79	1.39	1.32
13	6	214	ILE	CA-C	-6.79	1.44	1.52
21	N	864	LYS	C-O	6.79	1.31	1.24
7	g	184	PRO	N-CA	-6.79	1.38	1.47
11	k	20	ALA	CA-C	-6.78	1.44	1.52
30	K	66	ASP	CA-C	6.78	1.61	1.52
4	d	42	VAL	C-O	-6.78	1.17	1.24
12	5	77	THR	CA-C	-6.78	1.44	1.52
3	C	77	VAL	CA-C	-6.78	1.44	1.52
11	4	47	ALA	N-CA	-6.78	1.37	1.45
15	W	194	GLU	CA-C	-6.78	1.44	1.52
28	H	168	ILE	N-CA	-6.78	1.38	1.46
9	i	129	VAL	CA-C	-6.77	1.44	1.52
10	j	196	VAL	CA-CB	-6.77	1.45	1.54
2	B	156	TYR	CA-C	-6.77	1.44	1.52
21	N	674	GLN	CA-C	-6.77	1.44	1.52
7	g	107	ILE	N-CA	-6.77	1.38	1.46
31	L	64	LEU	CA-CB	6.77	1.64	1.53
26	U	158	PRO	N-CA	-6.77	1.39	1.47
28	H	140	ASP	CA-C	-6.77	1.46	1.53
7	G	24	VAL	C-N	6.76	1.42	1.33
28	H	192	ASP	CA-C	-6.76	1.44	1.52
13	m	144	CYS	N-CA	-6.76	1.38	1.46
21	N	585	ARG	CZ-NH1	6.76	1.42	1.32
4	D	120	TYR	C-N	6.76	1.42	1.33
9	2	140	PHE	CA-C	-6.76	1.44	1.52
29	I	262	ARG	CZ-NH1	6.76	1.42	1.32
29	I	355	LEU	CA-C	6.76	1.61	1.52
16	V	55	GLY	CA-C	-6.76	1.42	1.51
33	J	35	ARG	CD-NE	6.76	1.55	1.46
2	b	199	SER	CA-C	-6.76	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	89	SER	CA-C	6.76	1.61	1.52
11	k	192	VAL	C-N	6.76	1.42	1.33
11	k	2	ASP	C-N	6.75	1.44	1.33
12	5	80	ALA	CA-C	-6.75	1.44	1.52
20	Z	524	ALA	CA-C	-6.75	1.44	1.52
25	R	42	GLN	N-CA	-6.75	1.38	1.46
27	O	204	SER	CA-C	-6.75	1.44	1.52
6	F	152	ASN	CA-C	-6.75	1.44	1.52
5	e	168	ASN	C-N	6.75	1.41	1.33
29	I	246	ARG	CD-NE	6.75	1.55	1.46
3	c	143	ARG	CZ-NH2	6.75	1.42	1.33
4	d	147	LEU	N-CA	-6.75	1.38	1.46
10	3	31	SER	N-CA	6.74	1.54	1.46
17	T	8	THR	CA-C	-6.74	1.43	1.52
21	N	343	THR	CA-C	-6.74	1.44	1.52
20	Z	948	TRP	CE2-CZ2	6.74	1.54	1.39
23	P	148	LYS	CA-C	-6.74	1.44	1.52
25	R	146	ASP	C-N	6.74	1.43	1.33
26	U	68	LEU	N-CA	-6.74	1.37	1.46
3	C	202	ASP	C-N	6.74	1.43	1.33
27	O	273	GLN	C-N	6.74	1.42	1.33
29	I	313	LEU	N-CA	-6.74	1.38	1.46
4	d	120	TYR	CA-C	-6.73	1.44	1.52
7	G	232	LYS	CA-C	-6.73	1.44	1.52
23	P	115	ARG	CD-NE	6.73	1.55	1.46
4	D	156	TYR	CA-C	-6.73	1.44	1.52
6	F	74	LEU	CA-C	-6.73	1.44	1.52
11	4	177	LYS	CA-C	-6.73	1.44	1.53
21	N	31	VAL	CA-CB	6.73	1.62	1.54
6	F	179	PHE	CA-C	-6.73	1.43	1.52
13	m	211	GLU	CA-C	-6.73	1.44	1.52
31	L	393	ASN	N-CA	-6.73	1.38	1.46
15	W	164	PRO	N-CA	-6.72	1.39	1.47
9	2	122	HIS	CA-C	-6.72	1.43	1.52
31	L	69	ARG	NE-CZ	6.72	1.40	1.33
8	1	85	GLU	C-N	6.72	1.42	1.33
33	J	223	ILE	C-N	6.72	1.42	1.33
20	Z	798	ARG	CZ-NH1	6.72	1.42	1.32
22	S	421	TYR	CA-C	6.72	1.61	1.52
3	c	143	ARG	NE-CZ	6.71	1.40	1.33
5	e	179	ALA	CA-C	-6.71	1.44	1.52
31	L	220	LEU	CA-C	-6.71	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	39	ARG	NE-CZ	6.71	1.40	1.33
20	Z	545	SER	CA-CB	6.71	1.64	1.53
4	d	224	LEU	CA-C	-6.71	1.44	1.52
11	k	85	ARG	CD-NE	6.71	1.55	1.46
14	7	205	VAL	CA-C	-6.71	1.44	1.52
21	N	298	TYR	N-CA	-6.71	1.37	1.46
26	U	122	ILE	C-N	6.71	1.42	1.33
20	Z	55	ARG	NE-CZ	6.70	1.40	1.33
7	G	207	ASN	N-CA	-6.70	1.38	1.46
1	A	243	GLU	CA-C	-6.70	1.44	1.52
30	K	400	TYR	CA-C	-6.70	1.47	1.52
4	D	41	CYS	CA-C	-6.70	1.44	1.52
30	K	260	LEU	N-CA	-6.70	1.38	1.46
12	l	128	GLN	N-CA	-6.69	1.38	1.46
4	D	7	ALA	CA-C	-6.69	1.44	1.52
20	Z	534	PHE	C-N	6.69	1.42	1.33
33	J	253	ILE	C-N	6.69	1.41	1.33
21	N	473	ASP	N-CA	-6.69	1.37	1.46
30	K	88	ARG	CZ-NH1	6.69	1.42	1.32
2	b	191	ILE	N-CA	6.69	1.54	1.46
13	m	103	HIS	CE1-NE2	6.69	1.39	1.32
3	C	75	VAL	N-CA	-6.68	1.38	1.46
2	b	236	ARG	C-N	6.68	1.42	1.33
18	X	63	PRO	C-N	6.68	1.42	1.33
27	O	61	LEU	CA-CB	6.68	1.63	1.53
27	O	163	ILE	C-N	6.68	1.41	1.33
32	M	268	ALA	N-CA	6.68	1.54	1.46
4	d	83	ARG	CD-NE	6.68	1.55	1.46
25	R	223	ASN	N-CA	-6.68	1.37	1.46
1	a	187	LYS	C-N	6.68	1.43	1.33
4	D	42	VAL	N-CA	-6.68	1.38	1.46
2	b	209	ILE	CA-C	-6.68	1.44	1.52
26	U	239	LEU	C-N	6.68	1.42	1.33
32	M	316	SER	C-N	6.68	1.43	1.33
8	1	88	ALA	C-N	6.67	1.43	1.34
11	4	68	SER	CA-C	-6.67	1.44	1.52
25	R	124	ASP	CA-CB	6.67	1.64	1.53
7	G	187	LEU	C-O	-6.67	1.15	1.24
19	Y	1	MET	SD-CE	6.67	1.96	1.79
28	H	390	ARG	NE-CZ	6.67	1.40	1.33
5	e	80	GLY	C-O	-6.67	1.19	1.24
14	n	95	HIS	CG-CD2	6.67	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	130	ILE	C-N	6.67	1.42	1.33
20	Z	26	ASN	C-N	6.67	1.42	1.33
20	Z	249	MET	C-N	6.67	1.42	1.33
20	Z	849	ARG	CZ-NH1	6.67	1.42	1.32
21	N	547	LEU	N-CA	-6.67	1.37	1.46
25	R	29	LYS	N-CA	-6.67	1.38	1.46
7	g	199	ILE	C-N	6.67	1.42	1.33
5	e	136	ARG	CD-NE	6.66	1.55	1.46
6	f	3	ARG	NE-CZ	6.66	1.40	1.33
30	K	258	PHE	CA-CB	6.66	1.63	1.53
33	J	403	LEU	N-CA	-6.66	1.37	1.46
3	C	41	SER	CA-CB	6.66	1.64	1.53
27	O	88	ASP	CA-C	-6.66	1.43	1.52
1	A	236	LEU	CA-C	-6.66	1.44	1.52
8	1	31	THR	C-N	6.66	1.43	1.33
26	U	227	GLY	C-N	6.66	1.43	1.33
17	T	237	ASN	CA-CB	6.65	1.63	1.53
13	m	57	ASN	CA-C	-6.65	1.44	1.53
32	M	279	PHE	CA-C	-6.65	1.44	1.52
16	V	198	SER	C-N	6.65	1.41	1.33
17	T	202	LEU	C-O	-6.65	1.16	1.24
22	S	148	ASP	N-CA	-6.65	1.38	1.46
8	h	45	ARG	CD-NE	6.64	1.55	1.46
21	N	559	TYR	CA-CB	6.64	1.62	1.53
20	Z	360	SER	C-N	6.64	1.43	1.33
21	N	528	ARG	CA-C	-6.64	1.43	1.52
2	B	187	ASP	C-N	6.64	1.42	1.34
2	B	225	THR	CA-C	-6.64	1.44	1.52
17	T	224	ARG	CA-C	-6.64	1.43	1.52
29	I	356	SER	CA-CB	6.64	1.63	1.53
13	m	221	ARG	CZ-NH1	6.64	1.42	1.32
30	K	123	LEU	N-CA	-6.64	1.38	1.46
17	T	104	LYS	CA-C	-6.63	1.44	1.52
29	I	388	SER	CA-C	-6.63	1.43	1.52
6	F	31	GLN	C-N	6.63	1.42	1.33
12	5	249	SER	CA-C	-6.63	1.44	1.52
9	2	164	MET	CA-CB	6.63	1.63	1.53
14	7	81	ASN	CA-C	-6.63	1.43	1.52
30	K	352	ILE	C-N	6.62	1.43	1.33
26	U	94	HIS	CG-ND1	6.62	1.45	1.38
29	I	181	TYR	CA-CB	6.62	1.63	1.53
33	J	202	VAL	C-N	6.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	7	ALA	N-CA	-6.62	1.37	1.46
28	H	373	ARG	CD-NE	6.62	1.55	1.46
21	N	375	HIS	CA-C	-6.62	1.43	1.52
27	O	210	ARG	CA-C	-6.61	1.44	1.52
3	c	129	ARG	NE-CZ	6.61	1.40	1.33
9	2	83	ALA	CA-C	-6.61	1.44	1.52
21	N	43	LEU	N-CA	-6.61	1.39	1.46
2	B	43	VAL	N-CA	-6.61	1.38	1.46
3	C	240	VAL	C-N	6.61	1.42	1.33
14	7	161	ARG	CD-NE	6.61	1.55	1.46
11	k	84	VAL	CA-CB	6.61	1.62	1.54
6	F	126	ARG	CA-C	-6.61	1.45	1.53
11	4	102	VAL	CA-C	-6.61	1.44	1.52
4	d	169	LYS	C-O	6.60	1.31	1.24
6	f	104	ALA	C-N	6.60	1.42	1.33
22	S	484	ASP	CA-C	-6.60	1.44	1.52
2	B	211	LEU	N-CA	-6.60	1.37	1.46
10	3	63	LEU	C-N	6.60	1.42	1.33
7	g	183	HIS	N-CA	-6.60	1.36	1.46
16	V	45	VAL	CA-CB	-6.60	1.45	1.54
29	I	290	LYS	CA-C	6.60	1.61	1.52
30	K	358	SER	N-CA	-6.60	1.38	1.46
29	I	219	VAL	N-CA	-6.60	1.38	1.46
12	l	182	LYS	CA-CB	6.59	1.62	1.53
16	V	304	ALA	CA-C	-6.59	1.44	1.52
21	N	705	ILE	CA-C	-6.59	1.44	1.52
23	P	123	ARG	NE-CZ	6.59	1.40	1.33
4	D	20	VAL	C-N	6.59	1.42	1.33
20	Z	430	LEU	N-CA	-6.59	1.38	1.46
32	M	284	ASP	C-N	6.59	1.43	1.33
10	j	123	GLY	CA-C	-6.59	1.46	1.52
13	6	83	TYR	CA-CB	6.59	1.63	1.53
23	P	300	VAL	CA-CB	-6.58	1.46	1.54
1	a	83	VAL	CA-C	6.58	1.60	1.52
12	l	196	ARG	NE-CZ	6.58	1.40	1.33
7	g	196	ALA	C-N	6.58	1.42	1.33
1	A	230	LYS	CA-C	-6.58	1.44	1.52
8	1	110	GLY	C-N	6.58	1.42	1.33
24	Q	415	LEU	CA-CB	6.58	1.63	1.53
8	1	38	ARG	NE-CZ	6.57	1.40	1.33
12	5	110	ILE	CA-C	-6.57	1.44	1.52
25	R	209	ARG	CD-NE	6.57	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	492	GLY	CA-C	-6.57	1.43	1.51
31	L	71	ASP	N-CA	-6.57	1.38	1.46
32	M	374	ILE	CA-C	-6.57	1.45	1.52
11	4	64	ILE	CA-C	-6.57	1.44	1.52
18	X	46	TRP	CA-CB	6.57	1.62	1.53
29	I	106	ILE	C-N	6.57	1.41	1.33
33	J	81	ASP	CA-C	-6.57	1.44	1.52
29	I	204	HIS	CA-C	-6.56	1.44	1.52
30	K	291	GLU	C-N	6.56	1.42	1.34
6	F	110	HIS	ND1-CE1	6.56	1.39	1.32
30	K	252	ARG	CZ-NH1	6.56	1.42	1.32
8	1	110	GLY	N-CA	-6.56	1.38	1.45
21	N	340	HIS	CA-CB	6.56	1.62	1.53
31	L	364	HIS	CD2-NE2	6.56	1.45	1.37
20	Z	801	HIS	CB-CG	-6.56	1.41	1.50
4	d	32	CYS	C-N	6.55	1.42	1.33
10	3	46	TYR	CA-C	-6.55	1.44	1.52
25	R	390	THR	CA-C	-6.55	1.44	1.52
1	A	194	ILE	CA-C	-6.55	1.45	1.52
20	Z	935	THR	C-N	6.55	1.41	1.33
26	U	236	LEU	CA-CB	6.55	1.63	1.52
17	T	210	PHE	CA-CB	6.55	1.63	1.53
30	K	49	PHE	N-CA	6.55	1.54	1.46
33	J	198	LEU	CA-C	-6.55	1.44	1.52
21	N	637	ALA	CA-C	-6.54	1.44	1.52
20	Z	904	LEU	CA-C	-6.54	1.46	1.52
22	S	261	HIS	N-CA	-6.54	1.37	1.46
6	f	128	TYR	CA-C	-6.54	1.44	1.53
5	e	174	SER	N-CA	-6.54	1.38	1.46
1	A	75	ILE	C-N	6.54	1.41	1.33
33	J	348	GLU	CA-C	-6.54	1.44	1.52
9	i	64	HIS	CA-C	-6.53	1.44	1.52
4	D	111	ARG	NE-CZ	6.53	1.40	1.33
4	D	174	PHE	CA-CB	6.53	1.63	1.53
20	Z	44	LYS	C-N	6.53	1.42	1.33
20	Z	774	ARG	NE-CZ	6.53	1.40	1.33
23	P	218	LEU	CA-C	-6.53	1.44	1.52
29	I	319	ARG	N-CA	-6.53	1.38	1.45
10	3	22	ALA	CA-C	-6.53	1.44	1.52
32	M	34	ALA	C-N	6.53	1.43	1.34
33	J	394	GLN	CA-CB	6.53	1.63	1.53
8	h	47	HIS	CA-C	-6.53	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	124	SER	CA-C	-6.53	1.45	1.52
4	D	161	ALA	C-N	6.53	1.41	1.33
22	S	428	ARG	CZ-NH2	6.53	1.42	1.33
24	Q	149	LYS	CA-C	-6.53	1.44	1.53
1	a	188	LYS	CA-CB	6.53	1.63	1.53
14	n	258	ILE	CA-C	-6.52	1.46	1.53
14	n	45	ILE	CA-C	-6.52	1.44	1.52
10	3	168	SER	N-CA	-6.52	1.38	1.46
30	K	310	THR	C-N	6.52	1.42	1.33
4	d	159	TRP	CA-C	-6.52	1.44	1.52
27	O	71	ASP	N-CA	-6.52	1.38	1.46
32	M	232	ALA	N-CA	-6.52	1.38	1.46
10	j	77	LYS	N-CA	6.52	1.54	1.46
13	m	99	ARG	C-N	6.52	1.42	1.33
2	b	243	ILE	C-N	6.51	1.42	1.33
12	l	119	THR	CA-C	-6.51	1.44	1.52
11	4	153	THR	N-CA	-6.51	1.37	1.46
33	J	229	MET	CA-C	-6.51	1.43	1.52
10	j	105	VAL	CA-C	-6.51	1.44	1.52
7	G	206	ASP	CA-C	-6.51	1.44	1.52
28	H	154	LYS	N-CA	-6.51	1.38	1.46
30	K	336	ARG	CA-CB	6.51	1.62	1.53
32	M	331	ASP	CA-C	-6.51	1.44	1.53
20	Z	573	LEU	C-N	-6.50	1.25	1.33
1	a	87	ILE	CA-C	6.50	1.58	1.52
13	6	21	LEU	C-N	6.50	1.41	1.32
23	P	50	SER	CA-C	-6.50	1.43	1.52
3	C	150	THR	N-CA	-6.50	1.37	1.45
1	A	15	HIS	CA-C	-6.50	1.44	1.52
5	E	53	ARG	NE-CZ	6.50	1.40	1.33
10	3	183	TRP	CA-C	-6.50	1.44	1.52
7	g	214	LEU	N-CA	-6.50	1.38	1.46
2	B	60	THR	CA-CB	6.50	1.63	1.53
3	C	82	ALA	CA-C	-6.49	1.44	1.52
12	l	267	ASP	C-N	6.49	1.42	1.33
26	U	18	ALA	C-N	6.49	1.42	1.33
10	j	98	ARG	CA-C	-6.49	1.44	1.52
12	5	100	TRP	N-CA	6.49	1.54	1.45
11	4	163	LEU	CA-C	6.49	1.61	1.52
12	5	124	ALA	CA-C	-6.49	1.44	1.52
21	N	566	SER	CA-CB	6.49	1.63	1.53
25	R	207	ARG	CZ-NH2	6.49	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	221	ILE	CA-CB	6.49	1.61	1.53
32	M	318	ASP	CA-C	-6.49	1.44	1.52
32	M	430	VAL	N-CA	6.49	1.53	1.46
21	N	259	PHE	CA-CB	6.48	1.63	1.53
21	N	193	ALA	N-CA	-6.48	1.38	1.46
32	M	411	LYS	CA-C	-6.48	1.44	1.52
33	J	389	VAL	CA-CB	6.48	1.62	1.54
2	b	115	ALA	N-CA	-6.48	1.38	1.46
23	P	185	GLU	CA-C	-6.48	1.44	1.52
24	Q	66	VAL	CA-C	-6.48	1.43	1.52
4	d	111	ARG	CA-CB	6.48	1.63	1.53
13	6	179	PRO	CA-C	-6.48	1.43	1.52
20	Z	885	ALA	C-N	6.48	1.41	1.33
22	S	382	ARG	CZ-NH2	6.48	1.41	1.33
23	P	264	ILE	CA-CB	6.48	1.62	1.54
25	R	263	ARG	C-N	6.48	1.42	1.33
20	Z	767	TYR	C-N	6.47	1.42	1.34
23	P	171	MET	CA-CB	6.47	1.62	1.53
16	V	141	VAL	CA-C	-6.47	1.44	1.52
17	T	138	ASP	C-N	6.47	1.42	1.33
23	P	69	ARG	N-CA	-6.47	1.38	1.46
7	g	169	ARG	CD-NE	6.47	1.55	1.46
17	T	91	SER	CA-C	-6.47	1.45	1.52
4	D	151	GLU	N-CA	-6.47	1.39	1.45
7	G	86	ARG	NE-CZ	6.47	1.40	1.33
25	R	389	GLU	CA-C	6.47	1.61	1.53
14	n	257	ASP	C-N	6.47	1.39	1.33
30	K	158	ILE	CA-CB	-6.47	1.47	1.54
21	N	804	LEU	CA-CB	6.46	1.63	1.53
6	f	89	ARG	CA-C	-6.46	1.44	1.52
6	F	88	LEU	C-N	6.46	1.42	1.33
11	k	21	VAL	C-N	6.46	1.42	1.33
29	I	227	THR	C-N	6.46	1.41	1.33
15	W	47	ASN	CA-CB	6.46	1.61	1.53
22	S	57	LEU	N-CA	-6.46	1.38	1.46
23	P	76	ASN	CA-CB	6.46	1.63	1.53
24	Q	308	ASN	C-N	6.45	1.43	1.33
20	Z	316	ALA	CA-C	-6.45	1.44	1.52
2	B	179	TRP	NE1-CE2	6.45	1.44	1.37
22	S	55	ARG	NE-CZ	6.45	1.40	1.33
13	6	145	ARG	CZ-NH2	6.45	1.41	1.33
31	L	305	LEU	C-N	6.45	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	60	VAL	C-N	6.44	1.41	1.33
20	Z	538	CYS	C-N	6.44	1.42	1.33
20	Z	42	ASP	C-N	6.44	1.42	1.33
20	Z	489	ALA	N-CA	-6.44	1.38	1.46
26	U	269	THR	CA-C	-6.44	1.44	1.52
2	b	227	ILE	C-N	6.44	1.40	1.34
19	Y	83	ARG	NE-CZ	6.44	1.40	1.33
31	L	370	LYS	CA-C	-6.44	1.45	1.52
33	J	287	ASN	CA-C	6.44	1.60	1.52
33	J	299	ILE	CA-CB	-6.44	1.46	1.54
18	X	124	LYS	CA-C	-6.44	1.44	1.52
20	Z	516	THR	C-N	6.44	1.42	1.33
24	Q	370	THR	C-N	6.44	1.42	1.33
15	W	178	PRO	CA-C	6.44	1.58	1.52
15	W	120	ASP	N-CA	-6.43	1.37	1.45
33	J	166	LEU	CA-C	6.43	1.60	1.52
33	J	357	ASP	CA-C	-6.43	1.44	1.52
10	j	131	ASP	CA-CB	6.43	1.63	1.53
13	m	113	TYR	CA-C	-6.43	1.44	1.53
8	1	25	ALA	N-CA	-6.43	1.38	1.46
24	Q	102	GLU	CA-CB	6.43	1.63	1.53
28	H	346	ARG	C-N	6.43	1.41	1.33
13	m	220	VAL	CA-C	6.43	1.60	1.52
5	E	212	LEU	CA-C	-6.43	1.44	1.52
20	Z	244	ARG	NE-CZ	6.43	1.40	1.33
20	Z	513	ALA	CA-CB	6.43	1.64	1.53
31	L	359	GLU	C-N	6.43	1.42	1.33
12	5	177	CYS	N-CA	-6.43	1.38	1.46
22	S	225	HIS	CE1-NE2	6.43	1.39	1.32
2	B	94	HIS	ND1-CE1	6.42	1.39	1.32
16	V	141	VAL	CA-CB	-6.42	1.46	1.54
9	2	253	GLN	CA-CB	6.42	1.63	1.53
21	N	14	ARG	CD-NE	6.42	1.55	1.46
11	k	90	LYS	C-N	6.42	1.42	1.34
2	B	107	THR	CA-CB	-6.42	1.43	1.53
4	d	188	VAL	N-CA	-6.42	1.38	1.46
6	F	41	ASN	CA-C	-6.42	1.44	1.52
12	5	195	THR	CA-CB	-6.42	1.43	1.53
20	Z	53	VAL	CA-CB	6.42	1.62	1.54
11	4	50	ALA	C-N	6.42	1.42	1.33
20	Z	189	ALA	CA-CB	6.42	1.63	1.54
22	S	271	ARG	C-N	6.42	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	69	ARG	C-N	6.42	1.42	1.33
5	e	119	LEU	C-N	6.42	1.42	1.34
9	i	161	LEU	CA-C	6.41	1.61	1.52
1	A	187	LYS	N-CA	-6.41	1.38	1.46
11	k	70	ARG	CA-CB	6.41	1.63	1.53
28	H	374	LYS	CA-C	-6.41	1.44	1.52
2	b	224	TYR	CA-C	-6.41	1.44	1.52
5	E	192	THR	CA-C	6.41	1.60	1.52
7	g	112	PHE	CA-C	-6.41	1.44	1.52
19	Y	27	LYS	C-N	6.41	1.42	1.33
22	S	171	TYR	N-CA	-6.41	1.38	1.46
20	Z	966	GLU	N-CA	6.41	1.53	1.46
10	j	40	PHE	CA-CB	6.41	1.61	1.53
10	j	152	SER	N-CA	-6.41	1.38	1.46
15	W	77	HIS	ND1-CE1	6.41	1.39	1.32
20	Z	710	SER	CA-CB	6.41	1.63	1.53
21	N	88	ARG	NE-CZ	6.41	1.40	1.33
29	I	413	ALA	CA-C	-6.41	1.44	1.52
22	S	141	LEU	C-N	6.40	1.41	1.33
23	P	294	GLU	C-N	6.40	1.43	1.33
6	f	3	ARG	CZ-NH2	6.40	1.41	1.33
11	k	77	PRO	C-N	6.40	1.42	1.33
9	2	121	GLY	N-CA	6.40	1.53	1.45
18	X	64	ILE	CA-C	-6.40	1.44	1.52
24	Q	138	SER	N-CA	-6.40	1.38	1.46
20	Z	417	SER	C-N	6.40	1.42	1.33
29	I	151	HIS	ND1-CE1	6.40	1.39	1.32
27	O	23	HIS	C-N	6.39	1.42	1.34
12	l	265	ASN	CA-C	-6.39	1.45	1.52
16	V	189	ILE	C-N	6.39	1.42	1.33
33	J	66	GLN	C-O	6.39	1.32	1.24
7	G	91	ARG	CZ-NH2	6.39	1.41	1.33
11	4	183	ILE	CA-C	-6.39	1.44	1.52
20	Z	773	ARG	NE-CZ	6.39	1.40	1.33
4	d	228	GLU	CA-CB	6.39	1.63	1.53
10	3	194	GLU	C-N	6.39	1.42	1.33
10	3	34	LEU	CA-C	-6.39	1.44	1.52
8	1	59	ALA	N-CA	-6.39	1.38	1.46
9	2	111	MET	C-N	6.39	1.42	1.33
20	Z	187	SER	CA-C	-6.39	1.44	1.52
20	Z	533	VAL	CA-CB	6.39	1.62	1.54
27	O	250	TRP	CD2-CE3	-6.39	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	183	ILE	CA-CB	-6.39	1.46	1.54
15	W	69	PHE	N-CA	-6.38	1.37	1.46
1	a	245	LEU	CA-CB	6.38	1.63	1.53
28	H	375	VAL	N-CA	-6.38	1.38	1.46
32	M	342	ARG	NE-CZ	6.38	1.40	1.33
20	Z	101	SER	CA-C	-6.38	1.43	1.52
8	h	67	ILE	CA-CB	-6.38	1.46	1.54
9	2	249	ILE	CA-C	-6.38	1.44	1.52
20	Z	338	HIS	C-N	6.38	1.42	1.33
30	K	44	ASN	N-CA	6.38	1.54	1.46
14	7	220	ARG	NE-CZ	6.37	1.40	1.33
21	N	184	LYS	CA-C	-6.37	1.44	1.52
27	O	184	ASP	N-CA	-6.37	1.38	1.46
31	L	214	PRO	C-N	6.37	1.41	1.33
9	2	190	ALA	C-N	6.37	1.42	1.33
4	D	90	ARG	CD-NE	6.37	1.55	1.46
4	D	235	GLN	CA-C	-6.37	1.44	1.52
9	2	106	VAL	N-CA	-6.37	1.39	1.46
20	Z	892	SER	CA-C	-6.37	1.46	1.53
21	N	664	LEU	C-N	6.37	1.41	1.33
2	b	133	SER	CA-C	-6.36	1.44	1.52
1	A	78	THR	C-N	6.36	1.41	1.33
2	b	83	ARG	C-N	6.36	1.41	1.33
21	N	47	GLU	C-N	6.36	1.42	1.34
10	3	196	VAL	N-CA	-6.36	1.38	1.46
16	V	295	VAL	C-N	6.36	1.42	1.33
7	G	112	PHE	CA-CB	6.35	1.63	1.53
28	H	364	ALA	C-N	6.35	1.42	1.34
13	6	181	LYS	N-CA	-6.35	1.38	1.46
23	P	349	ASN	CA-C	-6.35	1.44	1.52
2	b	88	LYS	C-N	6.35	1.42	1.33
13	m	58	ILE	C-N	6.35	1.41	1.33
13	m	129	ALA	C-N	6.35	1.42	1.33
20	Z	941	ARG	CZ-NH2	6.35	1.41	1.33
24	Q	24	GLU	CA-CB	6.35	1.63	1.53
31	L	148	LEU	N-CA	-6.35	1.38	1.45
10	j	192	LYS	N-CA	-6.35	1.38	1.46
16	V	194	ARG	CA-CB	6.35	1.64	1.53
22	S	327	ILE	C-N	6.35	1.41	1.33
25	R	302	ALA	N-CA	-6.35	1.37	1.46
32	M	42	ARG	CZ-NH2	6.35	1.41	1.33
10	3	29	LEU	CA-C	-6.35	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	209	GLU	C-N	6.35	1.42	1.33
8	h	197	PHE	N-CA	-6.34	1.38	1.46
22	S	403	SER	CA-C	-6.34	1.44	1.52
11	k	64	ILE	C-N	6.34	1.42	1.33
14	7	105	THR	CA-CB	-6.34	1.43	1.53
19	Y	53	ALA	C-N	6.34	1.41	1.33
24	Q	164	GLU	CA-C	-6.34	1.44	1.52
24	Q	218	LEU	CA-CB	6.34	1.63	1.53
28	H	358	PRO	CA-C	-6.34	1.46	1.52
33	J	221	LYS	CA-C	-6.34	1.44	1.52
14	n	95	HIS	CD2-NE2	6.34	1.44	1.37
5	E	179	ALA	CA-C	-6.34	1.44	1.52
5	e	99	HIS	C-N	6.34	1.42	1.34
14	n	202	THR	CA-C	-6.34	1.44	1.52
4	D	6	ARG	CZ-NH2	6.34	1.41	1.33
12	5	180	THR	CA-C	-6.34	1.44	1.53
16	V	275	ASP	CA-CB	6.34	1.62	1.53
31	L	209	ARG	CD-NE	6.34	1.55	1.46
5	E	78	MET	CA-C	-6.33	1.44	1.52
10	3	177	ARG	NE-CZ	6.33	1.40	1.33
4	d	134	LEU	CA-C	-6.33	1.45	1.52
5	e	72	ARG	CA-CB	6.33	1.62	1.53
12	l	196	ARG	C-N	6.33	1.42	1.33
24	Q	39	SER	CA-CB	6.33	1.64	1.53
4	D	192	VAL	CA-CB	-6.33	1.46	1.54
24	Q	322	GLU	C-N	6.33	1.42	1.33
13	6	51	VAL	CA-CB	-6.33	1.46	1.54
23	P	249	ALA	N-CA	6.33	1.53	1.46
30	K	122	ILE	N-CA	-6.33	1.38	1.46
2	b	49	LYS	CA-C	-6.33	1.45	1.52
13	m	193	ARG	CA-CB	6.33	1.63	1.53
21	N	317	SER	CA-C	-6.33	1.43	1.52
14	n	260	GLY	C-N	6.32	1.42	1.33
32	M	124	ARG	NE-CZ	6.32	1.40	1.33
3	c	118	ILE	CA-CB	-6.32	1.46	1.54
8	h	119	VAL	N-CA	-6.32	1.38	1.46
13	m	51	VAL	CA-C	-6.32	1.45	1.52
33	J	293	ALA	C-N	6.32	1.41	1.33
3	c	221	ASN	C-N	6.32	1.41	1.33
6	f	58	SER	C-N	6.32	1.42	1.33
10	j	61	THR	CA-CB	-6.32	1.43	1.53
2	B	68	THR	N-CA	-6.32	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	313	ILE	CA-CB	-6.32	1.46	1.54
1	A	105	ARG	CA-C	-6.32	1.44	1.52
25	R	64	LYS	N-CA	-6.32	1.38	1.46
11	4	70	ARG	CZ-NH1	6.31	1.41	1.32
23	P	159	ILE	CA-C	-6.31	1.45	1.52
29	I	73	GLU	CA-CB	6.31	1.63	1.53
14	n	151	GLY	CA-C	-6.31	1.44	1.51
6	F	12	THR	CA-C	-6.31	1.45	1.52
14	7	36	GLN	CA-CB	6.31	1.61	1.54
20	Z	837	TYR	CA-C	-6.31	1.44	1.52
2	b	128	ARG	NE-CZ	6.31	1.40	1.33
9	i	82	GLU	CA-C	-6.31	1.44	1.52
16	V	181	ASN	N-CA	-6.31	1.38	1.46
20	Z	849	ARG	CD-NE	6.31	1.55	1.46
3	c	192	LEU	CA-C	-6.31	1.44	1.52
13	6	38	ILE	C-N	6.31	1.41	1.33
24	Q	332	ARG	CD-NE	6.31	1.55	1.46
33	J	238	ARG	CD-NE	6.31	1.55	1.46
3	C	76	ALA	CA-C	-6.30	1.45	1.52
15	W	45	PRO	CA-CB	-6.30	1.45	1.53
16	V	217	HIS	ND1-CE1	6.30	1.38	1.32
18	X	68	LEU	C-N	6.30	1.38	1.33
26	U	140	ILE	CA-C	-6.30	1.46	1.52
31	L	180	PHE	CA-CB	6.30	1.63	1.53
6	f	74	LEU	CA-C	-6.30	1.44	1.52
7	g	123	HIS	C-O	-6.30	1.14	1.24
8	h	38	ARG	NE-CZ	6.30	1.40	1.33
12	5	82	ARG	C-N	6.30	1.41	1.33
12	5	85	GLY	C-N	6.30	1.42	1.33
20	Z	948	TRP	CD2-CE2	6.30	1.52	1.41
33	J	263	GLY	N-CA	6.30	1.54	1.45
5	e	99	HIS	CB-CG	6.30	1.58	1.50
9	2	152	TYR	N-CA	-6.30	1.38	1.46
25	R	334	ARG	CD-NE	6.30	1.55	1.46
12	l	133	TRP	CA-C	-6.30	1.44	1.52
21	N	548	ARG	NE-CZ	6.30	1.40	1.33
21	N	479	GLU	N-CA	-6.29	1.38	1.46
24	Q	268	SER	CA-C	6.29	1.60	1.52
20	Z	19	SER	CA-C	6.29	1.60	1.52
21	N	350	LYS	N-CA	-6.29	1.38	1.46
32	M	82	VAL	C-N	6.29	1.41	1.33
6	F	145	LEU	CA-CB	6.29	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	160	LEU	CA-C	-6.29	1.45	1.52
3	C	160	TRP	CA-C	-6.29	1.45	1.52
20	Z	466	GLU	CA-C	-6.29	1.44	1.52
33	J	153	LEU	C-N	6.29	1.42	1.33
11	k	13	VAL	N-CA	-6.28	1.39	1.46
11	k	159	ASP	CA-CB	6.28	1.63	1.53
17	T	270	ILE	CA-C	-6.28	1.44	1.52
20	Z	213	LYS	CA-C	-6.28	1.44	1.52
33	J	350	MET	N-CA	-6.28	1.38	1.46
23	P	421	GLU	CA-CB	6.28	1.64	1.53
6	f	43	HIS	CA-C	-6.28	1.44	1.52
29	I	425	LYS	N-CA	-6.28	1.37	1.46
4	D	222	VAL	C-O	-6.28	1.17	1.23
11	4	103	LEU	N-CA	-6.28	1.38	1.46
22	S	275	TYR	CA-C	-6.28	1.44	1.52
21	N	51	ASP	CA-C	6.28	1.60	1.52
22	S	472	HIS	CG-ND1	6.28	1.45	1.38
11	k	171	ARG	CD-NE	6.27	1.55	1.46
10	3	28	ARG	NE-CZ	6.27	1.40	1.33
22	S	273	PHE	CA-C	-6.27	1.44	1.52
27	O	68	LYS	CA-C	-6.27	1.46	1.52
6	f	89	ARG	C-N	6.27	1.42	1.33
20	Z	217	GLU	N-CA	-6.27	1.38	1.46
22	S	127	THR	C-N	6.27	1.42	1.33
29	I	107	GLY	N-CA	-6.27	1.39	1.45
3	C	174	THR	C-O	-6.27	1.16	1.24
6	F	182	ILE	C-O	-6.27	1.17	1.23
30	K	130	LEU	C-N	6.27	1.42	1.33
15	W	100	HIS	ND1-CE1	6.27	1.38	1.32
4	D	58	ARG	CZ-NH2	6.26	1.41	1.33
13	6	20	ILE	CA-C	-6.26	1.45	1.52
28	H	356	ASN	CA-C	-6.26	1.44	1.52
3	c	92	ARG	CD-NE	6.26	1.55	1.46
20	Z	369	PHE	C-N	6.26	1.44	1.33
5	e	94	THR	CA-CB	-6.26	1.43	1.53
8	h	28	ARG	CZ-NH1	6.26	1.41	1.32
20	Z	93	ARG	NE-CZ	6.26	1.40	1.33
27	O	271	LYS	CA-CB	6.26	1.63	1.53
29	I	400	GLY	CA-C	6.26	1.59	1.51
31	L	67	HIS	ND1-CE1	6.26	1.38	1.32
1	A	36	ASN	CA-C	-6.26	1.44	1.52
2	B	41	ASN	C-N	6.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	242	GLN	CA-CB	6.26	1.63	1.53
5	E	167	TYR	CA-C	-6.25	1.45	1.52
6	F	225	TYR	CA-CB	6.25	1.63	1.53
10	3	129	CYS	CA-C	-6.25	1.44	1.52
20	Z	212	LEU	CA-C	-6.25	1.45	1.52
22	S	466	LYS	N-CA	-6.25	1.38	1.46
5	e	148	ASP	CA-C	-6.25	1.45	1.52
7	G	35	THR	C-N	6.25	1.42	1.33
8	1	169	SER	CA-CB	6.25	1.63	1.53
14	n	35	GLN	C-N	-6.25	1.25	1.32
7	G	229	LYS	CA-C	-6.25	1.44	1.52
4	d	5	ASP	CA-C	-6.25	1.44	1.52
2	B	66	LEU	CA-CB	6.25	1.61	1.53
10	3	159	GLU	CA-C	6.25	1.60	1.52
12	5	242	ARG	NE-CZ	6.25	1.40	1.33
21	N	106	ILE	N-CA	6.25	1.53	1.46
33	J	283	GLU	CA-C	-6.25	1.44	1.52
13	m	38	ILE	C-N	6.25	1.41	1.33
9	2	246	ILE	C-N	6.25	1.41	1.33
20	Z	257	PRO	CA-CB	-6.25	1.45	1.54
20	Z	318	LYS	CA-C	-6.25	1.44	1.52
23	P	114	THR	C-N	6.25	1.41	1.33
1	a	176	GLN	CA-C	-6.24	1.44	1.52
5	e	143	LEU	C-O	-6.24	1.16	1.24
9	i	133	ASP	CA-CB	6.24	1.62	1.53
14	n	40	THR	CA-C	-6.24	1.44	1.52
29	I	305	THR	N-CA	-6.24	1.38	1.46
1	a	130	GLN	C-N	6.24	1.42	1.33
2	b	237	LYS	CA-C	-6.24	1.45	1.52
2	B	104	TYR	CA-C	6.24	1.60	1.52
23	P	237	VAL	CA-CB	-6.24	1.47	1.54
31	L	126	ARG	NE-CZ	6.24	1.40	1.33
1	a	91	ARG	NE-CZ	6.24	1.40	1.33
6	f	69	HIS	ND1-CE1	6.24	1.38	1.32
14	n	172	SER	CA-CB	6.24	1.63	1.54
9	2	72	CYS	CA-CB	6.24	1.64	1.53
1	a	15	HIS	CG-ND1	6.24	1.45	1.38
14	n	69	PHE	CA-C	-6.24	1.45	1.52
9	2	208	GLU	N-CA	-6.24	1.38	1.45
21	N	921	ARG	NE-CZ	6.24	1.40	1.33
27	O	176	SER	CA-C	-6.24	1.44	1.52
8	h	50	ILE	CA-CB	-6.23	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	139	HIS	CB-CG	6.23	1.58	1.50
29	I	304	ARG	CZ-NH1	6.23	1.41	1.32
30	K	346	ARG	NE-CZ	6.23	1.40	1.33
33	J	228	ARG	CD-NE	6.23	1.54	1.46
2	B	190	HIS	CG-CD2	6.23	1.42	1.35
9	2	84	VAL	C-N	6.22	1.42	1.33
15	W	30	ILE	N-CA	-6.22	1.38	1.46
16	V	254	ARG	NE-CZ	6.22	1.39	1.33
22	S	142	VAL	C-N	6.22	1.42	1.33
9	i	97	LEU	C-N	6.22	1.42	1.33
20	Z	66	ALA	N-CA	-6.22	1.38	1.46
20	Z	963	ALA	C-N	6.22	1.41	1.33
15	W	25	ARG	NE-CZ	6.22	1.39	1.33
22	S	362	SER	CA-C	-6.22	1.44	1.52
31	L	80	ASN	CA-CB	6.22	1.63	1.53
22	S	302	HIS	C-N	6.22	1.41	1.33
11	k	92	ILE	CA-CB	6.21	1.62	1.54
9	2	64	HIS	ND1-CE1	6.21	1.38	1.32
18	X	26	PRO	CA-C	-6.21	1.45	1.52
25	R	58	GLU	CA-C	-6.21	1.46	1.53
33	J	15	HIS	CA-CB	6.21	1.63	1.53
7	G	190	ARG	N-CA	-6.21	1.39	1.46
19	Y	47	GLU	C-N	6.21	1.42	1.33
33	J	211	ILE	N-CA	-6.21	1.38	1.46
28	H	46	ALA	CA-C	-6.21	1.45	1.52
5	e	108	ASN	C-N	6.21	1.41	1.33
15	W	13	SER	CA-C	-6.21	1.44	1.52
6	F	142	ALA	N-CA	-6.21	1.38	1.46
21	N	653	ARG	NE-CZ	6.21	1.39	1.33
29	I	225	PRO	CA-CB	6.21	1.61	1.53
16	V	155	ALA	N-CA	-6.20	1.38	1.46
32	M	401	ILE	CA-C	-6.20	1.44	1.52
5	E	71	ASP	C-N	-6.20	1.25	1.33
5	E	34	GLY	CA-C	6.20	1.58	1.52
11	4	81	SER	C-N	6.20	1.42	1.33
12	5	96	THR	C-N	6.20	1.41	1.33
20	Z	181	GLY	CA-C	-6.20	1.43	1.51
11	4	85	ARG	CZ-NH1	6.20	1.41	1.32
4	d	99	THR	CA-CB	6.19	1.63	1.53
11	4	124	THR	C-N	6.19	1.42	1.33
15	W	179	ARG	CD-NE	6.19	1.54	1.46
16	V	223	SER	CA-CB	6.19	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	511	PRO	N-CA	-6.19	1.39	1.47
22	S	120	SER	C-N	6.19	1.41	1.33
32	M	303	ARG	NE-CZ	6.19	1.39	1.33
5	e	200	VAL	C-N	6.19	1.42	1.34
1	A	105	ARG	NE-CZ	6.19	1.39	1.33
1	A	124	LEU	CA-CB	6.19	1.62	1.53
15	W	114	VAL	C-O	-6.19	1.17	1.24
18	X	112	ASN	CA-CB	6.19	1.62	1.53
22	S	240	ASP	N-CA	-6.19	1.39	1.46
2	b	203	GLU	N-CA	-6.19	1.38	1.46
3	c	94	HIS	CD2-NE2	6.19	1.44	1.37
1	A	228	ALA	C-N	6.19	1.42	1.33
16	V	146	SER	N-CA	-6.19	1.38	1.46
27	O	115	ARG	CZ-NH1	6.19	1.41	1.32
23	P	431	HIS	ND1-CE1	6.19	1.38	1.32
12	l	89	VAL	CA-C	-6.18	1.44	1.52
13	m	45	SER	CA-C	-6.18	1.44	1.52
4	D	119	ARG	CD-NE	6.18	1.54	1.46
29	I	161	GLN	C-N	6.18	1.41	1.33
31	L	110	LYS	C-N	6.18	1.41	1.33
4	D	190	GLU	N-CA	-6.18	1.38	1.46
23	P	111	ASP	CA-C	-6.18	1.45	1.52
23	P	216	LEU	C-N	6.18	1.42	1.33
31	L	217	GLY	N-CA	-6.18	1.36	1.45
1	a	91	ARG	CA-CB	6.18	1.62	1.53
33	J	318	PRO	C-N	-6.18	1.25	1.33
30	K	205	PRO	CA-CB	-6.18	1.48	1.53
14	7	170	TYR	CA-C	-6.18	1.45	1.52
18	X	27	ILE	CA-C	6.18	1.59	1.52
3	c	36	ILE	CA-C	-6.17	1.45	1.52
4	D	133	THR	CA-CB	-6.17	1.44	1.53
23	P	346	ILE	CA-C	-6.17	1.45	1.52
5	E	20	ARG	CA-C	-6.17	1.45	1.52
17	T	198	ASP	CA-CB	6.17	1.62	1.53
20	Z	143	VAL	CA-CB	6.17	1.62	1.54
14	7	98	ARG	CZ-NH2	6.17	1.41	1.33
12	l	144	ARG	CD-NE	6.17	1.54	1.46
7	G	199	ILE	CA-CB	-6.17	1.47	1.54
33	J	379	GLN	N-CA	-6.17	1.39	1.46
6	f	158	GLY	CA-C	-6.17	1.43	1.51
28	H	341	ASP	C-N	6.17	1.41	1.33
28	H	362	ASP	N-CA	-6.17	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	67	ILE	N-CA	-6.17	1.39	1.46
6	F	195	GLU	CA-C	-6.17	1.44	1.52
15	W	143	ASN	CA-CB	6.17	1.61	1.53
1	A	36	ASN	CA-CB	6.17	1.61	1.53
21	N	518	ALA	CA-CB	6.17	1.62	1.53
7	G	220	SER	CA-C	-6.16	1.44	1.52
30	K	133	PRO	C-N	6.16	1.42	1.33
9	i	101	ARG	CZ-NH1	6.16	1.41	1.32
20	Z	303	ASP	N-CA	-6.16	1.40	1.46
7	g	190	ARG	CZ-NH1	6.16	1.41	1.32
12	l	241	HIS	CA-C	-6.16	1.45	1.52
22	S	19	HIS	CE1-NE2	-6.16	1.26	1.32
10	3	80	ARG	NE-CZ	6.16	1.39	1.33
9	i	83	ALA	C-N	6.16	1.41	1.33
16	V	137	VAL	N-CA	-6.16	1.38	1.46
17	T	11	LEU	C-N	6.16	1.42	1.33
20	Z	396	ASN	CA-C	-6.16	1.45	1.52
28	H	303	ALA	C-N	6.16	1.41	1.33
30	K	189	GLU	CA-C	-6.16	1.44	1.52
32	M	85	VAL	CA-C	-6.15	1.45	1.52
20	Z	381	LEU	N-CA	-6.15	1.39	1.46
27	O	330	ARG	NE-CZ	6.15	1.39	1.33
31	L	78	ARG	NE-CZ	6.15	1.39	1.33
6	F	115	LYS	N-CA	-6.15	1.39	1.46
30	K	128	ARG	N-CA	-6.15	1.40	1.46
14	7	68	ARG	CD-NE	6.15	1.54	1.46
11	4	96	ARG	CZ-NH1	6.14	1.41	1.32
11	4	172	MET	CA-C	-6.14	1.46	1.52
22	S	254	ILE	C-N	6.14	1.41	1.33
32	M	203	ARG	NE-CZ	6.14	1.39	1.33
3	c	50	ARG	CA-CB	6.14	1.62	1.53
11	k	85	ARG	NE-CZ	6.14	1.39	1.33
8	1	11	SER	CA-C	-6.14	1.45	1.52
20	Z	952	SER	C-N	6.14	1.40	1.33
32	M	370	THR	C-N	6.14	1.41	1.33
1	a	13	ASP	N-CA	6.14	1.54	1.46
7	g	84	ASP	N-CA	-6.14	1.38	1.46
21	N	373	VAL	N-CA	-6.14	1.39	1.46
4	d	171	VAL	CA-C	-6.14	1.43	1.52
1	A	32	PHE	CA-CB	6.14	1.63	1.53
22	S	55	ARG	CZ-NH1	6.13	1.41	1.32
23	P	225	VAL	CA-CB	-6.13	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	416	SER	N-CA	6.13	1.53	1.46
17	T	61	ILE	N-CA	6.13	1.53	1.46
20	Z	226	GLU	C-N	6.13	1.41	1.33
32	M	64	ASP	C-N	6.13	1.41	1.33
23	P	49	ALA	CA-C	-6.13	1.44	1.52
26	U	141	GLU	CA-C	-6.13	1.45	1.52
10	3	178	ASP	CA-CB	6.12	1.63	1.53
24	Q	222	SER	N-CA	-6.12	1.39	1.46
26	U	156	HIS	CE1-NE2	6.12	1.38	1.32
13	m	10	PHE	CA-C	-6.12	1.45	1.52
26	U	204	LEU	C-N	6.12	1.42	1.33
32	M	410	VAL	C-N	6.12	1.42	1.33
23	P	64	ASP	N-CA	6.12	1.53	1.46
1	a	168	ALA	N-CA	-6.12	1.38	1.46
10	j	68	ARG	CZ-NH2	6.12	1.41	1.33
4	D	105	THR	C-N	6.12	1.41	1.33
9	2	247	VAL	CA-C	-6.12	1.45	1.52
31	L	357	ARG	CD-NE	6.12	1.54	1.46
13	m	209	GLY	N-CA	-6.12	1.39	1.45
7	G	230	PHE	C-N	6.12	1.41	1.33
20	Z	332	ASN	N-CA	-6.12	1.38	1.45
13	m	99	ARG	CZ-NH1	6.11	1.41	1.32
14	n	177	THR	N-CA	6.11	1.53	1.45
7	g	216	ILE	N-CA	-6.11	1.39	1.46
3	C	136	ILE	N-CA	-6.11	1.38	1.46
27	O	248	TYR	CA-C	-6.11	1.43	1.52
2	b	11	THR	C-N	6.11	1.42	1.33
22	S	137	PHE	CA-CB	6.11	1.63	1.53
24	Q	179	LEU	CA-C	-6.11	1.44	1.52
2	b	177	LYS	CA-C	-6.10	1.45	1.52
6	f	202	ARG	NE-CZ	6.10	1.39	1.33
8	h	134	ALA	C-N	6.10	1.40	1.33
8	1	25	ALA	CA-C	-6.10	1.45	1.52
13	6	175	LYS	CA-C	-6.10	1.44	1.52
22	S	64	ARG	C-N	6.10	1.42	1.33
27	O	218	SER	CA-C	-6.10	1.45	1.52
3	C	170	SER	C-N	6.10	1.41	1.33
3	c	244	ILE	CA-CB	-6.10	1.46	1.54
9	2	138	HIS	CE1-NE2	6.10	1.38	1.32
15	W	80	GLN	CA-C	-6.10	1.45	1.52
22	S	456	ASP	N-CA	6.10	1.53	1.46
24	Q	20	TYR	CA-CB	6.10	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	219	LEU	CA-C	-6.10	1.45	1.52
2	b	8	SER	N-CA	-6.10	1.38	1.45
8	1	63	ALA	N-CA	-6.10	1.38	1.46
4	d	198	SER	CA-CB	6.09	1.62	1.53
11	k	190	ARG	NE-CZ	6.09	1.39	1.33
6	F	218	LYS	N-CA	-6.09	1.38	1.46
23	P	306	ASN	CA-C	-6.09	1.45	1.52
30	K	268	ILE	CA-C	-6.09	1.45	1.52
33	J	86	VAL	CA-C	-6.09	1.45	1.52
33	J	270	ARG	CZ-NH1	6.09	1.41	1.32
13	6	220	VAL	C-N	6.09	1.42	1.33
21	N	471	TYR	CA-C	6.09	1.61	1.52
23	P	216	LEU	N-CA	-6.09	1.38	1.46
27	O	225	ASP	CA-CB	6.09	1.63	1.53
3	c	114	ARG	CA-C	-6.09	1.45	1.52
5	e	244	LYS	C-N	6.09	1.42	1.33
3	C	18	ARG	NE-CZ	6.09	1.39	1.33
24	Q	135	HIS	CE1-NE2	-6.09	1.26	1.32
27	O	286	PHE	CA-C	-6.09	1.45	1.52
27	O	301	PHE	C-N	6.09	1.41	1.33
28	H	323	ALA	N-CA	-6.09	1.38	1.46
13	6	199	ALA	CA-C	-6.09	1.44	1.52
25	R	213	TYR	CA-C	-6.09	1.45	1.52
7	G	11	SER	CA-C	-6.09	1.45	1.52
14	7	40	THR	CA-C	-6.09	1.45	1.52
20	Z	928	ARG	CA-CB	6.09	1.62	1.53
32	M	179	THR	N-CA	6.09	1.54	1.46
16	V	176	ASN	C-N	6.08	1.42	1.34
20	Z	268	ALA	N-CA	-6.08	1.39	1.46
29	I	117	HIS	CA-C	-6.08	1.45	1.52
11	4	73	TYR	N-CA	-6.08	1.38	1.46
3	C	36	ILE	CA-C	-6.08	1.45	1.52
7	G	115	ARG	N-CA	-6.08	1.38	1.46
13	6	133	PHE	CA-C	-6.08	1.45	1.52
30	K	417	THR	CA-C	-6.08	1.44	1.52
7	G	202	LEU	CA-C	-6.08	1.44	1.52
20	Z	268	ALA	CA-C	-6.08	1.44	1.52
3	C	238	ILE	CA-CB	-6.07	1.45	1.54
8	1	31	THR	N-CA	-6.07	1.39	1.46
21	N	385	VAL	CA-C	6.07	1.61	1.52
13	m	79	SER	C-N	6.07	1.41	1.33
20	Z	453	LEU	CA-CB	6.07	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	89	SER	CA-C	-6.07	1.45	1.52
32	M	289	LYS	CA-CB	6.07	1.63	1.53
1	a	217	GLU	CA-CB	6.07	1.63	1.53
5	e	177	GLU	CA-C	-6.07	1.44	1.52
6	f	32	GLY	CA-C	6.07	1.61	1.52
7	g	149	TYR	CA-C	-6.07	1.45	1.52
14	n	98	ARG	NE-CZ	6.07	1.39	1.33
12	5	263	HIS	CA-CB	6.07	1.61	1.53
20	Z	196	SER	N-CA	-6.07	1.39	1.46
23	P	337	HIS	CB-CG	6.07	1.58	1.50
11	k	49	GLU	C-N	6.06	1.42	1.33
9	2	217	ARG	CD-NE	6.06	1.54	1.46
23	P	384	VAL	C-N	6.06	1.42	1.33
27	O	325	GLU	CA-C	-6.06	1.44	1.52
31	L	333	LEU	N-CA	-6.06	1.38	1.45
1	a	161	GLY	N-CA	6.06	1.53	1.44
2	b	178	ARG	NE-CZ	6.06	1.39	1.33
16	V	217	HIS	CG-CD2	6.06	1.42	1.35
17	T	238	GLN	CA-CB	6.06	1.62	1.53
29	I	309	LEU	CA-CB	6.06	1.62	1.53
4	d	141	ARG	NE-CZ	6.06	1.39	1.33
11	k	114	PRO	N-CD	-6.06	1.39	1.47
2	B	241	GLN	CA-C	-6.06	1.44	1.52
11	4	62	ALA	N-CA	-6.06	1.39	1.46
20	Z	121	ILE	CA-C	-6.06	1.45	1.52
12	l	118	GLY	CA-C	-6.05	1.46	1.52
7	G	20	ARG	CA-CB	6.05	1.63	1.53
21	N	443	LEU	CA-CB	6.05	1.63	1.53
2	B	85	LEU	CA-CB	6.05	1.62	1.53
6	f	197	ILE	C-N	6.05	1.42	1.33
3	C	56	LEU	CA-C	-6.05	1.44	1.52
21	N	666	GLN	C-N	6.05	1.42	1.33
22	S	471	LEU	C-N	6.05	1.41	1.33
27	O	283	HIS	N-CA	-6.05	1.39	1.46
31	L	360	ILE	C-N	6.05	1.41	1.33
6	f	225	TYR	C-N	6.05	1.41	1.33
12	l	166	LYS	C-N	6.05	1.42	1.33
5	E	26	TYR	N-CA	-6.05	1.38	1.46
22	S	51	ARG	CA-C	-6.05	1.45	1.52
23	P	27	LEU	C-N	6.05	1.41	1.33
5	e	242	GLU	C-O	-6.05	1.17	1.24
10	3	141	THR	C-N	6.05	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	48	GLU	CA-CB	6.04	1.60	1.53
17	T	103	SER	CA-CB	6.04	1.62	1.53
17	T	105	LEU	C-N	6.04	1.41	1.34
25	R	59	MET	CA-CB	6.04	1.61	1.53
28	H	254	THR	C-O	6.04	1.31	1.24
28	H	93	GLU	CA-CB	6.04	1.60	1.52
16	V	68	VAL	CA-CB	-6.04	1.45	1.54
21	N	655	ALA	C-N	6.04	1.41	1.33
3	C	216	ILE	CA-C	-6.04	1.44	1.52
23	P	326	ASP	CA-CB	6.04	1.63	1.53
25	R	219	LEU	C-N	6.04	1.41	1.33
31	L	142	LYS	CA-C	-6.04	1.44	1.52
10	j	119	PRO	CA-C	6.04	1.59	1.52
11	k	136	SER	CA-C	-6.04	1.45	1.52
22	S	69	LEU	C-O	-6.04	1.17	1.24
10	j	108	VAL	CA-CB	6.04	1.62	1.54
20	Z	349	THR	CA-C	-6.04	1.45	1.52
21	N	112	GLU	CA-C	6.04	1.60	1.52
24	Q	301	ALA	CA-C	-6.04	1.45	1.52
28	H	282	LYS	C-N	6.04	1.41	1.33
2	b	186	GLU	CA-CB	6.03	1.62	1.53
8	1	21	VAL	CA-C	-6.03	1.45	1.52
33	J	181	GLN	CA-CB	6.03	1.62	1.54
12	l	94	ARG	CA-CB	6.03	1.62	1.53
13	6	42	SER	N-CA	-6.03	1.38	1.46
13	6	225	TYR	N-CA	-6.03	1.38	1.46
24	Q	75	ARG	CD-NE	6.03	1.54	1.46
31	L	369	LYS	CA-C	-6.03	1.45	1.52
6	f	202	ARG	CZ-NH1	6.03	1.41	1.32
3	C	155	GLY	C-N	6.03	1.41	1.33
24	Q	129	LYS	C-N	6.03	1.41	1.33
4	d	90	ARG	CD-NE	6.03	1.54	1.46
18	X	101	LEU	CA-C	-6.02	1.45	1.52
25	R	224	PHE	CA-C	-6.02	1.44	1.52
4	d	253	ASN	C-N	6.02	1.41	1.33
12	5	129	PHE	CA-CB	6.02	1.62	1.53
22	S	19	HIS	CG-ND1	-6.02	1.31	1.38
23	P	30	ASN	C-N	6.02	1.41	1.33
24	Q	42	ALA	N-CA	-6.02	1.38	1.46
27	O	359	SER	CA-C	-6.02	1.45	1.53
28	H	400	ARG	CA-C	-6.02	1.45	1.53
2	b	146	SER	C-N	6.02	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	204	GLN	CA-C	6.02	1.60	1.52
9	2	48	ARG	CA-CB	6.02	1.62	1.53
9	2	226	GLU	C-N	6.02	1.41	1.33
10	j	203	ARG	NE-CZ	6.02	1.39	1.33
22	S	91	ASN	C-N	6.02	1.41	1.33
6	F	148	GLN	C-N	-6.02	1.27	1.34
6	F	164	ARG	CD-NE	6.02	1.54	1.46
33	J	363	THR	C-N	6.02	1.42	1.33
6	f	218	LYS	CA-CB	6.01	1.62	1.54
11	4	133	HIS	ND1-CE1	6.01	1.38	1.32
3	C	177	GLN	N-CA	-6.01	1.38	1.46
4	D	63	LYS	CA-C	-6.01	1.44	1.52
11	4	190	ARG	NE-CZ	6.01	1.39	1.33
29	I	166	PRO	CA-CB	6.01	1.62	1.53
5	e	196	ALA	N-CA	-6.01	1.39	1.46
16	V	302	SER	CA-CB	6.01	1.62	1.53
25	R	227	ALA	N-CA	-6.01	1.39	1.46
8	h	198	TYR	CA-C	-6.01	1.45	1.52
10	3	195	VAL	N-CA	-6.01	1.39	1.46
20	Z	105	LYS	CA-CB	6.01	1.63	1.53
9	i	104	ARG	CD-NE	6.00	1.54	1.46
22	S	198	SER	C-N	6.00	1.42	1.33
6	f	175	THR	C-N	6.00	1.41	1.33
10	j	131	ASP	C-N	6.00	1.41	1.33
10	3	48	HIS	CG-ND1	6.00	1.44	1.38
22	S	481	TYR	CA-CB	6.00	1.62	1.53
30	K	149	ILE	CA-C	-6.00	1.45	1.52
13	m	36	ARG	NE-CZ	6.00	1.39	1.33
3	C	113	ARG	CZ-NH2	6.00	1.41	1.33
5	e	188	HIS	C-N	6.00	1.41	1.33
3	C	114	ARG	CA-C	-6.00	1.45	1.52
32	M	333	LEU	N-CA	-6.00	1.38	1.46
6	f	110	HIS	ND1-CE1	6.00	1.38	1.32
20	Z	295	ARG	CZ-NH1	6.00	1.41	1.32
21	N	64	ILE	CA-C	-6.00	1.45	1.52
22	S	222	SER	CA-C	-6.00	1.45	1.52
26	U	24	ARG	CD-NE	6.00	1.54	1.46
29	I	345	ASP	CA-CB	6.00	1.60	1.52
32	M	57	VAL	CA-C	-6.00	1.44	1.52
20	Z	928	ARG	C-N	6.00	1.41	1.33
29	I	70	LEU	C-N	6.00	1.41	1.33
7	g	72	ARG	CZ-NH2	5.99	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	280	LEU	CA-C	-5.99	1.45	1.52
11	k	180	ILE	N-CA	-5.99	1.38	1.46
10	3	67	PHE	N-CA	-5.99	1.39	1.46
23	P	376	THR	N-CA	-5.99	1.39	1.46
6	f	227	GLY	CA-C	-5.99	1.43	1.51
21	N	502	PHE	CA-C	-5.99	1.45	1.52
21	N	815	LYS	C-N	5.99	1.42	1.33
33	J	345	LYS	C-N	5.99	1.41	1.33
17	T	76	ASP	CA-CB	5.99	1.62	1.53
5	e	162	GLY	C-N	5.99	1.41	1.33
5	E	132	ARG	CD-NE	5.99	1.54	1.46
10	3	36	VAL	CA-CB	-5.99	1.46	1.54
20	Z	269	TYR	CZ-OH	5.99	1.50	1.38
21	N	88	ARG	CZ-NH2	5.99	1.41	1.33
7	G	123	HIS	ND1-CE1	5.98	1.38	1.32
21	N	197	VAL	CA-C	-5.98	1.46	1.52
9	i	82	GLU	N-CA	-5.98	1.39	1.46
18	X	101	LEU	CA-CB	5.98	1.63	1.53
22	S	419	VAL	CA-C	5.98	1.60	1.52
28	H	309	ASP	CA-C	-5.98	1.45	1.52
21	N	891	VAL	CA-CB	-5.98	1.46	1.54
22	S	465	ILE	N-CA	-5.98	1.39	1.46
3	c	125	HIS	CG-ND1	5.98	1.44	1.38
16	V	112	PRO	CA-C	-5.98	1.44	1.52
21	N	843	LYS	CA-C	-5.98	1.45	1.52
10	j	50	PHE	CA-C	-5.98	1.45	1.52
14	n	168	VAL	N-CA	5.98	1.53	1.46
24	Q	76	GLU	C-O	-5.98	1.17	1.24
3	C	42	ASP	CA-CB	5.97	1.62	1.53
4	D	197	ARG	C-N	5.97	1.41	1.33
21	N	737	SER	CA-C	-5.97	1.44	1.52
3	c	94	HIS	ND1-CE1	5.97	1.38	1.32
18	X	89	LEU	CA-C	-5.97	1.45	1.52
26	U	150	THR	CA-C	-5.97	1.44	1.52
17	T	118	ASN	CA-CB	5.97	1.60	1.53
21	N	857	TYR	C-N	5.97	1.42	1.33
23	P	357	TYR	N-CA	-5.97	1.38	1.46
14	7	78	VAL	N-CA	-5.97	1.38	1.46
18	X	37	PRO	C-N	5.97	1.39	1.33
28	H	392	HIS	CE1-NE2	-5.97	1.26	1.32
5	e	193	LEU	CA-C	-5.97	1.45	1.52
7	g	47	VAL	CA-CB	-5.97	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	206	GLY	N-CA	-5.97	1.36	1.45
21	N	239	LEU	CA-C	-5.97	1.45	1.52
21	N	672	ASN	C-N	5.97	1.41	1.34
7	g	213	GLU	CA-C	-5.96	1.45	1.52
4	d	100	LEU	CA-C	-5.96	1.44	1.52
14	7	95	HIS	CA-C	-5.96	1.45	1.52
20	Z	948	TRP	C-N	5.96	1.41	1.33
29	I	117	HIS	CD2-NE2	5.96	1.44	1.37
13	6	65	PHE	CA-CB	5.96	1.61	1.53
1	a	163	TYR	CA-CB	5.96	1.64	1.53
8	h	108	VAL	CA-CB	-5.96	1.46	1.53
13	6	107	GLY	N-CA	-5.96	1.36	1.45
14	7	85	GLY	CA-C	-5.96	1.48	1.52
22	S	239	ARG	NE-CZ	5.96	1.39	1.33
6	F	214	ALA	CA-C	-5.96	1.45	1.52
15	W	107	HIS	N-CA	-5.96	1.38	1.45
1	a	100	GLU	C-N	5.96	1.42	1.33
13	6	115	VAL	CA-C	-5.96	1.45	1.52
21	N	58	ARG	CZ-NH1	5.96	1.41	1.32
7	g	9	ASP	CA-C	-5.95	1.44	1.52
1	A	209	HIS	CA-CB	5.95	1.62	1.53
11	4	133	HIS	CB-CG	5.95	1.58	1.50
28	H	260	ALA	N-CA	-5.95	1.38	1.46
20	Z	581	VAL	C-N	5.95	1.42	1.33
25	R	401	HIS	CA-C	-5.95	1.45	1.52
9	i	55	VAL	N-CA	-5.95	1.39	1.46
21	N	357	GLY	C-N	5.95	1.42	1.33
33	J	196	THR	N-CA	-5.95	1.39	1.46
2	b	242	GLU	CA-C	-5.95	1.45	1.52
4	d	183	GLU	CA-CB	5.95	1.59	1.53
14	7	187	LEU	CA-CB	5.95	1.62	1.53
20	Z	406	TRP	CA-C	-5.95	1.44	1.52
20	Z	478	VAL	CA-C	5.95	1.60	1.52
20	Z	928	ARG	CD-NE	5.95	1.54	1.46
22	S	71	ALA	CA-C	-5.95	1.44	1.52
25	R	20	ARG	NE-CZ	5.95	1.39	1.33
10	j	166	THR	N-CA	-5.94	1.39	1.46
14	7	76	ILE	N-CA	-5.94	1.41	1.45
28	H	462	ARG	CZ-NH2	5.94	1.41	1.33
23	P	314	VAL	CA-C	5.94	1.60	1.52
4	d	166	ARG	CZ-NH1	5.94	1.41	1.32
3	C	82	ALA	N-CA	-5.94	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	55	ARG	C-N	5.94	1.40	1.33
21	N	725	LEU	CA-C	5.94	1.60	1.52
32	M	65	ASN	CA-C	-5.94	1.45	1.52
5	e	25	GLU	CA-CB	5.94	1.62	1.53
8	h	29	THR	CA-C	-5.94	1.45	1.52
28	H	218	ILE	CA-CB	-5.94	1.46	1.54
4	D	221	ILE	CA-C	-5.93	1.45	1.52
15	W	114	VAL	CA-C	5.93	1.60	1.52
23	P	423	LEU	C-N	5.93	1.41	1.33
25	R	90	GLU	CA-C	-5.93	1.44	1.52
14	n	176	ALA	CA-C	-5.93	1.45	1.52
8	1	137	GLY	C-O	-5.93	1.20	1.24
16	V	147	VAL	CA-CB	-5.93	1.48	1.54
1	a	120	ARG	CZ-NH1	5.93	1.41	1.32
13	6	52	PHE	N-CA	-5.93	1.39	1.46
20	Z	772	ILE	N-CA	-5.93	1.38	1.46
27	O	210	ARG	C-N	5.93	1.41	1.33
31	L	300	GLU	C-N	5.93	1.41	1.33
7	g	101	LYS	CA-C	-5.93	1.45	1.52
4	d	151	GLU	C-N	5.92	1.40	1.34
14	n	248	GLU	CA-C	-5.92	1.45	1.52
15	W	171	LEU	CA-C	-5.92	1.45	1.52
31	L	291	PHE	C-O	-5.92	1.17	1.24
5	E	217	ALA	CA-C	-5.92	1.45	1.52
12	5	231	LEU	C-N	5.92	1.41	1.33
12	l	250	VAL	CA-C	-5.92	1.45	1.52
9	2	115	HIS	CG-CD2	5.92	1.42	1.35
29	I	150	HIS	CE1-NE2	-5.92	1.26	1.32
32	M	153	TYR	CA-CB	5.92	1.60	1.52
1	A	40	ILE	CA-CB	-5.92	1.46	1.54
20	Z	195	PHE	CA-C	5.92	1.60	1.52
28	H	292	ARG	CD-NE	5.92	1.54	1.46
30	K	74	HIS	CA-CB	5.92	1.62	1.53
29	I	291	ARG	C-N	5.92	1.41	1.33
30	K	297	ILE	CA-CB	5.92	1.61	1.54
3	c	231	LYS	C-N	5.91	1.41	1.33
5	e	135	SER	CA-C	-5.91	1.45	1.52
18	X	59	ARG	NE-CZ	5.91	1.39	1.33
20	Z	372	ALA	CA-C	-5.91	1.44	1.53
21	N	666	GLN	N-CA	5.91	1.53	1.46
24	Q	38	SER	CA-C	-5.91	1.45	1.52
25	R	367	ASP	CA-C	5.91	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	133	HIS	CA-C	-5.91	1.45	1.52
20	Z	124	MET	CA-CB	5.91	1.62	1.53
32	M	258	GLU	CA-CB	5.91	1.63	1.53
6	f	65	LYS	N-CA	-5.91	1.38	1.46
11	4	125	LYS	C-N	5.91	1.40	1.33
22	S	107	SER	C-N	5.91	1.42	1.33
9	i	114	GLN	N-CA	5.91	1.53	1.46
20	Z	738	TYR	CE1-CZ	5.91	1.52	1.38
4	d	77	GLY	CA-C	-5.91	1.45	1.52
7	G	190	ARG	CZ-NH1	5.91	1.41	1.32
24	Q	331	THR	N-CA	-5.91	1.39	1.46
1	a	213	ALA	CA-C	-5.90	1.45	1.52
5	e	41	ALA	CA-CB	5.90	1.62	1.53
5	e	204	LEU	CA-CB	5.90	1.62	1.53
12	l	252	LEU	C-N	5.90	1.42	1.33
18	X	76	VAL	CA-CB	5.90	1.61	1.54
32	M	233	ARG	CD-NE	5.90	1.54	1.46
7	G	153	PRO	N-CD	-5.90	1.39	1.47
11	4	41	HIS	N-CA	-5.90	1.41	1.46
14	7	137	ARG	CA-CB	5.90	1.62	1.53
21	N	534	ASP	N-CA	-5.90	1.39	1.46
23	P	105	LYS	CA-C	-5.90	1.45	1.52
16	V	273	ARG	NE-CZ	5.90	1.39	1.33
29	I	201	PRO	C-N	5.90	1.41	1.33
32	M	163	PHE	CA-CB	5.90	1.66	1.54
13	6	127	LYS	CA-C	-5.89	1.45	1.52
22	S	49	ASP	C-O	-5.89	1.19	1.24
6	F	175	THR	C-N	5.89	1.41	1.33
14	7	64	GLY	CA-C	-5.89	1.43	1.51
21	N	343	THR	N-CA	-5.89	1.39	1.46
28	H	222	ARG	CZ-NH1	5.89	1.41	1.32
29	I	407	ARG	CA-C	-5.89	1.44	1.52
26	U	64	ASP	CA-CB	5.89	1.61	1.53
31	L	215	PRO	N-CD	-5.89	1.39	1.47
13	6	38	ILE	CA-C	-5.89	1.45	1.52
32	M	382	SER	CA-C	5.89	1.60	1.52
33	J	12	LEU	CA-C	-5.89	1.44	1.52
6	f	146	GLU	CA-C	-5.89	1.45	1.52
5	e	10	ARG	CD-NE	5.88	1.54	1.46
6	f	133	LEU	N-CA	-5.88	1.39	1.46
14	n	95	HIS	ND1-CE1	5.88	1.38	1.32
32	M	371	ASP	N-CA	-5.88	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	ASP	CA-C	-5.88	1.45	1.52
11	4	77	PRO	C-N	5.88	1.41	1.33
12	5	160	ASN	N-CA	-5.88	1.39	1.46
17	T	186	ARG	NE-CZ	5.88	1.39	1.33
22	S	298	ARG	CZ-NH2	5.88	1.41	1.33
22	S	484	ASP	N-CA	5.88	1.53	1.46
25	R	246	TYR	C-N	5.88	1.42	1.33
12	l	100	TRP	CA-C	-5.88	1.45	1.52
8	1	181	VAL	CA-C	-5.88	1.46	1.52
14	7	218	TYR	C-O	-5.88	1.17	1.24
33	J	83	LYS	N-CA	-5.88	1.37	1.46
2	B	188	ALA	C-N	-5.88	1.26	1.34
17	T	61	ILE	CA-CB	-5.88	1.47	1.54
23	P	432	LEU	C-N	5.88	1.41	1.33
25	R	204	TRP	CZ2-CH2	5.88	1.48	1.37
33	J	186	ILE	C-N	5.88	1.41	1.33
13	m	30	VAL	C-N	5.87	1.41	1.33
13	m	199	ALA	C-O	-5.87	1.17	1.24
20	Z	35	GLU	CA-CB	5.87	1.62	1.53
30	K	318	THR	CA-C	-5.87	1.45	1.52
25	R	99	TYR	CA-C	-5.87	1.45	1.52
27	O	376	GLN	C-N	5.87	1.41	1.33
30	K	262	ARG	CD-NE	5.87	1.54	1.46
30	K	315	ILE	CA-C	-5.87	1.45	1.52
31	L	194	ARG	NE-CZ	5.87	1.39	1.33
17	T	98	GLU	CA-C	-5.87	1.46	1.53
7	G	144	ASN	CA-C	-5.87	1.44	1.52
24	Q	50	ARG	CZ-NH1	5.87	1.41	1.32
30	K	361	SER	N-CA	-5.87	1.39	1.46
32	M	45	ARG	C-N	5.87	1.42	1.33
1	a	50	CYS	N-CA	-5.87	1.38	1.45
17	T	137	GLU	CA-C	-5.87	1.45	1.52
1	a	168	ALA	CA-C	-5.86	1.45	1.52
6	F	167	GLY	C-N	5.86	1.42	1.33
14	7	148	ILE	C-N	5.86	1.41	1.33
12	l	160	ASN	C-N	5.86	1.41	1.33
11	4	169	GLU	CA-CB	5.86	1.62	1.53
21	N	139	ARG	CD-NE	5.86	1.54	1.46
15	W	167	GLU	N-CA	-5.86	1.38	1.46
21	N	704	GLY	C-N	5.86	1.41	1.33
1	A	227	VAL	C-N	5.86	1.41	1.33
19	Y	54	VAL	CA-C	-5.86	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	117	HIS	ND1-CE1	5.86	1.38	1.32
2	b	190	HIS	CA-CB	5.86	1.63	1.53
13	6	69	GLY	N-CA	-5.86	1.38	1.45
16	V	93	ASP	N-CA	-5.86	1.39	1.46
20	Z	291	GLU	CA-C	-5.86	1.45	1.52
20	Z	946	THR	CA-C	-5.86	1.45	1.52
6	F	77	LEU	CA-C	-5.85	1.45	1.52
27	O	123	GLY	C-N	5.85	1.41	1.33
27	O	356	ARG	CD-NE	5.85	1.54	1.46
6	f	148	GLN	N-CA	-5.85	1.39	1.45
12	l	134	LEU	CA-CB	5.85	1.62	1.53
28	H	403	ARG	NE-CZ	5.85	1.39	1.33
15	W	58	ASN	N-CA	-5.85	1.38	1.46
4	d	74	SER	CA-C	-5.85	1.45	1.52
16	V	209	GLU	C-N	5.85	1.41	1.33
30	K	43	VAL	CA-C	-5.85	1.45	1.52
1	a	247	ALA	C-N	5.85	1.41	1.33
30	K	85	GLU	CA-CB	5.85	1.62	1.53
13	m	123	ASP	N-CA	5.85	1.53	1.45
14	n	68	ARG	NE-CZ	5.85	1.39	1.33
13	6	214	ILE	CB-CG1	5.85	1.65	1.53
23	P	412	LEU	C-N	5.85	1.41	1.33
2	b	199	SER	C-N	5.84	1.41	1.33
14	7	81	ASN	N-CA	-5.84	1.38	1.46
21	N	457	SER	CA-C	-5.84	1.44	1.52
28	H	449	LYS	CA-C	5.84	1.60	1.52
29	I	156	ILE	CA-C	-5.84	1.46	1.52
8	h	77	SER	CA-C	-5.84	1.45	1.52
3	C	193	ALA	CA-CB	5.84	1.62	1.53
16	V	305	ILE	C-N	5.84	1.41	1.33
17	T	228	ILE	C-N	5.84	1.41	1.33
20	Z	434	GLN	CA-CB	-5.84	1.44	1.53
24	Q	261	VAL	C-N	-5.84	1.26	1.33
14	n	249	ASN	CA-CB	5.84	1.62	1.53
24	Q	265	MET	C-O	-5.84	1.17	1.24
11	k	135	TYR	CA-C	-5.84	1.45	1.52
6	F	29	ILE	C-N	5.84	1.41	1.33
22	S	319	CYS	C-N	5.84	1.41	1.33
24	Q	184	VAL	N-CA	5.83	1.53	1.46
11	k	29	LYS	CA-C	-5.83	1.45	1.52
11	k	182	LYS	CA-C	5.83	1.59	1.52
9	2	177	LYS	N-CA	-5.83	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	756	MET	CA-C	-5.83	1.45	1.52
21	N	703	GLN	CA-CB	5.83	1.62	1.53
9	i	129	VAL	C-N	5.83	1.40	1.33
3	C	127	GLY	CA-C	-5.83	1.43	1.51
8	1	184	MET	C-N	5.83	1.41	1.33
5	E	136	ARG	CD-NE	5.83	1.54	1.46
7	G	145	GLY	CA-C	-5.83	1.45	1.52
11	4	11	ASP	N-CA	5.83	1.52	1.46
14	7	144	TRP	CA-CB	5.83	1.60	1.53
24	Q	406	ASP	N-CA	-5.83	1.38	1.45
27	O	141	ASN	CA-CB	5.83	1.63	1.53
31	L	420	ARG	CA-C	-5.83	1.45	1.52
2	B	128	ARG	CD-NE	5.83	1.54	1.46
4	D	41	CYS	N-CA	-5.83	1.39	1.46
25	R	222	ARG	CD-NE	5.83	1.54	1.46
9	i	187	ALA	C-N	5.83	1.41	1.33
1	A	226	GLY	CA-C	-5.83	1.48	1.52
4	D	27	VAL	CA-C	-5.83	1.45	1.52
10	3	115	LYS	CA-C	-5.83	1.44	1.52
20	Z	523	ALA	N-CA	5.83	1.52	1.46
30	K	311	ASN	N-CA	-5.83	1.38	1.45
5	e	170	LYS	CA-CB	5.82	1.63	1.53
10	3	198	ARG	CD-NE	5.82	1.54	1.46
1	a	19	PHE	N-CA	5.82	1.53	1.45
13	6	120	ALA	C-N	5.82	1.40	1.33
23	P	52	LEU	CA-C	-5.82	1.44	1.52
12	l	276	LYS	N-CA	5.82	1.53	1.46
13	m	109	ARG	CZ-NH1	5.82	1.40	1.32
13	6	213	LEU	C-N	5.82	1.40	1.33
25	R	209	ARG	CZ-NH2	5.82	1.41	1.33
27	O	191	THR	N-CA	-5.82	1.39	1.46
31	L	369	LYS	C-N	5.82	1.40	1.33
4	d	33	ALA	CA-CB	5.82	1.63	1.53
15	W	179	ARG	C-N	5.82	1.41	1.33
32	M	50	ARG	CZ-NH1	5.82	1.40	1.32
3	c	5	ARG	CD-NE	5.82	1.54	1.46
8	h	22	ILE	C-O	-5.82	1.17	1.24
7	G	147	HIS	ND1-CE1	5.82	1.38	1.32
21	N	183	VAL	N-CA	-5.82	1.39	1.46
27	O	128	LEU	C-N	5.82	1.41	1.33
14	n	104	VAL	CA-CB	-5.82	1.47	1.54
20	Z	464	ASP	CA-C	-5.82	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	166	ALA	CA-C	-5.82	1.44	1.52
5	E	127	ALA	CA-C	-5.81	1.45	1.52
14	7	171	SER	CA-C	-5.81	1.45	1.52
4	D	172	ARG	CA-CB	5.81	1.62	1.53
20	Z	129	ASN	CA-CB	5.81	1.62	1.53
13	m	116	HIS	ND1-CE1	5.81	1.38	1.32
1	A	87	ILE	CA-C	5.81	1.57	1.52
20	Z	354	PRO	N-CD	-5.81	1.39	1.47
3	C	58	GLU	CA-C	-5.81	1.45	1.52
24	Q	37	GLN	CA-C	-5.81	1.45	1.52
1	A	103	GLU	C-O	-5.80	1.17	1.24
5	E	27	SER	C-N	5.80	1.42	1.33
21	N	701	VAL	C-N	5.80	1.41	1.33
24	Q	239	PHE	N-CA	5.80	1.53	1.46
2	b	78	MET	C-O	-5.80	1.17	1.23
8	h	148	ASP	CA-CB	5.80	1.62	1.53
4	D	83	ARG	C-N	5.80	1.41	1.33
22	S	417	GLN	C-N	5.80	1.41	1.33
14	n	189	ARG	CA-CB	5.80	1.63	1.53
1	A	18	ILE	CA-C	-5.80	1.45	1.52
21	N	446	ALA	N-CA	5.80	1.53	1.46
22	S	144	LEU	N-CA	-5.80	1.39	1.46
32	M	210	MET	N-CA	-5.80	1.39	1.46
33	J	157	ILE	CA-C	-5.80	1.45	1.52
11	4	108	ASP	CA-C	5.80	1.60	1.52
10	3	197	LYS	C-N	5.80	1.41	1.33
16	V	228	TYR	CA-C	-5.80	1.45	1.52
20	Z	111	LEU	N-CA	-5.80	1.38	1.46
7	G	15	PHE	CA-C	-5.79	1.45	1.52
4	d	217	PRO	CA-C	-5.79	1.45	1.52
5	e	106	ASP	CA-C	-5.79	1.45	1.52
4	D	16	HIS	CA-C	5.79	1.61	1.53
17	T	19	ASP	C-O	5.79	1.30	1.24
17	T	90	PHE	CA-CB	5.79	1.62	1.53
20	Z	387	ASN	CA-C	-5.79	1.45	1.52
4	d	152	PRO	N-CA	-5.79	1.39	1.47
9	i	71	TRP	CA-C	-5.79	1.45	1.52
18	X	27	ILE	CA-CB	-5.79	1.46	1.54
21	N	303	LEU	N-CA	-5.79	1.39	1.46
23	P	201	ARG	CZ-NH2	5.79	1.41	1.33
14	7	241	PHE	CA-CB	5.79	1.61	1.53
2	b	114	VAL	CA-C	-5.79	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	152	ASN	CA-CB	5.79	1.62	1.53
14	n	246	GLN	CA-C	-5.79	1.45	1.52
2	B	44	VAL	N-CA	-5.79	1.39	1.46
5	E	122	ARG	CZ-NH2	5.79	1.41	1.33
20	Z	147	GLU	N-CA	-5.79	1.39	1.46
20	Z	764	LEU	CA-C	-5.79	1.45	1.52
21	N	669	GLU	CA-CB	5.79	1.63	1.53
30	K	189	GLU	C-O	5.79	1.30	1.24
2	b	83	ARG	CZ-NH1	5.79	1.40	1.32
3	c	242	THR	C-N	5.79	1.41	1.33
7	g	186	GLY	C-N	5.79	1.41	1.33
22	S	281	ALA	CA-C	-5.79	1.45	1.52
30	K	212	TYR	N-CA	-5.79	1.38	1.46
10	j	198	ARG	CZ-NH1	5.78	1.40	1.32
9	2	231	SER	N-CA	-5.78	1.38	1.46
13	6	90	LYS	N-CA	-5.78	1.39	1.46
15	W	127	ARG	CD-NE	5.78	1.54	1.46
20	Z	504	GLU	C-O	-5.78	1.17	1.24
28	H	170	GLU	CA-C	-5.78	1.45	1.52
30	K	363	ALA	CA-CB	5.78	1.62	1.53
21	N	49	LEU	CA-C	-5.78	1.45	1.52
5	e	134	MET	CA-C	-5.78	1.45	1.52
4	D	224	LEU	C-N	5.78	1.41	1.33
12	5	185	PRO	N-CA	5.78	1.54	1.47
20	Z	340	LEU	CA-C	-5.78	1.45	1.52
21	N	394	ARG	C-N	5.78	1.41	1.33
28	H	49	LEU	CA-C	-5.78	1.45	1.52
28	H	134	THR	C-N	5.78	1.41	1.33
16	V	32	ILE	C-N	5.78	1.41	1.33
16	V	58	VAL	C-N	5.78	1.39	1.33
17	T	266	TYR	CA-C	-5.78	1.45	1.52
1	A	200	GLU	C-N	5.78	1.42	1.33
10	3	93	SER	CA-C	-5.78	1.45	1.52
21	N	141	ILE	CA-CB	-5.78	1.47	1.54
28	H	94	GLU	CA-C	-5.78	1.45	1.52
24	Q	140	LYS	C-N	5.78	1.41	1.33
30	K	195	ALA	CA-C	-5.78	1.44	1.52
33	J	346	VAL	N-CA	-5.78	1.39	1.46
5	e	93	ARG	C-N	5.77	1.41	1.33
9	i	76	GLY	CA-C	-5.77	1.44	1.51
2	B	101	TYR	CA-CB	5.77	1.62	1.54
10	j	166	THR	C-N	5.77	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	30	THR	C-N	5.77	1.41	1.33
27	O	116	ASN	N-CA	-5.77	1.39	1.46
30	K	54	LEU	CA-C	5.77	1.60	1.52
11	k	44	MET	C-N	5.77	1.41	1.33
20	Z	762	GLY	CA-C	-5.77	1.45	1.52
3	C	70	ASN	CA-C	-5.77	1.45	1.52
23	P	164	GLN	CA-C	-5.77	1.44	1.52
30	K	66	ASP	N-CA	-5.77	1.39	1.46
32	M	184	GLY	CA-C	-5.77	1.43	1.51
7	G	12	ASN	N-CA	-5.77	1.39	1.46
20	Z	208	VAL	N-CA	-5.77	1.39	1.46
20	Z	80	SER	CA-C	5.76	1.60	1.52
30	K	241	GLU	CA-CB	5.76	1.62	1.53
31	L	111	GLU	CA-CB	5.76	1.63	1.53
15	W	193	GLU	CA-C	-5.76	1.45	1.52
17	T	174	PHE	CA-C	-5.76	1.45	1.52
27	O	47	LYS	C-N	5.76	1.41	1.33
33	J	42	ARG	NE-CZ	5.76	1.39	1.33
1	a	95	LEU	C-N	-5.76	1.26	1.33
4	d	113	VAL	N-CA	-5.76	1.39	1.46
10	j	99	ARG	CA-C	-5.76	1.45	1.52
13	6	200	THR	CA-CB	-5.76	1.44	1.53
21	N	248	GLU	CA-C	-5.76	1.45	1.52
24	Q	411	SER	C-N	5.76	1.41	1.33
28	H	56	LEU	CA-C	-5.76	1.45	1.52
30	K	374	ARG	CD-NE	5.76	1.54	1.46
4	d	22	TYR	C-N	5.76	1.41	1.33
20	Z	36	GLU	CA-CB	5.76	1.62	1.54
21	N	368	THR	C-N	5.76	1.41	1.33
30	K	121	ARG	N-CA	-5.76	1.38	1.46
4	D	32	CYS	CA-C	-5.76	1.45	1.53
27	O	169	ASN	N-CA	-5.76	1.39	1.46
10	j	5	SER	N-CA	-5.76	1.39	1.46
4	D	218	ASP	CB-CG	5.76	1.66	1.52
11	4	133	HIS	CD2-NE2	5.76	1.44	1.37
17	T	64	VAL	C-N	5.76	1.40	1.34
31	L	81	ILE	C-N	5.76	1.41	1.33
4	d	48	ARG	N-CA	-5.75	1.39	1.46
26	U	29	GLU	CA-C	5.75	1.61	1.52
27	O	147	ARG	CD-NE	5.75	1.54	1.46
11	4	96	ARG	CA-C	5.75	1.58	1.52
21	N	787	MET	CA-C	5.75	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	ARG	NE-CZ	5.75	1.39	1.33
12	5	234	ARG	CZ-NH2	5.75	1.41	1.33
21	N	614	ASN	CA-C	-5.75	1.45	1.52
26	U	230	GLN	CA-C	-5.75	1.45	1.52
32	M	140	LEU	N-CA	-5.75	1.39	1.46
32	M	365	SER	CA-C	-5.75	1.44	1.52
30	K	371	LEU	CB-CG	5.75	1.65	1.53
33	J	146	THR	N-CA	-5.75	1.38	1.45
6	F	88	LEU	CA-C	5.75	1.60	1.52
8	1	198	TYR	CA-CB	5.75	1.62	1.53
23	P	310	ARG	CD-NE	5.75	1.54	1.46
12	l	176	ILE	CA-CB	5.75	1.60	1.54
26	U	248	ASP	N-CA	-5.75	1.39	1.46
33	J	76	ILE	C-N	5.75	1.40	1.33
23	P	265	VAL	CA-C	5.75	1.59	1.52
28	H	393	SER	C-N	5.75	1.41	1.33
6	f	197	ILE	CA-CB	-5.74	1.47	1.54
13	m	25	GLY	N-CA	-5.74	1.39	1.45
22	S	100	HIS	CD2-NE2	5.74	1.44	1.37
26	U	33	CYS	CA-C	-5.74	1.45	1.52
33	J	285	SER	N-CA	-5.74	1.39	1.46
11	k	66	LEU	C-N	5.74	1.41	1.34
13	m	28	PHE	CA-C	-5.74	1.45	1.52
3	C	214	ALA	N-CA	-5.74	1.38	1.45
10	3	86	THR	CA-CB	-5.74	1.44	1.53
1	A	44	ALA	C-N	5.74	1.41	1.33
30	K	349	ARG	CZ-NH2	5.74	1.41	1.33
31	L	80	ASN	CA-C	-5.74	1.45	1.52
33	J	55	VAL	C-N	5.74	1.41	1.33
7	g	126	TYR	CZ-OH	5.74	1.50	1.38
8	h	104	ALA	C-N	5.74	1.36	1.33
13	m	222	LYS	CA-C	-5.74	1.45	1.52
11	4	97	PRO	N-CD	-5.74	1.39	1.47
21	N	97	PHE	CA-CB	5.74	1.62	1.53
21	N	660	LEU	CB-CG	5.74	1.65	1.53
32	M	288	THR	N-CA	-5.74	1.38	1.45
4	d	68	ASP	CA-C	-5.74	1.46	1.53
10	3	164	PHE	N-CA	-5.74	1.39	1.46
33	J	13	GLU	N-CA	-5.74	1.39	1.46
13	m	93	SER	CA-C	-5.74	1.45	1.53
2	B	137	ALA	C-O	-5.74	1.17	1.23
5	E	101	LEU	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	176	SER	N-CA	-5.74	1.39	1.46
29	I	89	GLN	C-N	5.74	1.41	1.33
4	d	216	LYS	CA-CB	5.73	1.61	1.54
10	3	47	GLY	C-N	5.73	1.41	1.33
14	7	161	ARG	NE-CZ	5.73	1.39	1.33
22	S	212	SER	N-CA	-5.73	1.39	1.46
23	P	386	GLN	C-N	5.73	1.41	1.33
22	S	19	HIS	N-CA	-5.73	1.39	1.46
24	Q	48	ASP	N-CA	-5.73	1.38	1.46
33	J	133	LEU	C-N	5.73	1.41	1.33
4	d	24	LEU	CA-CB	5.73	1.62	1.53
7	g	38	ILE	N-CA	5.73	1.52	1.46
9	i	72	CYS	CA-CB	5.73	1.64	1.53
17	T	138	ASP	CA-C	-5.73	1.48	1.53
29	I	84	PRO	C-N	5.73	1.41	1.33
32	M	430	VAL	CA-CB	-5.73	1.47	1.54
5	e	222	ILE	CB-CG1	5.73	1.65	1.53
1	A	155	TYR	CA-C	-5.73	1.45	1.52
9	2	100	SER	N-CA	-5.73	1.38	1.46
10	3	15	MET	N-CA	-5.73	1.38	1.45
11	4	76	SER	N-CA	-5.73	1.38	1.45
16	V	163	ALA	CA-CB	5.73	1.62	1.53
17	T	213	ASN	CA-CB	5.73	1.63	1.53
20	Z	817	LEU	CA-C	-5.73	1.45	1.52
25	R	324	ARG	CA-C	-5.73	1.44	1.52
33	J	237	ALA	CA-C	-5.73	1.45	1.52
11	k	159	ASP	CA-C	-5.73	1.45	1.52
19	Y	57	THR	CA-CB	-5.73	1.45	1.53
29	I	353	PRO	N-CD	-5.73	1.39	1.47
12	l	264	GLY	C-N	5.72	1.41	1.33
13	m	203	HIS	CB-CG	5.72	1.58	1.50
4	D	33	ALA	N-CA	-5.72	1.38	1.45
10	3	161	GLU	N-CA	-5.72	1.38	1.46
12	5	81	PHE	CA-CB	5.72	1.64	1.53
23	P	419	VAL	C-N	5.72	1.41	1.33
28	H	420	ARG	NE-CZ	5.72	1.39	1.33
32	M	408	SER	CA-C	-5.72	1.46	1.52
20	Z	614	VAL	CA-C	-5.72	1.45	1.52
14	7	41	GLY	C-N	5.72	1.41	1.33
2	B	140	ASP	CA-CB	-5.72	1.43	1.53
7	G	205	GLU	C-N	5.72	1.42	1.33
22	S	371	LEU	CA-C	-5.72	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	231	TYR	N-CA	-5.72	1.38	1.45
21	N	457	SER	N-CA	-5.72	1.39	1.46
21	N	511	GLY	CA-C	5.72	1.59	1.51
6	F	82	ARG	CD-NE	5.72	1.54	1.46
12	5	241	HIS	ND1-CE1	5.72	1.38	1.32
25	R	378	ASN	CA-C	-5.72	1.47	1.53
29	I	238	ASN	CG-ND2	5.72	1.45	1.33
13	m	151	ALA	CA-C	-5.71	1.45	1.52
21	N	23	TYR	C-N	5.71	1.41	1.33
22	S	357	LEU	CA-CB	5.71	1.62	1.53
6	F	3	ARG	NE-CZ	5.71	1.39	1.33
22	S	351	ALA	CA-C	-5.71	1.45	1.52
5	e	241	LYS	N-CA	-5.71	1.39	1.46
20	Z	448	LYS	CA-CB	5.71	1.62	1.53
24	Q	105	GLU	C-N	5.71	1.41	1.33
31	L	208	GLN	CA-C	-5.71	1.45	1.52
2	b	103	GLU	CA-C	-5.71	1.45	1.52
8	1	75	TYR	CA-C	-5.71	1.45	1.52
13	6	158	LEU	N-CA	-5.71	1.38	1.46
20	Z	586	GLU	C-N	5.71	1.41	1.33
24	Q	333	SER	CA-C	-5.71	1.45	1.52
31	L	207	PHE	C-N	5.71	1.41	1.34
2	b	239	THR	CA-CB	-5.71	1.45	1.53
30	K	86	VAL	CA-C	-5.71	1.45	1.52
33	J	244	ILE	CA-C	-5.71	1.46	1.52
6	F	103	LEU	C-N	5.71	1.41	1.33
4	d	59	ILE	C-N	5.70	1.41	1.33
6	F	114	ASP	CA-C	-5.70	1.45	1.52
13	6	76	PHE	C-N	5.70	1.41	1.33
23	P	439	MET	C-N	5.70	1.41	1.33
7	g	216	ILE	CA-CB	-5.70	1.47	1.54
14	7	191	VAL	CA-C	-5.70	1.46	1.52
20	Z	123	ALA	CA-C	-5.70	1.45	1.52
28	H	158	GLY	CA-C	-5.70	1.44	1.51
33	J	156	GLN	C-N	5.70	1.41	1.33
1	a	186	PHE	N-CA	5.70	1.53	1.46
4	d	97	ARG	N-CA	-5.70	1.38	1.46
4	d	179	TYR	CA-CB	5.70	1.63	1.53
5	e	99	HIS	CE1-NE2	-5.70	1.26	1.32
3	C	49	GLU	N-CA	-5.70	1.39	1.46
29	I	300	ARG	NE-CZ	5.70	1.39	1.33
32	M	141	LYS	CA-C	-5.70	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	247	GLU	C-O	-5.70	1.17	1.24
30	K	337	LYS	N-CA	-5.70	1.39	1.46
1	A	163	TYR	CA-C	-5.70	1.45	1.52
5	E	70	ILE	CA-CB	5.70	1.60	1.54
10	3	66	MET	N-CA	-5.70	1.39	1.46
25	R	355	SER	CA-CB	5.70	1.62	1.53
30	K	134	SER	CA-C	5.70	1.60	1.52
30	K	211	LEU	CA-CB	5.70	1.62	1.53
11	k	22	THR	CA-C	-5.69	1.46	1.52
22	S	106	GLY	CA-C	5.69	1.59	1.51
23	P	399	ILE	N-CA	-5.69	1.39	1.46
28	H	276	GLY	C-O	-5.69	1.18	1.24
30	K	124	SER	N-CA	5.69	1.53	1.45
1	a	236	LEU	C-N	5.69	1.41	1.33
5	e	8	TYR	N-CA	5.69	1.53	1.46
12	l	286	ILE	CA-CB	-5.69	1.48	1.54
1	A	104	PHE	C-N	5.69	1.41	1.33
24	Q	86	MET	CA-CB	5.69	1.62	1.53
25	R	364	LEU	CA-C	-5.69	1.45	1.52
30	K	148	ASP	N-CA	-5.69	1.39	1.46
10	3	146	LEU	CA-C	-5.69	1.45	1.52
29	I	253	ILE	CA-CB	-5.69	1.47	1.54
30	K	72	GLN	CA-CB	5.69	1.62	1.53
6	F	135	ILE	C-O	-5.69	1.18	1.24
9	2	175	LEU	CA-C	-5.69	1.45	1.53
15	W	46	GLU	CA-C	5.69	1.60	1.52
22	S	111	ARG	CD-NE	5.69	1.54	1.46
27	O	265	LYS	N-CA	-5.69	1.39	1.46
32	M	115	LYS	N-CA	-5.69	1.39	1.46
8	h	71	HIS	CG-ND1	5.69	1.44	1.38
9	i	245	SER	C-N	5.69	1.40	1.33
9	i	98	TYR	CZ-OH	5.68	1.50	1.38
11	k	33	ASP	CA-C	-5.68	1.45	1.52
13	6	23	ILE	CA-C	-5.68	1.45	1.52
20	Z	203	LEU	CA-CB	5.68	1.62	1.54
27	O	250	TRP	C-N	5.68	1.41	1.33
3	c	217	ARG	CZ-NH1	5.68	1.40	1.32
7	g	203	ALA	CA-C	-5.68	1.44	1.52
5	E	196	ALA	C-N	5.68	1.41	1.33
20	Z	441	TYR	C-N	5.68	1.41	1.33
26	U	227	GLY	C-O	5.68	1.30	1.23
30	K	63	LEU	C-N	5.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	280	MET	N-CA	-5.68	1.39	1.46
32	M	166	ARG	CZ-NH2	5.68	1.40	1.33
3	c	31	HIS	ND1-CE1	5.68	1.38	1.32
4	d	29	ARG	CZ-NH2	5.68	1.40	1.33
4	d	199	LEU	C-N	5.68	1.41	1.33
10	3	150	CYS	N-CA	-5.68	1.39	1.46
26	U	208	VAL	CA-C	-5.68	1.46	1.52
27	O	358	ILE	C-N	5.68	1.41	1.33
30	K	73	ARG	CD-NE	5.68	1.54	1.46
21	N	834	GLU	N-CA	-5.68	1.38	1.46
25	R	270	VAL	C-N	5.68	1.40	1.33
29	I	271	ALA	CA-CB	5.68	1.62	1.53
11	k	68	SER	CA-C	-5.68	1.45	1.52
2	B	177	LYS	CA-C	-5.68	1.45	1.52
13	m	18	GLY	N-CA	-5.68	1.39	1.45
13	m	143	GLN	C-O	-5.68	1.16	1.24
2	B	6	SER	CA-C	-5.68	1.45	1.53
4	D	98	LEU	N-CA	-5.68	1.39	1.46
10	3	171	LEU	CA-C	-5.68	1.45	1.52
20	Z	803	ALA	N-CA	-5.68	1.39	1.46
21	N	128	ILE	N-CA	-5.68	1.39	1.46
4	D	49	ARG	NE-CZ	5.67	1.39	1.33
22	S	160	ARG	NE-CZ	5.67	1.39	1.33
32	M	246	LEU	N-CA	-5.67	1.39	1.46
7	g	201	TYR	C-N	5.67	1.42	1.33
14	n	263	THR	CA-C	-5.67	1.46	1.52
4	D	29	ARG	CZ-NH1	5.67	1.40	1.32
5	E	159	GLU	N-CA	-5.67	1.40	1.46
16	V	136	ALA	CA-C	-5.67	1.45	1.52
21	N	81	TYR	CA-CB	5.67	1.62	1.53
21	N	229	VAL	CA-CB	-5.67	1.47	1.54
24	Q	35	SER	N-CA	-5.67	1.39	1.46
5	e	97	VAL	CA-CB	-5.67	1.47	1.54
11	k	156	GLU	CA-C	-5.67	1.45	1.52
23	P	326	ASP	CA-C	-5.67	1.45	1.53
14	7	117	GLU	CA-CB	5.67	1.63	1.54
20	Z	264	PHE	C-N	5.67	1.41	1.34
30	K	395	VAL	CA-CB	-5.67	1.47	1.54
10	j	150	CYS	C-O	-5.67	1.17	1.24
6	F	135	ILE	C-N	5.67	1.41	1.33
6	F	174	ARG	NE-CZ	5.67	1.39	1.33
10	3	193	ASP	CA-C	-5.67	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	266	TYR	CA-CB	5.67	1.62	1.53
28	H	432	ARG	NE-CZ	5.67	1.39	1.33
1	a	96	ARG	NE-CZ	5.66	1.39	1.33
8	1	201	GLU	C-N	5.66	1.41	1.33
12	5	261	ILE	C-N	5.66	1.41	1.33
7	G	104	LYS	CA-C	-5.66	1.46	1.53
16	V	241	THR	N-CA	-5.66	1.39	1.46
1	a	72	ILE	N-CA	-5.66	1.39	1.46
1	A	225	VAL	C-N	5.66	1.39	1.33
24	Q	262	LEU	C-O	-5.66	1.17	1.24
25	R	412	THR	CA-C	-5.66	1.45	1.52
33	J	344	ARG	NE-CZ	5.66	1.39	1.33
2	b	28	VAL	N-CA	5.66	1.53	1.46
12	5	188	TYR	CZ-OH	5.66	1.50	1.38
22	S	209	ILE	CA-C	-5.66	1.45	1.52
1	a	204	GLU	CA-C	-5.66	1.45	1.52
2	B	68	THR	CA-CB	5.66	1.61	1.54
20	Z	404	ASP	CA-CB	5.66	1.63	1.53
23	P	73	ASP	N-CA	-5.66	1.39	1.46
25	R	131	ALA	CA-CB	-5.66	1.44	1.53
29	I	100	ARG	CZ-NH1	5.66	1.40	1.32
8	1	147	CYS	C-N	5.65	1.41	1.33
16	V	234	GLU	C-N	5.65	1.41	1.33
10	j	104	PHE	C-N	5.65	1.38	1.33
25	R	350	LEU	C-N	5.65	1.41	1.33
28	H	400	ARG	CZ-NH1	5.65	1.40	1.32
31	L	260	ALA	CA-C	-5.65	1.45	1.52
5	E	89	ILE	C-N	5.65	1.41	1.33
8	1	129	HIS	CA-C	-5.65	1.47	1.53
11	4	96	ARG	CD-NE	5.65	1.54	1.46
20	Z	567	ALA	C-N	5.65	1.41	1.33
24	Q	39	SER	C-N	5.65	1.42	1.33
25	R	392	ARG	CZ-NH2	5.65	1.40	1.33
29	I	122	SER	N-CA	5.65	1.50	1.45
9	i	152	TYR	N-CA	-5.65	1.38	1.46
16	V	81	GLU	N-CA	-5.65	1.38	1.46
3	c	222	ASP	C-N	5.65	1.41	1.33
4	d	200	LEU	N-CA	-5.65	1.39	1.46
24	Q	360	SER	CA-CB	5.65	1.62	1.53
10	3	124	PHE	C-O	-5.65	1.17	1.23
18	X	93	SER	CA-CB	5.65	1.62	1.53
32	M	156	LEU	CA-CB	5.65	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	45	ILE	N-CA	-5.64	1.39	1.46
13	m	229	ARG	CA-CB	5.64	1.61	1.53
3	c	86	ILE	CA-CB	5.64	1.61	1.54
11	k	172	MET	C-N	-5.64	1.29	1.33
14	n	262	GLY	N-CA	-5.64	1.37	1.45
20	Z	762	GLY	C-N	5.64	1.42	1.33
24	Q	113	ASP	CA-CB	5.64	1.62	1.53
6	F	172	LEU	N-CA	-5.64	1.39	1.46
4	D	135	ILE	N-CA	-5.64	1.38	1.46
20	Z	304	PRO	CA-CB	5.64	1.61	1.53
25	R	359	VAL	CA-C	-5.64	1.46	1.52
32	M	189	GLN	C-N	5.64	1.41	1.33
33	J	297	LEU	CA-C	-5.64	1.45	1.52
10	j	13	VAL	C-N	5.64	1.40	1.33
10	j	28	ARG	CA-C	-5.64	1.45	1.52
12	5	111	GLU	CA-CB	5.64	1.60	1.52
29	I	323	LYS	C-O	-5.64	1.17	1.23
29	I	432	LEU	N-CA	5.64	1.53	1.46
30	K	101	GLU	N-CA	-5.64	1.40	1.45
13	m	168	TYR	CZ-OH	5.63	1.49	1.38
16	V	117	TRP	CA-C	-5.63	1.45	1.52
33	J	94	TYR	CA-CB	5.63	1.63	1.53
20	Z	606	CYS	CA-C	5.63	1.60	1.52
22	S	68	LEU	CA-CB	5.63	1.61	1.53
4	d	142	ASP	CA-C	-5.63	1.45	1.52
5	e	218	GLN	C-N	5.63	1.41	1.33
6	f	33	SER	CA-C	-5.63	1.45	1.52
3	C	109	GLU	N-CA	5.63	1.53	1.46
19	Y	85	LYS	CA-C	-5.63	1.45	1.52
21	N	62	ALA	N-CA	-5.63	1.38	1.46
24	Q	331	THR	CA-C	-5.63	1.45	1.52
8	1	121	THR	C-N	5.63	1.38	1.33
19	Y	33	ASP	N-CA	-5.63	1.39	1.46
12	5	245	TYR	CA-C	-5.63	1.45	1.52
18	X	37	PRO	N-CA	-5.63	1.40	1.47
21	N	604	ARG	NE-CZ	5.63	1.39	1.33
26	U	287	ALA	N-CA	-5.63	1.39	1.46
4	d	111	ARG	CD-NE	5.63	1.54	1.46
5	e	119	LEU	CA-C	-5.63	1.45	1.52
5	E	64	ILE	CA-C	-5.63	1.45	1.52
6	F	29	ILE	CA-C	-5.63	1.46	1.52
20	Z	454	GLY	CA-C	-5.63	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	196	THR	CA-C	-5.62	1.45	1.53
24	Q	320	GLN	CA-C	-5.62	1.45	1.52
7	G	113	ALA	C-N	5.62	1.41	1.33
21	N	26	GLU	N-CA	-5.62	1.39	1.46
1	a	210	MET	CA-CB	5.62	1.62	1.53
4	d	88	LYS	CA-C	-5.62	1.45	1.52
5	e	27	SER	CA-C	-5.62	1.44	1.52
8	h	43	LEU	N-CA	-5.62	1.39	1.46
10	j	120	PHE	C-N	5.62	1.41	1.33
32	M	187	ASP	N-CA	-5.62	1.39	1.46
2	b	91	LYS	CA-CB	5.62	1.62	1.53
5	E	69	GLU	CA-CB	5.62	1.61	1.53
20	Z	195	PHE	N-CA	-5.62	1.39	1.46
21	N	623	PHE	N-CA	5.62	1.53	1.46
30	K	95	VAL	N-CA	-5.62	1.39	1.46
31	L	383	SER	C-N	5.62	1.41	1.33
24	Q	209	TYR	CA-C	-5.62	1.45	1.52
8	h	86	THR	CA-C	-5.62	1.45	1.52
4	D	6	ARG	NE-CZ	5.62	1.39	1.33
6	F	47	VAL	CA-CB	-5.62	1.47	1.54
16	V	50	MET	CA-C	-5.62	1.46	1.52
30	K	128	ARG	NE-CZ	5.62	1.39	1.33
1	A	225	VAL	N-CA	-5.61	1.39	1.46
21	N	16	ASN	CA-C	-5.61	1.46	1.52
27	O	15	ARG	CD-NE	5.61	1.54	1.46
29	I	325	ILE	C-N	5.61	1.41	1.33
5	e	199	LEU	C-N	5.61	1.41	1.33
17	T	174	PHE	CA-CB	5.61	1.62	1.53
11	4	136	SER	CA-C	-5.61	1.45	1.52
12	5	114	PRO	N-CD	-5.61	1.39	1.47
29	I	346	ARG	N-CA	-5.61	1.39	1.45
31	L	435	GLN	N-CA	-5.61	1.38	1.45
5	e	132	ARG	NE-CZ	5.61	1.39	1.33
17	T	57	ILE	N-CA	-5.61	1.39	1.46
24	Q	281	ILE	CA-C	5.61	1.59	1.52
12	l	255	VAL	C-N	5.61	1.42	1.33
18	X	7	VAL	CA-C	-5.61	1.41	1.52
21	N	340	HIS	CA-C	-5.61	1.44	1.52
13	m	74	LYS	CA-C	-5.61	1.45	1.52
23	P	278	ASN	CA-CB	5.61	1.62	1.53
25	R	28	GLU	C-N	5.61	1.41	1.33
29	I	381	VAL	C-N	5.61	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	345	ARG	CD-NE	5.61	1.54	1.46
7	g	69	VAL	CA-CB	5.60	1.62	1.54
12	5	261	ILE	C-O	-5.60	1.18	1.24
2	b	88	LYS	N-CA	-5.60	1.39	1.46
3	c	37	GLY	C-N	5.60	1.40	1.33
14	n	83	VAL	N-CA	-5.60	1.39	1.46
2	B	193	LEU	N-CA	-5.60	1.39	1.46
3	C	245	THR	N-CA	-5.60	1.35	1.46
15	W	121	SER	CA-C	-5.60	1.45	1.53
20	Z	771	HIS	ND1-CE1	5.60	1.38	1.32
7	G	60	VAL	CA-C	-5.60	1.47	1.52
25	R	151	GLU	N-CA	-5.60	1.39	1.46
30	K	177	LEU	CA-C	-5.60	1.47	1.53
33	J	399	SER	CA-C	-5.60	1.45	1.52
3	C	210	ARG	CD-NE	5.60	1.54	1.46
4	D	109	LEU	CA-C	-5.60	1.45	1.52
23	P	233	GLU	N-CA	-5.60	1.39	1.46
4	d	18	PHE	CA-CB	5.60	1.62	1.53
9	i	187	ALA	CA-CB	5.60	1.62	1.53
12	5	282	PHE	CA-CB	5.60	1.61	1.53
13	6	36	ARG	CD-NE	5.60	1.54	1.46
31	L	70	TYR	CA-C	-5.60	1.45	1.52
3	c	86	ILE	CA-C	-5.59	1.46	1.52
14	7	90	ILE	C-N	5.59	1.41	1.33
24	Q	342	LEU	N-CA	5.59	1.53	1.46
31	L	375	ASP	N-CA	-5.59	1.39	1.46
32	M	57	VAL	C-N	5.59	1.41	1.33
4	d	233	VAL	CA-CB	-5.59	1.47	1.54
4	D	163	THR	N-CA	-5.59	1.39	1.46
7	G	230	PHE	N-CA	-5.59	1.39	1.46
13	6	145	ARG	CD-NE	5.59	1.54	1.46
32	M	53	HIS	CD2-NE2	-5.59	1.31	1.37
9	i	56	ALA	N-CA	-5.59	1.39	1.46
2	B	83	ARG	CZ-NH2	5.59	1.40	1.33
24	Q	27	TYR	N-CA	5.59	1.53	1.46
28	H	244	LYS	CA-C	-5.59	1.45	1.52
3	c	187	ASP	N-CA	5.59	1.53	1.46
3	C	149	TYR	C-N	5.59	1.40	1.33
22	S	268	LEU	N-CA	-5.59	1.39	1.46
22	S	310	LEU	CA-CB	5.59	1.62	1.53
9	i	217	ARG	CZ-NH2	5.59	1.40	1.33
3	C	224	GLU	C-N	5.59	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	195	SER	N-CA	-5.59	1.39	1.46
17	T	92	ASN	C-N	5.59	1.40	1.33
24	Q	137	LEU	CA-CB	5.59	1.62	1.53
30	K	350	ARG	NE-CZ	5.59	1.39	1.33
15	W	92	GLN	CA-C	-5.58	1.45	1.52
29	I	132	ILE	CA-C	-5.58	1.45	1.52
7	g	86	ARG	NE-CZ	5.58	1.39	1.33
1	A	96	ARG	NE-CZ	5.58	1.39	1.33
6	F	170	THR	N-CA	5.58	1.53	1.46
10	j	204	GLN	N-CA	-5.58	1.39	1.46
21	N	7	ALA	CA-C	5.58	1.59	1.52
23	P	247	THR	CA-C	-5.58	1.45	1.52
23	P	425	HIS	CG-CD2	-5.58	1.29	1.35
24	Q	403	PRO	CA-C	-5.58	1.45	1.52
17	T	41	ILE	N-CA	-5.58	1.39	1.46
13	m	38	ILE	CA-C	-5.58	1.46	1.52
10	3	200	LEU	C-N	5.58	1.41	1.33
11	4	144	LEU	C-N	5.58	1.41	1.33
21	N	231	ASN	C-N	5.58	1.42	1.33
27	O	166	ARG	C-N	5.58	1.41	1.33
4	d	143	ASP	N-CA	-5.58	1.40	1.46
16	V	54	LEU	CA-CB	5.58	1.62	1.53
3	C	73	ILE	N-CA	5.58	1.52	1.46
5	E	155	LEU	CA-C	-5.58	1.45	1.52
16	V	127	LYS	C-N	5.58	1.41	1.33
16	V	294	SER	C-N	-5.58	1.26	1.33
23	P	129	LYS	CA-C	-5.58	1.45	1.52
26	U	145	ASP	C-N	5.58	1.41	1.33
31	L	304	THR	CA-C	-5.58	1.45	1.52
32	M	357	ARG	CZ-NH2	5.58	1.40	1.33
2	B	72	GLY	CA-C	-5.57	1.45	1.52
31	L	279	PHE	N-CA	-5.57	1.39	1.46
11	k	158	LEU	C-N	5.57	1.41	1.34
4	D	106	VAL	CA-CB	-5.57	1.47	1.54
7	G	157	TYR	CA-C	-5.57	1.45	1.52
19	Y	23	GLU	CA-C	-5.57	1.45	1.52
22	S	211	ARG	CZ-NH2	5.57	1.40	1.33
5	E	123	PHE	CA-CB	5.57	1.62	1.54
30	K	132	LYS	N-CA	-5.57	1.42	1.46
1	A	185	HIS	CA-C	-5.57	1.45	1.52
13	m	125	ASP	CA-CB	5.57	1.63	1.53
7	G	107	ILE	N-CA	-5.57	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	116	GLN	C-N	5.57	1.41	1.33
26	U	68	LEU	C-N	5.57	1.41	1.33
31	L	326	ALA	CA-C	-5.57	1.45	1.52
6	F	35	THR	CA-C	-5.56	1.45	1.52
17	T	253	GLU	CA-C	5.56	1.59	1.52
29	I	264	CYS	C-N	5.56	1.41	1.33
16	V	43	ALA	N-CA	5.56	1.53	1.46
20	Z	440	LEU	C-N	5.56	1.40	1.33
28	H	344	ASP	CA-CB	5.56	1.61	1.53
31	L	210	VAL	C-N	5.56	1.42	1.33
31	L	329	ARG	CD-NE	5.56	1.54	1.46
4	d	155	ILE	N-CA	-5.56	1.39	1.46
9	i	212	ASP	C-N	5.56	1.42	1.33
13	m	149	ALA	N-CA	-5.56	1.39	1.46
1	A	199	TRP	N-CA	-5.56	1.39	1.46
2	B	23	TYR	CA-CB	5.56	1.62	1.53
2	B	207	ASP	C-N	5.56	1.41	1.33
25	R	337	VAL	CA-C	5.56	1.60	1.52
27	O	266	PHE	C-O	-5.56	1.17	1.24
13	6	103	HIS	ND1-CE1	5.56	1.38	1.32
15	W	147	ILE	CA-C	-5.56	1.45	1.52
18	X	75	TRP	NE1-CE2	5.56	1.43	1.37
23	P	30	ASN	CA-CB	5.56	1.62	1.53
28	H	352	MET	CA-C	-5.56	1.46	1.52
8	1	92	LYS	C-N	5.56	1.41	1.33
6	F	55	GLU	C-O	-5.55	1.16	1.24
7	G	219	CYS	C-N	5.55	1.40	1.33
13	6	34	ASP	CA-C	-5.55	1.45	1.52
16	V	168	LEU	CA-CB	5.55	1.62	1.53
23	P	313	ILE	CA-C	-5.55	1.45	1.52
27	O	23	HIS	ND1-CE1	5.55	1.38	1.32
13	m	75	ARG	N-CA	-5.55	1.39	1.46
7	G	187	LEU	C-N	5.55	1.40	1.33
27	O	145	LYS	CA-CB	5.55	1.61	1.53
5	e	38	ILE	C-O	-5.55	1.18	1.24
14	n	109	TYR	CA-C	-5.55	1.45	1.52
16	V	62	THR	N-CA	-5.55	1.39	1.46
20	Z	745	LEU	C-N	5.55	1.40	1.33
27	O	77	SER	C-O	-5.55	1.17	1.24
1	A	131	ARG	CZ-NH2	5.55	1.40	1.33
20	Z	279	THR	CA-C	-5.55	1.45	1.52
22	S	157	GLU	CA-CB	5.55	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	94	PHE	CA-CB	5.55	1.61	1.53
24	Q	221	MET	CA-C	-5.55	1.45	1.52
13	m	55	GLY	C-N	5.54	1.41	1.33
20	Z	1	MET	C-N	5.54	1.41	1.33
1	A	144	VAL	CA-C	-5.54	1.45	1.52
6	F	89	ARG	CZ-NH2	5.54	1.40	1.33
16	V	193	ASN	CA-C	-5.54	1.45	1.52
21	N	593	PHE	CA-C	-5.54	1.45	1.52
26	U	134	THR	CA-C	-5.54	1.45	1.52
30	K	141	ARG	NE-CZ	5.54	1.39	1.33
3	C	87	LEU	CA-C	-5.54	1.45	1.52
7	G	165	THR	CA-C	-5.54	1.46	1.52
8	1	109	ALA	CA-C	-5.54	1.45	1.52
13	6	183	LEU	CA-C	-5.54	1.46	1.52
15	W	2	VAL	C-N	5.54	1.40	1.33
24	Q	252	HIS	CA-CB	5.54	1.62	1.53
28	H	76	LEU	CA-C	-5.54	1.45	1.52
28	H	291	VAL	N-CA	-5.54	1.39	1.46
32	M	395	THR	CA-CB	5.54	1.62	1.53
20	Z	29	ASP	CA-CB	5.54	1.61	1.53
33	J	48	ARG	CZ-NH2	5.54	1.40	1.33
7	g	214	LEU	CA-C	-5.54	1.46	1.52
13	6	84	HIS	CG-CD2	5.54	1.42	1.35
20	Z	886	VAL	CA-CB	-5.54	1.48	1.54
22	S	294	ILE	C-N	5.54	1.41	1.33
31	L	202	LYS	CA-C	5.54	1.59	1.52
31	L	420	ARG	CD-NE	5.54	1.54	1.46
14	7	182	HIS	CA-CB	5.54	1.62	1.53
17	T	207	ALA	N-CA	-5.54	1.39	1.46
31	L	251	ILE	CA-C	-5.54	1.45	1.52
3	C	244	ILE	C-N	5.54	1.41	1.33
18	X	11	ARG	CD-NE	5.54	1.53	1.46
27	O	270	ILE	CA-CB	-5.54	1.46	1.54
29	I	148	LEU	C-N	5.54	1.40	1.33
29	I	390	ALA	C-O	-5.54	1.17	1.24
14	n	188	LEU	C-N	5.53	1.42	1.33
3	C	137	TYR	CA-C	-5.53	1.46	1.52
21	N	361	ASN	CA-C	5.53	1.60	1.52
24	Q	13	ARG	NE-CZ	5.53	1.39	1.33
26	U	65	VAL	N-CA	-5.53	1.39	1.46
7	g	232	LYS	N-CA	-5.53	1.39	1.46
31	L	156	MET	C-N	5.53	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	57	ALA	C-N	5.53	1.41	1.33
13	6	161	GLN	CA-CB	5.53	1.62	1.53
17	T	105	LEU	N-CA	-5.53	1.39	1.46
20	Z	287	ARG	CA-C	-5.53	1.45	1.52
20	Z	553	ARG	CZ-NH2	5.53	1.40	1.33
13	6	152	SER	CA-C	-5.53	1.45	1.52
15	W	122	ARG	NE-CZ	5.53	1.39	1.33
6	f	79	PRO	N-CA	-5.53	1.40	1.47
13	m	198	SER	CA-CB	5.53	1.61	1.53
7	G	179	LEU	C-N	5.53	1.40	1.33
9	2	115	HIS	CA-C	-5.53	1.45	1.52
20	Z	585	LEU	CA-CB	5.53	1.61	1.53
23	P	194	SER	C-N	5.53	1.41	1.33
24	Q	338	LEU	C-N	5.53	1.41	1.33
27	O	89	SER	C-N	5.53	1.41	1.33
31	L	95	ILE	CA-C	-5.53	1.45	1.52
33	J	101	ASP	C-N	5.53	1.41	1.33
11	k	42	THR	CA-C	5.52	1.59	1.52
7	G	178	LYS	CA-C	-5.52	1.45	1.52
20	Z	832	ARG	CZ-NH2	5.52	1.40	1.33
8	1	34	TYR	C-N	5.52	1.40	1.33
24	Q	309	ARG	CA-CB	5.52	1.61	1.53
30	K	335	ASP	C-N	5.52	1.41	1.33
2	b	115	ALA	CA-C	-5.52	1.45	1.52
25	R	196	SER	CA-C	-5.52	1.45	1.52
32	M	246	LEU	CA-C	-5.52	1.46	1.53
10	j	164	PHE	CA-C	-5.52	1.45	1.52
2	B	99	ARG	CD-NE	5.52	1.53	1.46
4	D	210	ILE	C-O	-5.52	1.18	1.24
6	F	178	THR	CA-CB	-5.52	1.44	1.53
21	N	122	GLN	N-CA	-5.52	1.38	1.45
24	Q	132	PHE	N-CA	-5.52	1.39	1.46
24	Q	399	VAL	N-CA	-5.52	1.39	1.46
12	l	235	SER	C-N	5.52	1.40	1.33
4	D	127	ARG	CZ-NH2	5.52	1.40	1.33
23	P	184	MET	C-N	5.52	1.41	1.33
22	S	53	ILE	N-CA	-5.51	1.39	1.46
24	Q	193	LYS	CA-C	-5.51	1.45	1.52
29	I	109	LEU	CA-C	-5.51	1.46	1.52
6	f	74	LEU	N-CA	-5.51	1.38	1.45
14	n	161	ARG	NE-CZ	5.51	1.39	1.33
10	3	169	GLN	C-N	5.51	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	87	LYS	N-CA	5.51	1.51	1.46
22	S	338	MET	C-N	5.51	1.42	1.33
28	H	312	ASP	N-CA	-5.51	1.39	1.46
4	d	183	GLU	CA-C	-5.51	1.46	1.52
6	f	229	ALA	C-N	5.51	1.41	1.33
26	U	32	ARG	CA-C	-5.51	1.45	1.53
28	H	200	VAL	N-CA	5.51	1.52	1.46
29	I	311	ASN	CA-CB	5.51	1.61	1.53
32	M	342	ARG	CZ-NH1	5.51	1.40	1.32
16	V	221	TRP	C-N	5.51	1.41	1.33
7	g	119	TYR	CA-CB	5.51	1.62	1.53
8	h	66	ASP	CA-C	-5.51	1.45	1.52
10	j	62	THR	N-CA	-5.51	1.39	1.46
7	G	125	LEU	CA-C	-5.51	1.45	1.52
15	W	71	LYS	C-N	5.51	1.40	1.33
18	X	130	ASN	C-N	5.51	1.40	1.33
20	Z	198	GLU	N-CA	-5.51	1.39	1.46
2	B	201	GLU	C-N	5.50	1.41	1.33
21	N	798	LYS	CA-CB	5.50	1.62	1.53
25	R	142	ALA	C-N	5.50	1.40	1.33
27	O	192	SER	CA-C	-5.50	1.45	1.52
13	6	225	TYR	C-N	5.50	1.40	1.33
32	M	227	GLY	CA-C	-5.50	1.44	1.51
7	G	11	SER	C-N	5.50	1.41	1.33
13	6	193	ARG	NE-CZ	5.50	1.39	1.33
20	Z	209	PRO	CA-C	5.50	1.60	1.52
25	R	263	ARG	NE-CZ	5.50	1.39	1.33
25	R	355	SER	N-CA	5.50	1.53	1.46
29	I	236	VAL	CA-C	-5.50	1.45	1.52
30	K	336	ARG	CZ-NH2	5.50	1.40	1.33
33	J	39	GLU	CA-CB	5.50	1.61	1.53
2	b	4	ARG	CD-NE	5.50	1.53	1.46
11	k	27	VAL	N-CA	-5.50	1.40	1.46
21	N	63	LEU	N-CA	-5.50	1.39	1.46
29	I	64	ARG	CD-NE	5.50	1.53	1.46
9	i	145	HIS	C-N	5.50	1.41	1.33
7	G	91	ARG	CZ-NH1	5.50	1.40	1.32
14	7	38	ILE	C-N	5.50	1.42	1.33
28	H	367	ARG	NE-CZ	5.50	1.39	1.33
33	J	5	VAL	C-N	5.50	1.38	1.33
2	B	36	GLY	CA-C	-5.50	1.46	1.51
8	1	159	GLU	N-CA	-5.50	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	91	ASP	C-O	-5.50	1.17	1.24
27	O	120	LYS	N-CA	-5.50	1.39	1.46
33	J	236	MET	CA-CB	5.50	1.61	1.53
5	e	162	GLY	CA-C	-5.49	1.44	1.51
9	2	48	ARG	CD-NE	5.49	1.53	1.46
23	P	325	ASP	N-CA	5.49	1.52	1.46
28	H	443	PHE	N-CA	-5.49	1.38	1.46
33	J	186	ILE	CA-C	-5.49	1.45	1.52
1	a	120	ARG	CD-NE	5.49	1.53	1.46
3	c	163	ILE	CA-CB	-5.49	1.49	1.55
6	F	83	VAL	C-O	-5.49	1.18	1.24
4	D	159	TRP	CD2-CE3	-5.49	1.31	1.40
20	Z	500	SER	CA-C	-5.49	1.45	1.52
28	H	49	LEU	C-N	5.49	1.41	1.34
2	b	236	ARG	CZ-NH1	5.49	1.40	1.32
9	i	88	ILE	N-CA	-5.49	1.40	1.46
12	5	137	GLN	N-CA	-5.49	1.39	1.46
21	N	427	ILE	CA-CB	-5.49	1.47	1.54
25	R	159	SER	C-N	5.49	1.40	1.33
30	K	149	ILE	C-N	5.49	1.39	1.32
7	g	61	PRO	CA-CB	5.49	1.60	1.53
14	n	133	MET	CA-C	-5.49	1.45	1.52
2	B	171	ALA	N-CA	5.49	1.52	1.46
4	d	111	ARG	CZ-NH2	5.49	1.40	1.33
10	j	28	ARG	CZ-NH1	5.49	1.40	1.32
5	E	221	CYS	CA-C	-5.49	1.46	1.52
11	4	171	ARG	N-CA	-5.49	1.40	1.46
17	T	14	ALA	N-CA	-5.49	1.39	1.46
20	Z	43	ALA	N-CA	-5.49	1.39	1.46
23	P	177	ILE	C-N	5.49	1.41	1.33
10	j	203	ARG	CZ-NH2	5.48	1.40	1.33
20	Z	823	ASN	CA-C	-5.48	1.45	1.52
22	S	369	GLN	N-CA	-5.48	1.39	1.46
11	k	95	ARG	NE-CZ	5.48	1.39	1.33
4	D	192	VAL	CA-C	-5.48	1.45	1.52
6	F	222	PHE	C-O	-5.48	1.17	1.24
14	7	115	ASP	CA-C	-5.48	1.46	1.52
21	N	393	SER	C-N	5.48	1.40	1.33
25	R	176	ARG	CD-NE	5.48	1.53	1.46
30	K	252	ARG	CD-NE	5.48	1.53	1.46
1	a	96	ARG	CZ-NH1	5.48	1.40	1.32
13	m	99	ARG	CA-C	-5.48	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	35	VAL	C-N	5.48	1.41	1.33
9	2	215	TYR	CA-C	-5.48	1.46	1.52
20	Z	147	GLU	C-N	5.48	1.41	1.33
3	c	73	ILE	CA-C	5.48	1.59	1.52
12	l	119	THR	N-CA	5.48	1.53	1.45
10	3	166	THR	CA-CB	5.48	1.61	1.53
18	X	106	SER	CA-CB	5.48	1.62	1.53
28	H	338	THR	N-CA	-5.48	1.38	1.46
33	J	359	LYS	C-O	-5.48	1.17	1.24
3	c	143	ARG	N-CA	-5.48	1.38	1.46
3	C	191	GLU	N-CA	5.48	1.52	1.46
4	D	105	THR	CA-C	-5.47	1.45	1.52
15	W	76	LEU	C-N	5.47	1.41	1.33
23	P	16	ILE	C-N	5.47	1.40	1.33
27	O	84	ALA	C-O	5.47	1.30	1.24
1	a	135	ARG	CA-C	-5.47	1.46	1.52
8	h	68	VAL	C-N	5.47	1.40	1.33
9	i	138	HIS	ND1-CE1	5.47	1.38	1.32
3	C	183	ASP	N-CA	-5.47	1.39	1.46
11	4	32	ASP	C-N	5.47	1.41	1.33
20	Z	898	HIS	CA-CB	5.47	1.60	1.53
29	I	294	SER	CA-C	-5.47	1.45	1.52
31	L	157	ARG	C-N	5.47	1.40	1.33
16	V	194	ARG	CZ-NH2	5.47	1.40	1.33
21	N	337	GLY	C-N	5.47	1.41	1.33
32	M	412	HIS	CG-ND1	5.47	1.44	1.38
12	l	248	GLY	C-N	5.47	1.40	1.33
14	7	209	ALA	C-N	5.47	1.40	1.33
22	S	394	ILE	C-N	5.47	1.40	1.33
25	R	96	GLN	N-CA	-5.47	1.39	1.46
27	O	159	LYS	C-N	5.47	1.41	1.33
30	K	235	ILE	C-N	5.47	1.41	1.33
32	M	65	ASN	N-CA	-5.47	1.39	1.46
3	c	47	ALA	C-N	5.47	1.40	1.33
5	E	42	THR	CA-C	-5.47	1.45	1.52
28	H	135	ASP	CA-CB	5.47	1.61	1.53
7	g	36	THR	CA-C	5.47	1.59	1.52
9	i	219	TYR	CA-CB	5.47	1.61	1.53
9	2	207	MET	N-CA	-5.47	1.39	1.46
17	T	75	PHE	CA-CB	5.47	1.61	1.53
30	K	131	LEU	CA-C	-5.47	1.45	1.52
7	G	215	GLU	CA-C	-5.46	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	68	SER	C-O	-5.46	1.17	1.24
21	N	770	LYS	N-CA	-5.46	1.39	1.46
22	S	375	ASP	CA-CB	5.46	1.60	1.53
17	T	157	TYR	CZ-OH	5.46	1.49	1.38
11	k	132	ALA	CA-C	-5.46	1.45	1.52
7	G	197	ALA	C-N	5.46	1.41	1.34
17	T	142	LEU	C-N	5.46	1.41	1.33
20	Z	870	ALA	C-N	5.46	1.40	1.33
33	J	179	ILE	N-CA	-5.46	1.40	1.46
9	2	184	ALA	CA-C	-5.46	1.45	1.52
26	U	144	LYS	CA-C	-5.46	1.46	1.52
29	I	292	TYR	CA-CB	5.46	1.62	1.53
9	i	115	HIS	CD2-NE2	5.46	1.43	1.37
12	l	139	ARG	CZ-NH2	5.46	1.40	1.33
21	N	356	LEU	CA-CB	5.46	1.62	1.53
21	N	764	SER	N-CA	-5.46	1.41	1.46
22	S	424	SER	C-N	5.46	1.41	1.33
25	R	97	GLU	N-CA	-5.46	1.39	1.46
26	U	47	ARG	NE-CZ	5.46	1.39	1.33
5	e	10	ARG	NE-CZ	5.46	1.39	1.33
13	m	20	ILE	CA-C	-5.46	1.46	1.52
30	K	236	ARG	NE-CZ	5.46	1.39	1.33
1	a	43	LEU	CA-C	-5.46	1.46	1.52
11	k	82	SER	CA-CB	5.46	1.61	1.53
1	A	132	ALA	CA-C	-5.46	1.44	1.52
22	S	258	GLU	N-CA	-5.46	1.38	1.46
2	b	191	ILE	CA-CB	-5.45	1.47	1.54
2	B	114	VAL	CA-CB	-5.45	1.47	1.54
7	G	221	LEU	CA-C	-5.45	1.45	1.52
22	S	317	HIS	CD2-NE2	5.45	1.43	1.37
24	Q	13	ARG	CZ-NH1	5.45	1.40	1.32
4	d	45	GLY	CA-C	-5.45	1.47	1.51
1	A	230	LYS	N-CA	-5.45	1.39	1.46
4	D	101	GLU	N-CA	-5.45	1.39	1.46
5	E	147	HIS	ND1-CE1	5.45	1.38	1.32
14	7	175	LEU	CA-C	-5.45	1.46	1.52
16	V	42	ARG	CD-NE	5.45	1.53	1.46
21	N	419	THR	CA-C	-5.45	1.45	1.52
21	N	528	ARG	CD-NE	5.45	1.53	1.46
12	l	285	VAL	C-N	5.45	1.39	1.33
4	D	104	VAL	CA-CB	-5.45	1.47	1.54
10	3	122	ALA	N-CA	-5.45	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	160	VAL	CA-C	-5.45	1.46	1.52
31	L	238	THR	CA-CB	-5.45	1.44	1.53
7	g	82	ILE	CA-C	5.45	1.57	1.52
20	Z	926	ASN	C-O	-5.45	1.18	1.24
1	A	90	ALA	CA-CB	5.45	1.61	1.53
20	Z	825	ALA	CA-C	-5.45	1.45	1.52
29	I	54	ARG	CA-CB	5.45	1.62	1.53
8	h	60	ASP	C-N	5.44	1.41	1.34
2	B	150	VAL	CA-C	-5.44	1.45	1.52
17	T	144	TYR	CA-C	-5.44	1.45	1.52
21	N	521	LEU	N-CA	-5.44	1.39	1.46
23	P	132	VAL	CA-C	-5.44	1.45	1.52
27	O	210	ARG	CZ-NH2	5.44	1.40	1.33
32	M	404	ARG	NE-CZ	5.44	1.39	1.33
29	I	193	GLU	C-N	5.44	1.40	1.33
29	I	384	LYS	CA-C	-5.44	1.45	1.52
6	f	46	LEU	N-CA	5.44	1.52	1.46
11	4	159	ASP	CA-CB	5.44	1.61	1.53
14	7	154	SER	C-N	5.44	1.41	1.33
21	N	513	ILE	N-CA	-5.44	1.40	1.46
31	L	91	THR	CA-C	-5.44	1.45	1.52
1	a	179	THR	CA-C	-5.44	1.45	1.52
2	b	13	SER	C-N	-5.44	1.28	1.33
11	k	160	LEU	CA-C	5.44	1.60	1.52
11	4	145	ASP	C-N	5.44	1.40	1.33
22	S	35	LEU	C-N	5.44	1.41	1.33
23	P	128	ASN	N-CA	-5.44	1.39	1.45
25	R	124	ASP	N-CA	-5.44	1.39	1.45
27	O	49	PHE	CA-CB	5.44	1.62	1.53
9	i	95	HIS	ND1-CE1	5.44	1.38	1.32
19	Y	20	LYS	C-N	5.44	1.41	1.33
21	N	843	LYS	C-O	-5.44	1.17	1.23
21	N	880	ARG	CD-NE	5.44	1.53	1.46
21	N	894	ARG	CZ-NH2	5.44	1.40	1.33
22	S	64	ARG	CZ-NH1	5.44	1.40	1.32
24	Q	224	ILE	CA-CB	5.44	1.61	1.54
13	6	18	GLY	C-O	-5.43	1.16	1.23
20	Z	721	ASN	CA-C	-5.43	1.46	1.52
21	N	119	LYS	CA-C	-5.43	1.46	1.52
6	f	117	GLN	C-N	5.43	1.41	1.34
9	i	104	ARG	NE-CZ	5.43	1.39	1.33
21	N	778	LYS	C-N	5.43	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	431	HIS	CB-CG	5.43	1.57	1.50
28	H	246	ILE	CA-C	-5.43	1.45	1.52
28	H	278	GLU	CA-C	-5.43	1.46	1.52
32	M	212	ILE	CA-C	-5.43	1.46	1.52
1	a	204	GLU	N-CA	5.43	1.52	1.46
21	N	524	ILE	C-O	-5.43	1.17	1.24
10	j	108	VAL	CA-C	-5.43	1.46	1.52
14	n	58	ASP	N-CA	-5.43	1.38	1.45
1	A	167	LYS	C-O	-5.43	1.17	1.23
21	N	880	ARG	CZ-NH2	5.43	1.40	1.33
24	Q	329	GLU	CA-C	5.43	1.60	1.52
32	M	70	LYS	CA-CB	5.43	1.62	1.53
33	J	329	ARG	C-N	5.43	1.40	1.33
12	5	149	ILE	C-N	5.43	1.40	1.33
24	Q	49	LYS	C-N	5.43	1.40	1.33
6	f	81	ALA	C-N	5.43	1.41	1.33
13	6	103	HIS	N-CA	-5.43	1.39	1.46
15	W	67	ALA	C-N	5.43	1.40	1.33
24	Q	291	TYR	CA-C	-5.43	1.46	1.52
28	H	433	ALA	CA-CB	5.43	1.62	1.53
13	m	106	TYR	N-CA	-5.42	1.39	1.46
2	B	216	ASP	CA-C	-5.42	1.45	1.52
7	G	136	THR	CA-C	-5.42	1.46	1.52
9	2	159	GLY	C-N	5.42	1.41	1.33
20	Z	115	LEU	C-N	5.42	1.41	1.33
10	3	120	PHE	CA-CB	5.42	1.63	1.53
13	m	221	ARG	CD-NE	5.42	1.53	1.46
11	4	114	PRO	CA-CB	5.42	1.61	1.53
12	5	267	ASP	CA-CB	5.42	1.62	1.53
2	B	12	PHE	CA-C	-5.42	1.45	1.53
2	B	83	ARG	CZ-NH1	5.42	1.40	1.32
27	O	54	SER	N-CA	-5.42	1.39	1.46
15	W	30	ILE	C-N	5.42	1.41	1.33
4	D	160	SER	CA-CB	5.42	1.61	1.53
15	W	166	GLU	CA-CB	5.42	1.65	1.54
16	V	33	ALA	C-O	-5.42	1.17	1.24
16	V	296	LEU	CA-C	-5.42	1.46	1.52
18	X	42	GLU	C-N	5.42	1.40	1.33
30	K	378	LEU	N-CA	5.42	1.52	1.46
2	b	139	HIS	CG-ND1	5.42	1.44	1.38
3	c	131	PHE	CA-C	-5.42	1.46	1.52
9	i	144	ALA	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	220	SER	CA-C	-5.41	1.45	1.52
13	6	188	VAL	C-N	5.41	1.40	1.33
15	W	157	PHE	N-CA	5.41	1.53	1.46
17	T	242	LYS	CA-C	-5.41	1.45	1.52
21	N	769	PRO	CA-CB	5.41	1.62	1.54
24	Q	304	GLU	N-CA	-5.41	1.39	1.46
27	O	298	GLU	CA-CB	5.41	1.61	1.53
29	I	108	THR	N-CA	-5.41	1.39	1.46
4	d	93	ALA	CA-C	-5.41	1.45	1.52
6	f	125	GLY	C-N	5.41	1.42	1.33
7	g	45	GLY	CA-C	-5.41	1.45	1.51
22	S	271	ARG	N-CA	-5.41	1.39	1.46
16	V	44	GLY	C-N	5.41	1.39	1.33
26	U	141	GLU	N-CA	-5.41	1.39	1.46
30	K	314	VAL	N-CA	-5.41	1.39	1.46
1	A	213	ALA	C-N	5.41	1.41	1.33
8	1	128	VAL	CA-C	-5.41	1.46	1.52
20	Z	228	GLU	CA-CB	5.41	1.62	1.53
30	K	408	GLU	CA-CB	5.41	1.62	1.53
33	J	12	LEU	C-N	5.41	1.41	1.34
21	N	464	GLU	CA-C	-5.41	1.45	1.52
3	c	193	ALA	N-CA	-5.41	1.40	1.46
4	D	23	ALA	C-O	-5.41	1.17	1.24
11	4	8	ARG	NE-CZ	5.41	1.39	1.33
16	V	273	ARG	CZ-NH1	5.41	1.40	1.32
21	N	646	LYS	CA-C	-5.41	1.45	1.52
32	M	324	LEU	C-N	5.41	1.40	1.33
8	1	179	GLY	CA-C	-5.40	1.45	1.52
11	k	153	THR	C-N	5.40	1.41	1.33
1	A	54	ILE	CA-C	-5.40	1.46	1.52
11	4	80	VAL	N-CA	5.40	1.52	1.46
22	S	150	LYS	CA-CB	5.40	1.62	1.53
33	J	170	HIS	ND1-CE1	5.40	1.38	1.32
10	j	45	HIS	ND1-CE1	5.40	1.38	1.32
18	X	88	ALA	CA-C	-5.40	1.46	1.52
20	Z	911	LYS	N-CA	5.40	1.52	1.46
23	P	62	ILE	C-N	5.40	1.40	1.33
25	R	200	LYS	CA-CB	5.40	1.61	1.53
28	H	83	ASP	CA-C	-5.40	1.45	1.52
12	5	252	LEU	C-N	5.40	1.40	1.33
29	I	325	ILE	CA-C	-5.40	1.46	1.52
31	L	206	ILE	CA-CB	-5.40	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	190	VAL	C-N	-5.40	1.25	1.33
17	T	50	ILE	C-O	-5.40	1.18	1.24
26	U	237	PRO	N-CA	-5.40	1.40	1.47
3	c	22	VAL	C-N	5.40	1.41	1.33
5	e	60	GLU	CA-C	-5.40	1.46	1.52
20	Z	27	LYS	CA-CB	5.40	1.61	1.53
32	M	339	ARG	N-CA	-5.40	1.39	1.46
5	e	65	GLU	CA-C	-5.39	1.46	1.52
13	m	28	PHE	N-CA	-5.39	1.39	1.46
13	6	13	TYR	N-CA	-5.39	1.40	1.46
16	V	131	GLN	CA-C	5.39	1.59	1.52
20	Z	365	SER	C-N	5.39	1.41	1.33
20	Z	479	THR	C-N	5.39	1.40	1.33
24	Q	234	THR	CA-CB	-5.39	1.44	1.53
8	h	179	GLY	N-CA	-5.39	1.37	1.45
9	2	101	ARG	CA-C	-5.39	1.45	1.52
1	a	118	ALA	C-N	5.39	1.41	1.33
8	1	100	ASP	C-N	5.39	1.42	1.33
8	1	133	TYR	N-CA	-5.39	1.39	1.46
12	5	94	ARG	N-CA	-5.39	1.39	1.46
19	Y	83	ARG	CZ-NH1	5.39	1.40	1.32
6	F	213	ILE	C-O	-5.39	1.18	1.24
20	Z	131	LYS	N-CA	-5.39	1.38	1.46
5	e	223	THR	N-CA	-5.39	1.39	1.46
2	B	174	PHE	N-CA	5.39	1.52	1.46
9	2	115	HIS	CD2-NE2	-5.39	1.31	1.37
22	S	332	PHE	C-O	-5.39	1.18	1.24
8	h	146	TYR	N-CA	-5.39	1.40	1.46
21	N	556	ALA	N-CA	-5.39	1.40	1.46
5	e	164	PHE	CA-C	-5.38	1.45	1.52
14	n	65	SER	C-N	5.38	1.41	1.33
7	G	216	ILE	N-CA	-5.38	1.39	1.46
13	6	36	ARG	CZ-NH1	5.38	1.40	1.32
15	W	39	ALA	N-CA	-5.38	1.40	1.46
21	N	365	PHE	CA-C	-5.38	1.45	1.52
23	P	370	ASP	CA-CB	5.38	1.61	1.53
25	R	28	GLU	C-O	-5.38	1.18	1.24
26	U	107	ASN	C-N	5.38	1.41	1.33
30	K	259	ARG	CA-C	-5.38	1.45	1.52
3	c	58	GLU	CA-CB	5.38	1.60	1.53
24	Q	320	GLN	CD-NE2	5.38	1.44	1.33
26	U	167	GLU	CA-CB	5.38	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	59	ILE	N-CA	-5.38	1.40	1.46
2	B	14	PRO	C-N	5.38	1.40	1.33
2	B	28	VAL	C-O	-5.38	1.18	1.24
3	C	113	ARG	CD-NE	5.38	1.53	1.46
3	C	130	PRO	CA-C	-5.38	1.45	1.52
17	T	27	LEU	C-N	5.38	1.39	1.33
29	I	346	ARG	CZ-NH2	5.38	1.40	1.33
6	f	226	ASP	C-N	5.38	1.41	1.33
28	H	90	ARG	CZ-NH2	5.38	1.40	1.33
32	M	312	LEU	CA-C	-5.38	1.45	1.52
8	h	118	GLU	C-N	5.38	1.40	1.33
12	l	88	ILE	CA-CB	5.38	1.60	1.54
11	4	9	VAL	N-CA	-5.38	1.39	1.46
22	S	455	GLU	CA-CB	5.38	1.63	1.53
26	U	256	ASN	CA-C	-5.38	1.45	1.52
33	J	339	ARG	N-CA	5.38	1.52	1.46
8	h	170	GLN	C-N	5.38	1.41	1.33
14	7	135	GLN	CD-NE2	5.38	1.44	1.33
28	H	292	ARG	CA-C	-5.38	1.45	1.52
31	L	77	ARG	CD-NE	5.38	1.53	1.46
4	d	119	ARG	C-N	5.38	1.41	1.33
24	Q	302	VAL	CA-CB	-5.38	1.47	1.54
28	H	266	ARG	CA-CB	5.38	1.61	1.53
6	f	161	ILE	C-N	5.37	1.41	1.33
7	g	109	ILE	CA-CB	-5.37	1.50	1.53
7	g	130	ARG	CZ-NH1	5.37	1.40	1.32
10	j	82	ILE	CA-CB	5.37	1.59	1.54
4	D	189	GLU	C-N	5.37	1.41	1.34
11	4	27	VAL	CA-CB	5.37	1.59	1.53
25	R	159	SER	CA-C	-5.37	1.45	1.52
25	R	251	THR	CA-C	-5.37	1.45	1.52
21	N	597	ARG	CD-NE	5.37	1.53	1.46
29	I	63	GLU	C-N	5.37	1.40	1.33
31	L	179	THR	CA-CB	-5.37	1.46	1.53
31	L	227	GLY	CA-C	-5.37	1.44	1.51
32	M	404	ARG	CD-NE	5.37	1.53	1.46
20	Z	291	GLU	C-O	-5.37	1.17	1.24
20	Z	799	PHE	C-N	5.37	1.41	1.33
22	S	320	ILE	CA-CB	5.37	1.61	1.54
26	U	89	LEU	N-CA	-5.37	1.39	1.46
28	H	247	LEU	N-CA	-5.37	1.40	1.46
8	h	193	GLU	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	55	ARG	CZ-NH2	5.37	1.40	1.33
21	N	885	ILE	CA-CB	-5.37	1.47	1.54
26	U	21	HIS	ND1-CE1	5.37	1.38	1.32
26	U	179	ARG	C-N	5.37	1.40	1.33
32	M	233	ARG	CZ-NH1	5.37	1.40	1.32
14	n	206	ALA	CA-C	-5.37	1.45	1.52
13	6	140	GLU	N-CA	-5.37	1.39	1.45
27	O	354	GLN	CA-CB	5.37	1.62	1.52
6	f	192	ALA	CA-CB	5.37	1.61	1.53
10	j	150	CYS	C-N	5.37	1.41	1.33
6	F	114	ASP	C-N	5.37	1.41	1.33
10	3	62	THR	N-CA	-5.37	1.39	1.46
17	T	130	ASP	CA-CB	5.37	1.62	1.53
21	N	176	GLN	C-N	5.37	1.41	1.34
27	O	94	GLU	C-N	5.37	1.41	1.33
27	O	354	GLN	C-N	5.37	1.40	1.33
7	g	25	GLU	C-O	-5.36	1.17	1.24
13	m	208	ASP	N-CA	-5.36	1.39	1.46
22	S	296	ALA	C-N	5.36	1.40	1.33
28	H	93	GLU	N-CA	-5.36	1.39	1.46
30	K	253	MET	CA-CB	5.36	1.61	1.53
32	M	299	ARG	CZ-NH2	5.36	1.40	1.33
2	B	140	ASP	CA-C	-5.36	1.45	1.52
20	Z	810	ASN	CA-CB	5.36	1.61	1.53
23	P	65	LEU	C-N	5.36	1.40	1.33
25	R	149	ASN	C-N	5.36	1.41	1.33
30	K	252	ARG	CA-CB	-5.36	1.44	1.53
6	f	86	ASN	CA-C	-5.36	1.46	1.52
9	i	182	LYS	CA-CB	5.36	1.61	1.53
14	7	134	TYR	CA-C	-5.36	1.45	1.52
17	T	101	LYS	CA-CB	5.36	1.62	1.53
29	I	75	PHE	C-N	5.36	1.40	1.33
1	a	101	ALA	CA-C	-5.36	1.45	1.52
5	e	171	ALA	CA-C	-5.36	1.46	1.52
7	g	47	VAL	C-O	-5.36	1.18	1.24
9	i	124	GLY	C-N	5.36	1.41	1.33
9	2	236	ARG	CD-NE	5.36	1.53	1.46
32	M	33	ARG	CZ-NH1	5.36	1.40	1.32
11	k	70	ARG	NE-CZ	5.36	1.39	1.33
6	F	158	GLY	N-CA	-5.36	1.37	1.45
10	3	31	SER	CA-C	-5.36	1.46	1.52
21	N	615	ALA	CA-C	-5.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	247	ILE	CA-C	-5.36	1.46	1.52
26	U	260	ASN	CA-CB	5.36	1.61	1.53
15	W	66	THR	CA-CB	5.35	1.62	1.53
25	R	130	GLN	C-N	5.35	1.41	1.33
5	E	87	SER	N-CA	-5.35	1.40	1.46
13	6	39	THR	N-CA	-5.35	1.39	1.46
19	Y	5	VAL	C-N	5.35	1.41	1.33
24	Q	95	LYS	C-N	5.35	1.40	1.33
25	R	121	GLU	N-CA	-5.35	1.39	1.46
32	M	320	ARG	CD-NE	5.35	1.53	1.46
33	J	68	PRO	N-CA	-5.35	1.40	1.47
14	7	224	SER	C-N	5.35	1.40	1.33
1	a	131	ARG	CD-NE	5.35	1.53	1.46
14	7	238	GLY	CA-C	-5.35	1.44	1.51
33	J	21	PRO	N-CD	-5.35	1.40	1.47
33	J	139	VAL	N-CA	-5.35	1.40	1.46
2	b	151	ASP	CA-C	5.35	1.59	1.53
11	k	22	THR	C-N	5.35	1.40	1.33
20	Z	489	ALA	C-N	5.35	1.40	1.33
29	I	54	ARG	NE-CZ	5.35	1.39	1.33
11	k	171	ARG	CZ-NH1	5.35	1.40	1.32
21	N	731	VAL	C-N	5.35	1.40	1.33
21	N	883	SER	CA-CB	5.35	1.63	1.53
22	S	239	ARG	CD-NE	5.35	1.53	1.46
13	m	193	ARG	NE-CZ	5.34	1.39	1.33
8	1	150	ASN	C-N	5.34	1.41	1.33
10	3	191	LYS	N-CA	-5.34	1.39	1.45
20	Z	338	HIS	CG-ND1	5.34	1.44	1.38
30	K	365	GLU	CA-CB	5.34	1.62	1.53
11	4	41	HIS	CE1-NE2	5.34	1.37	1.32
32	M	360	ILE	CA-CB	-5.34	1.47	1.54
1	a	37	GLN	CA-C	5.34	1.60	1.52
3	c	76	ALA	C-N	5.34	1.41	1.33
6	f	210	ASN	CA-CB	5.34	1.62	1.54
20	Z	618	GLN	N-CA	-5.34	1.39	1.46
21	N	160	GLY	CA-C	-5.34	1.44	1.51
27	O	189	TYR	N-CA	-5.34	1.40	1.46
30	K	66	ASP	CA-CB	5.34	1.61	1.53
10	j	54	THR	CA-CB	-5.34	1.45	1.53
14	n	242	LYS	C-N	5.34	1.41	1.33
6	F	147	PHE	CA-C	-5.34	1.46	1.52
15	W	33	VAL	C-N	5.34	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	379	LEU	C-N	5.34	1.41	1.34
12	l	177	CYS	C-N	5.34	1.40	1.33
10	3	137	ILE	CA-C	-5.34	1.46	1.52
20	Z	600	GLU	CA-CB	5.34	1.61	1.53
21	N	398	ARG	CZ-NH2	5.34	1.40	1.33
30	K	306	PHE	CG-CD2	5.34	1.50	1.38
4	d	6	ARG	CA-C	-5.34	1.45	1.52
9	i	249	ILE	CA-C	-5.34	1.46	1.52
5	E	184	LEU	CB-CG	-5.34	1.42	1.53
11	4	147	HIS	CB-CG	5.34	1.57	1.50
20	Z	766	HIS	CA-CB	5.34	1.61	1.53
22	S	449	LEU	CA-C	-5.34	1.48	1.53
31	L	396	THR	CA-C	-5.34	1.46	1.52
2	b	56	ALA	C-N	5.33	1.42	1.33
2	b	117	ILE	N-CA	5.33	1.52	1.46
14	n	226	ARG	CD-NE	5.33	1.53	1.46
1	A	244	ARG	CZ-NH1	5.33	1.40	1.32
2	B	62	SER	C-N	5.33	1.41	1.33
29	I	72	GLU	CA-CB	5.33	1.61	1.53
4	D	149	GLN	CA-C	-5.33	1.46	1.52
7	G	26	TYR	N-CA	-5.33	1.39	1.46
16	V	294	SER	CA-C	5.33	1.59	1.52
19	Y	19	LYS	C-N	5.33	1.41	1.33
20	Z	727	GLU	N-CA	-5.33	1.41	1.46
22	S	327	ILE	CB-CG1	5.33	1.64	1.53
25	R	324	ARG	C-N	5.33	1.41	1.33
28	H	317	ALA	C-N	5.33	1.40	1.33
29	I	277	SER	CA-CB	5.33	1.62	1.53
29	I	416	PHE	CA-C	-5.33	1.45	1.52
2	B	18	LEU	N-CA	-5.33	1.39	1.46
8	1	63	ALA	CA-C	-5.33	1.46	1.52
23	P	81	LEU	CA-CB	5.33	1.62	1.53
25	R	311	THR	N-CA	-5.33	1.40	1.46
4	d	135	ILE	C-N	5.33	1.41	1.33
2	B	85	LEU	CB-CG	5.33	1.64	1.53
10	3	98	ARG	CZ-NH2	5.33	1.40	1.33
13	6	84	HIS	C-N	-5.33	1.26	1.33
27	O	264	ASP	CA-C	-5.33	1.46	1.52
7	g	156	SER	CA-C	-5.33	1.46	1.52
9	i	181	ILE	N-CA	-5.33	1.39	1.46
7	G	174	ALA	C-N	5.33	1.41	1.33
9	2	173	GLN	N-CA	-5.33	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	20	TYR	CA-C	-5.33	1.45	1.52
21	N	35	LEU	CA-C	-5.33	1.46	1.52
21	N	348	PHE	CA-CB	5.33	1.61	1.53
26	U	189	ARG	CD-NE	5.33	1.53	1.46
27	O	200	GLU	C-N	5.33	1.40	1.34
28	H	59	ILE	CA-CB	-5.33	1.47	1.54
4	d	181	ARG	CZ-NH2	5.32	1.40	1.33
21	N	745	LEU	CA-C	-5.32	1.47	1.53
22	S	120	SER	CA-CB	5.32	1.62	1.53
23	P	348	HIS	C-N	5.32	1.40	1.33
24	Q	300	LYS	N-CA	-5.32	1.39	1.46
30	K	396	ARG	N-CA	-5.32	1.40	1.46
33	J	212	ARG	CZ-NH1	5.32	1.40	1.32
8	1	154	ASN	CA-C	-5.32	1.45	1.52
14	7	68	ARG	CZ-NH1	5.32	1.40	1.32
20	Z	436	LEU	CA-C	-5.32	1.45	1.52
21	N	415	PHE	C-N	5.32	1.41	1.33
23	P	32	CYS	N-CA	-5.32	1.40	1.46
1	a	139	VAL	CA-C	-5.32	1.46	1.53
8	h	183	ARG	NE-CZ	5.32	1.39	1.33
9	i	40	GLY	C-N	5.32	1.38	1.33
9	i	152	TYR	CA-CB	5.32	1.62	1.53
9	2	67	SER	CA-C	-5.32	1.47	1.52
9	2	224	VAL	N-CA	-5.32	1.39	1.46
21	N	50	TYR	CA-C	-5.32	1.45	1.52
31	L	349	ILE	CA-C	-5.32	1.48	1.52
13	m	229	ARG	CD-NE	5.32	1.53	1.46
14	n	189	ARG	CD-NE	5.32	1.53	1.46
21	N	886	LYS	C-N	-5.32	1.26	1.33
25	R	94	PHE	CA-C	-5.32	1.46	1.52
31	L	411	ASN	C-O	5.32	1.28	1.24
4	d	210	ILE	CA-C	-5.32	1.46	1.52
7	G	245	LYS	CA-CB	5.32	1.61	1.53
8	1	47	HIS	ND1-CE1	5.32	1.37	1.32
20	Z	532	HIS	ND1-CE1	5.32	1.37	1.32
27	O	99	LEU	CB-CG	5.32	1.64	1.53
20	Z	736	LEU	N-CA	-5.31	1.40	1.46
22	S	91	ASN	CA-CB	5.31	1.61	1.53
22	S	382	ARG	NE-CZ	5.31	1.38	1.33
28	H	306	ILE	CA-C	-5.31	1.45	1.52
30	K	46	ASP	C-N	5.31	1.40	1.33
33	J	108	LYS	C-N	5.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	298	ASP	C-N	5.31	1.41	1.34
14	n	201	THR	C-N	5.31	1.40	1.33
5	e	157	HIS	ND1-CE1	5.31	1.37	1.32
7	G	140	GLY	C-N	5.31	1.41	1.33
21	N	193	ALA	C-N	5.31	1.40	1.33
22	S	51	ARG	CD-NE	5.31	1.53	1.46
26	U	173	HIS	CE1-NE2	5.31	1.37	1.32
31	L	173	PHE	CA-CB	5.31	1.62	1.53
33	J	257	ARG	CZ-NH1	5.31	1.40	1.32
9	i	229	GLN	C-N	5.31	1.40	1.33
22	S	350	LYS	C-O	-5.31	1.17	1.24
23	P	282	HIS	N-CA	-5.31	1.39	1.46
25	R	149	ASN	CA-C	-5.31	1.45	1.52
27	O	218	SER	N-CA	-5.31	1.39	1.46
28	H	303	ALA	CA-CB	-5.31	1.44	1.53
20	Z	833	GLN	N-CA	-5.31	1.40	1.46
21	N	233	ASN	CA-C	-5.31	1.48	1.53
11	k	10	GLN	CA-CB	5.30	1.61	1.53
16	V	139	VAL	C-N	5.30	1.40	1.33
20	Z	25	PRO	CA-CB	5.30	1.61	1.53
24	Q	355	GLU	CA-C	-5.30	1.46	1.52
5	e	20	ARG	CZ-NH2	5.30	1.40	1.33
15	W	7	VAL	C-N	5.30	1.41	1.33
15	W	176	PRO	C-N	5.30	1.41	1.33
17	T	264	MET	N-CA	5.30	1.52	1.46
32	M	63	LYS	C-O	-5.30	1.17	1.24
2	b	132	VAL	CA-C	-5.30	1.46	1.52
8	h	65	ALA	CA-CB	5.30	1.61	1.53
1	A	92	ASN	CA-C	5.30	1.59	1.52
5	E	54	ALA	CA-C	-5.30	1.46	1.52
6	F	128	TYR	CA-C	-5.30	1.46	1.52
11	4	27	VAL	C-N	5.30	1.41	1.33
15	W	185	ILE	N-CA	-5.30	1.40	1.46
20	Z	296	SER	C-N	5.30	1.40	1.33
23	P	88	GLN	CD-NE2	5.30	1.44	1.33
32	M	265	ASP	CA-C	-5.30	1.46	1.52
1	a	95	LEU	N-CA	-5.30	1.40	1.46
1	A	22	GLU	CA-CB	5.30	1.62	1.53
26	U	196	SER	CA-C	-5.30	1.45	1.52
32	M	152	SER	CA-CB	5.30	1.62	1.53
4	D	70	HIS	N-CA	-5.30	1.40	1.46
4	D	139	ASP	N-CA	5.30	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	308	ASN	CA-CB	5.30	1.61	1.53
25	R	177	LEU	CA-C	5.30	1.59	1.52
6	F	100	ASN	C-N	5.30	1.41	1.33
21	N	609	LEU	C-O	-5.30	1.17	1.24
22	S	197	SER	CA-CB	5.30	1.61	1.53
22	S	394	ILE	N-CA	-5.30	1.40	1.46
31	L	151	THR	CA-C	-5.30	1.46	1.52
4	D	106	VAL	CA-C	-5.29	1.46	1.52
20	Z	915	ALA	CA-C	5.29	1.60	1.52
26	U	200	LEU	CA-C	-5.29	1.45	1.52
6	f	36	VAL	CA-CB	-5.29	1.48	1.54
1	A	210	MET	N-CA	-5.29	1.39	1.46
20	Z	418	ALA	C-N	5.29	1.40	1.33
22	S	480	ARG	CZ-NH1	5.29	1.40	1.32
26	U	258	SER	CA-C	-5.29	1.45	1.52
27	O	364	THR	CA-C	-5.29	1.45	1.52
1	a	24	ARG	CD-NE	5.29	1.53	1.46
3	c	172	ALA	C-N	5.29	1.41	1.33
5	e	86	ARG	C-N	5.29	1.40	1.33
14	n	166	LEU	N-CA	-5.29	1.39	1.46
13	6	99	ARG	CZ-NH1	5.29	1.40	1.32
21	N	678	ILE	CA-CB	-5.29	1.47	1.54
27	O	335	GLY	N-CA	-5.29	1.37	1.45
29	I	291	ARG	CZ-NH2	5.29	1.40	1.33
14	7	37	PRO	C-N	5.29	1.40	1.33
24	Q	379	GLN	N-CA	-5.29	1.40	1.46
29	I	150	HIS	CB-CG	5.29	1.57	1.50
21	N	81	TYR	C-N	5.29	1.40	1.33
24	Q	203	THR	C-O	-5.29	1.17	1.24
25	R	25	GLU	N-CA	-5.29	1.40	1.46
5	e	11	GLY	C-N	5.29	1.39	1.33
14	7	35	GLN	CA-C	-5.29	1.45	1.52
7	g	28	VAL	CA-CB	-5.29	1.47	1.54
9	i	163	ALA	N-CA	-5.29	1.40	1.46
9	i	170	HIS	CA-CB	5.29	1.60	1.53
29	I	140	LEU	CA-CB	5.29	1.63	1.53
29	I	409	MET	CA-C	-5.29	1.46	1.52
6	f	130	VAL	C-N	5.28	1.38	1.33
10	j	98	ARG	N-CA	-5.28	1.39	1.46
7	G	109	ILE	CA-C	5.28	1.57	1.52
15	W	161	VAL	N-CA	-5.28	1.40	1.46
13	m	123	ASP	C-N	5.28	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	845	LEU	N-CA	-5.28	1.39	1.46
4	d	183	GLU	N-CA	-5.28	1.41	1.46
8	h	47	HIS	ND1-CE1	5.28	1.37	1.32
1	A	199	TRP	C-N	5.28	1.40	1.33
4	D	234	THR	N-CA	-5.28	1.39	1.46
11	4	108	ASP	C-O	-5.28	1.17	1.24
20	Z	714	ASP	C-O	-5.28	1.18	1.24
27	O	294	MET	N-CA	-5.28	1.40	1.46
2	b	56	ALA	N-CA	-5.28	1.39	1.46
5	e	121	LEU	N-CA	-5.28	1.40	1.46
8	h	19	ASP	C-O	5.28	1.31	1.24
11	k	50	ALA	C-N	5.28	1.41	1.33
12	l	276	LYS	CA-C	-5.28	1.45	1.52
30	K	383	ILE	CA-CB	5.28	1.61	1.54
7	g	121	GLN	C-N	5.28	1.41	1.34
10	j	195	VAL	C-O	-5.28	1.18	1.24
2	B	235	PHE	CA-C	-5.28	1.46	1.52
6	F	35	THR	C-N	5.28	1.40	1.33
13	6	154	ILE	CA-CB	-5.28	1.47	1.54
16	V	47	MET	N-CA	-5.28	1.39	1.46
21	N	630	ALA	CA-C	5.28	1.59	1.52
24	Q	12	ARG	CD-NE	5.28	1.53	1.46
26	U	227	GLY	CA-C	-5.28	1.45	1.51
27	O	28	GLN	CD-NE2	5.28	1.44	1.33
6	f	135	ILE	CA-C	-5.28	1.46	1.52
6	f	205	SER	CA-C	-5.28	1.46	1.52
11	k	171	ARG	NE-CZ	5.28	1.38	1.33
4	D	220	ASP	CA-C	-5.28	1.46	1.52
19	Y	88	ASN	N-CA	-5.28	1.38	1.46
23	P	32	CYS	CA-C	5.28	1.59	1.52
2	B	99	ARG	C-N	5.27	1.40	1.33
7	G	198	LYS	CA-CB	5.27	1.61	1.53
17	T	233	VAL	C-N	5.27	1.40	1.33
21	N	217	MET	CA-C	-5.27	1.47	1.53
14	n	228	PHE	C-N	5.27	1.41	1.33
1	A	53	VAL	N-CA	-5.27	1.40	1.46
22	S	266	SER	C-N	5.27	1.40	1.33
22	S	438	HIS	ND1-CE1	5.27	1.37	1.32
26	U	82	LYS	N-CA	-5.27	1.40	1.46
31	L	302	GLN	CA-C	-5.27	1.46	1.52
4	d	6	ARG	CA-CB	5.27	1.61	1.53
6	f	196	ALA	N-CA	-5.27	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	381	ILE	CA-C	-5.27	1.46	1.52
25	R	43	ARG	C-N	5.27	1.41	1.33
3	C	126	GLY	CA-C	-5.27	1.44	1.52
13	6	213	LEU	CA-C	-5.27	1.46	1.52
24	Q	229	ASP	N-CA	5.27	1.53	1.46
29	I	378	GLU	CA-C	-5.27	1.45	1.52
20	Z	220	ALA	C-N	5.27	1.40	1.33
33	J	232	GLU	CA-C	-5.27	1.45	1.52
14	n	137	ARG	NE-CZ	5.27	1.38	1.33
5	E	223	THR	CA-C	-5.27	1.46	1.52
21	N	704	GLY	N-CA	-5.27	1.39	1.45
10	j	133	ALA	N-CA	-5.26	1.39	1.45
4	D	67	ILE	CA-C	-5.26	1.46	1.52
16	V	153	ILE	CB-CG1	5.26	1.64	1.53
31	L	78	ARG	CD-NE	5.26	1.53	1.46
3	C	91	ALA	N-CA	-5.26	1.39	1.46
6	F	61	LYS	CA-C	-5.26	1.45	1.52
12	5	227	ASP	CA-CB	5.26	1.62	1.53
20	Z	853	GLY	CA-C	-5.26	1.44	1.51
7	g	218	TRP	CA-C	-5.26	1.46	1.52
7	G	36	THR	CA-CB	-5.26	1.45	1.53
10	3	80	ARG	CZ-NH1	5.26	1.40	1.32
12	5	118	GLY	N-CA	-5.26	1.39	1.44
25	R	91	TRP	C-N	5.26	1.40	1.33
26	U	169	ILE	C-N	5.26	1.40	1.33
5	e	71	ASP	CA-CB	5.26	1.59	1.54
12	l	114	PRO	C-N	5.26	1.41	1.33
19	Y	72	ASP	C-N	5.26	1.41	1.33
26	U	82	LYS	CA-C	-5.26	1.46	1.52
30	K	397	LYS	C-N	5.26	1.41	1.33
33	J	81	ASP	C-N	5.26	1.41	1.33
8	h	137	GLY	C-N	5.26	1.41	1.33
9	2	156	LEU	CA-C	-5.26	1.46	1.52
25	R	22	PRO	C-N	5.26	1.40	1.33
26	U	51	SER	CA-C	-5.26	1.46	1.52
5	e	44	GLU	C-N	5.26	1.39	1.32
8	h	170	GLN	N-CA	-5.26	1.39	1.46
14	n	56	ALA	C-N	5.26	1.41	1.33
5	E	157	HIS	N-CA	-5.26	1.40	1.46
17	T	106	ILE	N-CA	-5.26	1.39	1.46
26	U	16	LEU	CA-CB	5.26	1.61	1.53
31	L	85	GLU	CA-C	-5.26	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	281	SER	C-N	5.25	1.40	1.33
14	n	98	ARG	CZ-NH1	5.25	1.40	1.32
21	N	309	ILE	C-N	5.25	1.40	1.33
32	M	112	ALA	CA-C	-5.25	1.46	1.53
3	c	21	GLN	C-N	5.25	1.40	1.33
1	A	238	ALA	N-CA	-5.25	1.40	1.46
21	N	788	TYR	C-N	5.25	1.40	1.33
32	M	410	VAL	CA-C	5.25	1.58	1.52
6	F	88	LEU	CA-CB	5.25	1.61	1.53
18	X	99	PHE	CA-C	-5.25	1.46	1.52
25	R	21	VAL	CA-CB	5.25	1.57	1.53
28	H	104	LYS	CA-C	-5.25	1.46	1.52
2	b	224	TYR	C-N	5.25	1.40	1.33
6	f	94	TYR	CA-CB	5.25	1.61	1.53
7	G	129	VAL	CA-CB	-5.25	1.46	1.54
21	N	15	GLU	CA-CB	-5.25	1.44	1.53
22	S	282	ILE	CA-CB	-5.25	1.48	1.54
23	P	291	LYS	CA-CB	5.25	1.60	1.53
29	I	301	GLU	C-N	5.25	1.40	1.33
14	n	262	GLY	C-N	5.25	1.40	1.33
9	2	73	ALA	CA-C	-5.25	1.46	1.52
27	O	326	HIS	C-N	5.25	1.41	1.33
28	H	400	ARG	CD-NE	5.25	1.53	1.46
31	L	141	LYS	C-N	5.25	1.40	1.33
31	L	412	PRO	N-CD	-5.25	1.40	1.47
8	h	175	ASP	CA-C	-5.25	1.46	1.52
12	l	163	TYR	CA-C	5.25	1.59	1.52
3	C	146	TYR	CA-C	-5.25	1.46	1.52
3	C	216	ILE	N-CA	-5.25	1.39	1.46
4	D	58	ARG	N-CA	-5.25	1.40	1.46
31	L	175	GLN	N-CA	-5.25	1.39	1.46
6	f	174	ARG	N-CA	-5.25	1.40	1.46
29	I	68	HIS	N-CA	-5.25	1.40	1.46
11	4	124	THR	CA-C	5.24	1.59	1.52
12	5	254	HIS	ND1-CE1	5.24	1.37	1.32
13	6	106	TYR	CZ-OH	5.24	1.49	1.38
20	Z	835	ALA	CA-C	-5.24	1.46	1.52
30	K	280	LYS	N-CA	5.24	1.52	1.46
32	M	296	SER	CA-CB	5.24	1.62	1.53
20	Z	882	LEU	C-N	5.24	1.41	1.33
6	f	222	PHE	N-CA	-5.24	1.39	1.46
7	g	106	PRO	C-N	5.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	90	SER	N-CA	-5.24	1.40	1.46
6	F	147	PHE	N-CA	-5.24	1.39	1.46
21	N	803	VAL	C-N	5.24	1.40	1.33
28	H	101	ARG	NE-CZ	5.24	1.38	1.33
4	d	175	LEU	C-N	5.24	1.40	1.33
7	g	246	GLU	C-N	5.24	1.40	1.33
8	h	129	HIS	CD2-NE2	5.24	1.43	1.37
10	j	62	THR	CA-C	-5.24	1.46	1.52
8	1	40	THR	C-N	5.24	1.41	1.33
10	3	32	GLN	CD-NE2	5.24	1.44	1.33
16	V	20	ARG	CA-C	-5.24	1.46	1.52
22	S	55	ARG	CD-NE	5.24	1.53	1.46
23	P	166	GLU	C-N	5.24	1.40	1.33
28	H	346	ARG	NE-CZ	5.24	1.38	1.33
29	I	184	ILE	CA-C	-5.24	1.46	1.52
30	K	381	ALA	CA-CB	-5.24	1.45	1.53
2	b	57	MET	C-N	5.24	1.40	1.33
13	m	199	ALA	N-CA	-5.24	1.40	1.46
22	S	485	LYS	C-N	5.24	1.41	1.34
10	j	26	ASP	N-CA	-5.24	1.39	1.45
1	A	135	ARG	CZ-NH2	5.24	1.40	1.33
5	E	12	VAL	CA-CB	5.24	1.60	1.54
28	H	403	ARG	CD-NE	5.24	1.53	1.46
5	E	157	HIS	CA-C	-5.23	1.46	1.52
21	N	425	ASN	N-CA	-5.23	1.40	1.46
30	K	367	ASP	CA-C	-5.23	1.46	1.52
12	5	190	VAL	C-N	5.23	1.40	1.33
14	7	227	ASN	N-CA	-5.23	1.39	1.45
17	T	188	GLU	CA-C	-5.23	1.46	1.52
31	L	262	ILE	C-N	5.23	1.40	1.33
6	f	11	VAL	C-N	5.23	1.40	1.33
22	S	462	ASP	C-N	5.23	1.41	1.34
11	k	65	GLN	N-CA	-5.23	1.40	1.46
16	V	265	GLU	C-N	5.23	1.40	1.33
19	Y	78	LYS	CA-C	-5.23	1.46	1.52
20	Z	832	ARG	CZ-NH1	5.23	1.40	1.32
6	F	199	GLN	N-CA	-5.23	1.40	1.46
8	1	182	ILE	CA-C	-5.23	1.46	1.52
21	N	7	ALA	N-CA	-5.23	1.41	1.46
24	Q	252	HIS	CD2-NE2	5.23	1.43	1.37
8	1	88	ALA	CA-CB	5.23	1.61	1.53
33	J	145	SER	CA-CB	5.23	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	44	LEU	CA-C	-5.22	1.46	1.52
1	A	68	THR	N-CA	-5.22	1.40	1.46
16	V	212	MET	CA-CB	5.22	1.61	1.53
23	P	238	ALA	N-CA	-5.22	1.40	1.46
30	K	79	LEU	CA-C	-5.22	1.46	1.52
30	K	334	LEU	CA-C	-5.22	1.45	1.52
33	J	43	ARG	C-N	5.22	1.41	1.34
9	2	151	GLY	C-N	5.22	1.41	1.33
27	O	313	ILE	C-N	5.22	1.40	1.33
8	1	95	CYS	N-CA	-5.22	1.39	1.46
13	6	75	ARG	CZ-NH1	5.22	1.40	1.32
16	V	171	ARG	NE-CZ	5.22	1.38	1.33
28	H	63	ILE	N-CA	5.22	1.52	1.46
30	K	321	ALA	N-CA	-5.22	1.39	1.46
14	7	166	LEU	CA-C	-5.22	1.45	1.52
19	Y	61	GLU	CA-CB	5.22	1.62	1.53
22	S	409	LEU	C-O	-5.22	1.18	1.24
31	L	404	ARG	CZ-NH1	5.22	1.40	1.32
32	M	203	ARG	C-N	5.22	1.41	1.34
27	O	196	LEU	C-N	5.22	1.41	1.33
13	m	141	ARG	CZ-NH2	5.22	1.40	1.33
1	A	224	GLU	N-CA	-5.22	1.39	1.46
7	G	76	CYS	CA-C	-5.22	1.46	1.52
18	X	64	ILE	CA-CB	5.22	1.61	1.54
30	K	87	LYS	C-O	5.22	1.30	1.24
31	L	246	SER	CA-CB	5.22	1.59	1.53
1	a	232	LYS	CA-C	-5.21	1.46	1.52
2	b	90	ARG	CZ-NH1	5.21	1.40	1.32
2	b	120	GLU	C-N	5.21	1.41	1.33
1	A	65	ASP	CA-CB	5.21	1.60	1.52
21	N	104	LYS	C-N	5.21	1.40	1.33
22	S	50	PRO	CA-CB	-5.21	1.46	1.53
23	P	107	SER	CA-C	-5.21	1.47	1.52
9	i	74	GLY	N-CA	-5.21	1.39	1.45
14	n	214	MET	N-CA	-5.21	1.40	1.46
32	M	428	LYS	CA-CB	5.21	1.61	1.53
3	c	45	VAL	CA-CB	5.21	1.61	1.54
6	f	69	HIS	CD2-NE2	5.21	1.43	1.37
6	f	143	HIS	CE1-NE2	-5.21	1.27	1.32
10	j	185	ALA	CA-C	-5.21	1.46	1.52
6	F	188	GLU	N-CA	-5.21	1.40	1.46
16	V	63	VAL	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	168	LEU	C-N	5.21	1.40	1.33
20	Z	826	ARG	N-CA	5.21	1.53	1.46
28	H	375	VAL	C-N	5.21	1.40	1.33
29	I	429	GLU	N-CA	-5.21	1.39	1.46
33	J	116	ARG	C-N	5.21	1.41	1.33
21	N	690	HIS	N-CA	-5.21	1.39	1.46
32	M	351	LEU	CA-C	-5.21	1.46	1.52
3	c	50	ARG	CD-NE	5.21	1.53	1.46
9	i	143	HIS	CA-C	-5.21	1.46	1.53
11	k	190	ARG	CD-NE	5.21	1.53	1.46
7	G	142	ASP	CA-CB	5.21	1.62	1.53
12	5	156	LYS	CA-C	5.21	1.59	1.52
20	Z	594	PRO	C-N	5.21	1.41	1.33
22	S	417	GLN	N-CA	-5.21	1.40	1.46
25	R	54	ILE	CA-CB	-5.21	1.48	1.54
30	K	142	HIS	N-CA	-5.21	1.39	1.46
28	H	460	THR	C-O	5.21	1.30	1.23
30	K	246	TYR	N-CA	-5.21	1.39	1.46
10	j	83	GLU	C-N	-5.21	1.27	1.33
23	P	348	HIS	ND1-CE1	5.21	1.37	1.32
1	a	156	LYS	C-O	-5.20	1.17	1.24
5	E	135	SER	N-CA	-5.20	1.39	1.45
15	W	102	GLN	C-N	5.20	1.40	1.33
20	Z	81	SER	C-N	5.20	1.41	1.33
22	S	44	THR	CA-CB	5.20	1.62	1.53
27	O	324	VAL	CA-C	-5.20	1.46	1.52
30	K	273	GLU	CA-CB	-5.20	1.44	1.53
14	n	111	ASN	CA-CB	5.20	1.61	1.54
6	F	73	SER	CA-C	-5.20	1.45	1.52
30	K	325	ASP	CA-C	-5.20	1.46	1.52
32	M	50	ARG	NE-CZ	5.20	1.38	1.33
10	3	61	THR	C-N	5.20	1.41	1.33
22	S	389	LYS	N-CA	-5.20	1.40	1.46
4	D	72	VAL	CA-CB	-5.20	1.46	1.54
8	1	89	SER	N-CA	-5.20	1.39	1.46
23	P	94	GLN	N-CA	-5.20	1.39	1.46
28	H	135	ASP	CA-C	5.20	1.59	1.52
28	H	144	LYS	N-CA	-5.20	1.40	1.46
32	M	263	VAL	CA-CB	-5.20	1.48	1.54
21	N	893	VAL	N-CA	-5.20	1.40	1.46
31	L	264	ARG	CA-CB	5.20	1.61	1.53
4	d	118	GLN	N-CA	-5.20	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	83	PHE	CA-C	5.20	1.59	1.52
12	l	128	GLN	CA-C	5.20	1.59	1.52
10	3	120	PHE	C-O	5.20	1.29	1.23
27	O	153	LEU	CB-CG	5.20	1.63	1.53
32	M	63	LYS	N-CA	-5.20	1.40	1.46
32	M	118	VAL	CA-C	-5.20	1.46	1.52
16	V	269	ARG	CZ-NH1	5.19	1.40	1.32
5	e	77	ALA	C-O	-5.19	1.16	1.23
1	A	183	GLU	C-N	5.19	1.40	1.33
9	i	225	ARG	N-CA	5.19	1.52	1.45
14	n	124	TYR	C-N	5.19	1.40	1.33
4	D	235	GLN	C-N	5.19	1.40	1.33
5	E	169	ALA	CA-CB	5.19	1.62	1.53
9	2	195	ASP	N-CA	-5.19	1.39	1.46
22	S	472	HIS	ND1-CE1	5.19	1.37	1.32
32	M	120	LYS	CA-C	-5.19	1.46	1.52
2	B	225	THR	C-N	5.19	1.40	1.33
6	F	208	VAL	C-N	5.19	1.40	1.33
12	5	138	CYS	CA-C	-5.19	1.46	1.52
2	b	141	GLU	N-CA	-5.19	1.39	1.46
20	Z	473	LEU	C-N	5.19	1.41	1.33
22	S	286	TYR	CA-C	-5.19	1.45	1.52
22	S	334	HIS	CA-C	-5.19	1.46	1.52
7	g	56	SER	CA-C	5.18	1.58	1.52
10	j	98	ARG	CD-NE	5.18	1.53	1.46
4	D	142	ASP	CA-C	-5.18	1.46	1.52
11	4	120	ASP	C-N	5.18	1.40	1.33
21	N	327	LEU	CA-CB	5.18	1.61	1.53
21	N	822	GLY	CA-C	5.18	1.55	1.51
12	5	82	ARG	CZ-NH1	5.18	1.40	1.32
20	Z	504	GLU	C-N	5.18	1.40	1.33
21	N	57	ASP	CA-C	-5.18	1.46	1.52
9	2	187	ALA	N-CA	-5.18	1.39	1.46
12	5	97	ALA	CA-C	-5.18	1.46	1.53
27	O	348	VAL	CA-CB	5.18	1.61	1.54
32	M	200	PRO	C-O	-5.18	1.17	1.24
2	b	178	ARG	CZ-NH1	5.18	1.40	1.32
7	g	6	THR	CA-CB	5.18	1.61	1.53
10	j	73	LEU	CB-CG	5.18	1.63	1.53
6	F	79	PRO	N-CD	-5.18	1.40	1.47
13	6	184	SER	CA-CB	5.18	1.61	1.53
17	T	38	ASN	C-N	5.18	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	192	ALA	CA-C	-5.18	1.46	1.52
12	l	168	ALA	CA-CB	5.18	1.60	1.53
13	6	223	GLU	CA-C	-5.18	1.46	1.52
26	U	124	ASP	C-N	5.18	1.39	1.33
5	e	176	SER	C-N	5.18	1.40	1.33
10	j	14	ALA	CA-C	-5.18	1.46	1.52
14	n	71	GLY	C-N	5.18	1.40	1.33
21	N	921	ARG	CA-CB	5.18	1.61	1.53
25	R	186	TYR	C-N	5.18	1.40	1.33
31	L	252	VAL	CA-CB	-5.18	1.48	1.53
32	M	233	ARG	CA-CB	5.18	1.61	1.53
4	d	183	GLU	C-O	-5.17	1.19	1.24
10	j	111	GLY	C-N	5.17	1.40	1.33
13	m	100	ASN	CA-C	-5.17	1.46	1.52
12	5	183	GLU	CA-C	-5.17	1.45	1.52
17	T	247	ASP	CA-CB	5.17	1.61	1.53
29	I	407	ARG	NE-CZ	5.17	1.38	1.33
30	K	52	LYS	C-N	5.17	1.40	1.33
32	M	166	ARG	NE-CZ	5.17	1.38	1.33
32	M	290	ARG	CZ-NH1	5.17	1.40	1.32
13	m	50	LYS	N-CA	-5.17	1.39	1.46
29	I	306	MET	C-N	5.17	1.40	1.33
7	g	113	ALA	N-CA	-5.17	1.40	1.46
12	l	285	VAL	CA-C	-5.17	1.46	1.52
27	O	182	LYS	C-N	5.17	1.41	1.33
31	L	229	THR	C-N	5.17	1.40	1.33
32	M	340	SER	CA-C	-5.17	1.46	1.52
1	a	63	LEU	CA-C	-5.17	1.46	1.52
2	b	104	TYR	CA-C	5.17	1.59	1.53
5	e	71	ASP	CA-C	5.17	1.58	1.53
20	Z	314	LEU	C-N	5.17	1.40	1.33
23	P	138	ARG	CZ-NH1	5.17	1.40	1.32
7	g	239	ALA	CA-CB	5.17	1.61	1.53
4	D	20	VAL	CA-C	5.17	1.59	1.52
21	N	524	ILE	CA-C	5.17	1.59	1.52
25	R	308	LEU	N-CA	-5.17	1.39	1.46
27	O	295	THR	CA-C	-5.17	1.46	1.52
33	J	331	HIS	CE1-NE2	-5.17	1.27	1.32
2	B	236	ARG	CD-NE	5.17	1.53	1.46
7	G	72	ARG	CZ-NH1	5.17	1.40	1.32
9	2	195	ASP	CA-CB	5.17	1.63	1.53
9	2	236	ARG	CZ-NH1	5.17	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	618	GLN	C-N	5.17	1.41	1.33
20	Z	705	GLU	CA-C	-5.17	1.46	1.52
21	N	84	ALA	CA-C	-5.17	1.45	1.52
21	N	898	GLY	C-N	5.17	1.40	1.33
24	Q	344	GLU	C-N	5.17	1.41	1.33
25	R	215	GLY	CA-C	5.17	1.57	1.52
1	a	31	ALA	CA-C	5.17	1.59	1.52
3	c	38	ILE	CA-C	-5.17	1.45	1.52
4	d	241	GLN	N-CA	-5.17	1.40	1.46
21	N	696	LYS	C-N	5.17	1.40	1.33
22	S	271	ARG	CZ-NH1	5.17	1.40	1.32
4	d	25	GLU	N-CA	5.16	1.52	1.46
10	j	164	PHE	C-N	5.16	1.40	1.33
12	l	212	TYR	CA-CB	5.16	1.61	1.53
2	B	6	SER	CA-CB	5.16	1.60	1.53
3	C	48	ALA	CA-C	-5.16	1.46	1.52
4	D	183	GLU	C-N	-5.16	1.27	1.33
9	2	79	ALA	C-N	5.16	1.41	1.33
24	Q	334	HIS	CG-ND1	5.16	1.44	1.38
29	I	377	LEU	C-N	5.16	1.40	1.34
12	l	281	SER	N-CA	-5.16	1.39	1.45
3	C	143	ARG	CA-C	-5.16	1.46	1.52
23	P	232	ARG	NE-CZ	5.16	1.38	1.33
3	C	217	ARG	CZ-NH1	5.16	1.40	1.32
20	Z	61	SER	C-N	5.16	1.41	1.34
21	N	493	GLY	CA-C	-5.16	1.44	1.51
23	P	144	VAL	CA-C	-5.16	1.46	1.52
28	H	331	ARG	CZ-NH1	5.16	1.40	1.32
31	L	281	ASP	CA-C	-5.16	1.46	1.52
33	J	255	SER	C-N	5.16	1.40	1.33
1	a	113	PRO	N-CA	5.16	1.53	1.47
9	i	166	VAL	C-N	5.16	1.40	1.33
10	j	24	ALA	C-N	5.16	1.40	1.33
1	A	105	ARG	C-O	-5.16	1.18	1.24
9	2	201	ASN	CA-CB	5.16	1.61	1.53
25	R	237	THR	CA-C	-5.16	1.46	1.52
27	O	37	LEU	CA-C	-5.16	1.46	1.52
30	K	271	ILE	CA-C	-5.16	1.46	1.52
32	M	144	ASP	CA-C	5.16	1.59	1.52
12	5	192	SER	C-N	5.16	1.42	1.33
23	P	430	GLY	CA-C	-5.16	1.45	1.52
1	A	40	ILE	N-CA	-5.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	PRO	C-N	5.16	1.40	1.33
9	2	37	PHE	C-N	5.16	1.41	1.33
21	N	544	GLU	C-N	5.16	1.40	1.34
21	N	873	ARG	NE-CZ	5.16	1.38	1.33
33	J	182	PRO	C-O	5.16	1.29	1.23
2	B	246	ARG	NE-CZ	5.15	1.38	1.33
21	N	820	GLU	CA-C	-5.15	1.46	1.52
25	R	98	LEU	N-CA	-5.15	1.40	1.46
10	3	34	LEU	CA-CB	5.15	1.60	1.53
12	5	203	CYS	CA-C	-5.15	1.46	1.52
17	T	132	HIS	N-CA	-5.15	1.39	1.46
20	Z	948	TRP	CD2-CE3	5.15	1.48	1.40
20	Z	959	HIS	CE1-NE2	5.15	1.37	1.32
22	S	396	SER	N-CA	5.15	1.52	1.46
27	O	53	LYS	CA-CB	5.15	1.62	1.53
28	H	346	ARG	CA-C	-5.15	1.45	1.52
29	I	82	LEU	CA-C	-5.15	1.46	1.52
2	b	148	TYR	CA-C	-5.15	1.46	1.52
3	c	95	ALA	CA-CB	-5.15	1.45	1.53
13	6	141	ARG	C-N	5.15	1.40	1.33
26	U	222	ASN	C-N	5.15	1.41	1.33
31	L	232	ALA	C-N	5.15	1.40	1.33
25	R	310	GLU	C-O	-5.15	1.18	1.24
2	b	197	LYS	CA-CB	5.15	1.62	1.53
4	d	117	GLN	C-N	5.15	1.40	1.33
1	A	137	LEU	CA-C	-5.15	1.46	1.52
14	7	226	ARG	CZ-NH1	5.15	1.40	1.32
20	Z	703	SER	CA-C	-5.15	1.46	1.52
20	Z	852	GLN	CA-C	-5.15	1.46	1.52
28	H	197	MET	CA-CB	5.15	1.61	1.53
31	L	104	LEU	CA-C	-5.15	1.46	1.52
12	l	170	LEU	CB-CG	5.14	1.63	1.53
8	1	163	PHE	CA-CB	5.14	1.61	1.53
25	R	24	TYR	CA-CB	5.14	1.61	1.53
27	O	392	TRP	NE1-CE2	5.14	1.43	1.37
33	J	324	ARG	CA-C	-5.14	1.46	1.52
8	h	36	ALA	N-CA	-5.14	1.40	1.46
6	F	154	THR	CA-C	-5.14	1.46	1.52
1	a	22	GLU	C-N	5.14	1.40	1.33
1	a	152	PRO	CA-CB	5.14	1.60	1.53
10	j	114	SER	CA-C	-5.14	1.45	1.52
14	n	109	TYR	CA-CB	5.14	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	33	ALA	C-N	5.14	1.40	1.33
23	P	310	ARG	C-N	5.14	1.41	1.33
25	R	219	LEU	CA-CB	5.14	1.61	1.53
28	H	432	ARG	CD-NE	5.14	1.53	1.46
30	K	55	GLU	CA-CB	5.14	1.61	1.53
1	a	177	GLU	C-N	5.14	1.40	1.33
5	E	107	ILE	CA-CB	-5.14	1.49	1.54
20	Z	286	VAL	CA-C	-5.14	1.46	1.52
21	N	562	THR	N-CA	-5.14	1.40	1.46
22	S	196	ARG	CZ-NH1	5.14	1.40	1.32
2	b	118	MET	C-N	5.14	1.40	1.33
3	C	113	ARG	CZ-NH1	5.14	1.40	1.32
13	6	184	SER	N-CA	-5.14	1.39	1.45
20	Z	775	MET	CA-C	-5.14	1.46	1.53
25	R	96	GLN	C-N	5.14	1.40	1.33
29	I	285	ASP	N-CA	-5.14	1.40	1.46
2	b	249	ALA	C-N	5.13	1.40	1.33
8	1	38	ARG	CZ-NH2	5.13	1.40	1.33
21	N	92	ASP	CA-C	-5.13	1.46	1.52
21	N	845	GLY	N-CA	5.13	1.51	1.45
25	R	107	GLU	CA-C	-5.13	1.46	1.52
28	H	89	GLN	C-N	5.13	1.41	1.33
28	H	434	ARG	NE-CZ	5.13	1.38	1.33
2	b	220	ASP	N-CA	-5.13	1.39	1.46
25	R	137	LEU	CA-CB	5.13	1.61	1.53
6	f	122	SER	CA-C	-5.13	1.46	1.53
7	g	128	SER	CA-CB	5.13	1.61	1.53
7	G	201	TYR	CA-C	5.13	1.59	1.52
17	T	130	ASP	N-CA	-5.13	1.40	1.46
7	g	49	ALA	CA-C	-5.13	1.46	1.52
10	j	176	ASP	CA-CB	5.13	1.61	1.53
7	G	63	LYS	C-O	-5.13	1.17	1.23
7	G	198	LYS	C-O	-5.13	1.17	1.24
22	S	277	SER	CA-C	-5.13	1.46	1.52
3	c	141	ASP	CA-C	-5.13	1.46	1.52
4	d	90	ARG	NE-CZ	5.13	1.38	1.33
5	e	170	LYS	N-CA	-5.13	1.39	1.46
13	m	46	ARG	NE-CZ	5.13	1.38	1.33
20	Z	316	ALA	C-O	5.13	1.30	1.24
24	Q	80	HIS	CD2-NE2	5.13	1.43	1.37
31	L	83	ASP	N-CA	-5.13	1.40	1.46
9	i	70	ILE	N-CA	-5.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	105	VAL	CA-C	-5.13	1.45	1.52
9	2	62	LYS	N-CA	-5.13	1.40	1.46
23	P	400	VAL	CA-C	-5.13	1.46	1.52
27	O	343	GLN	C-N	5.13	1.40	1.33
20	Z	160	GLU	C-O	-5.12	1.18	1.24
33	J	349	LYS	CA-C	5.12	1.59	1.52
4	D	57	THR	C-N	5.12	1.40	1.33
7	G	196	ALA	N-CA	-5.12	1.40	1.46
7	G	219	CYS	CA-CB	5.12	1.64	1.53
10	3	74	TYR	CA-CB	5.12	1.61	1.53
30	K	175	GLY	C-N	5.12	1.41	1.33
2	b	162	THR	CA-C	-5.12	1.46	1.52
8	h	27	SER	CA-CB	5.12	1.62	1.53
2	B	239	THR	C-N	5.12	1.40	1.33
19	Y	64	TRP	NE1-CE2	-5.12	1.31	1.37
14	n	150	ALA	C-N	5.12	1.38	1.33
7	G	153	PRO	N-CA	5.12	1.53	1.47
10	3	16	THR	CA-C	5.12	1.58	1.52
20	Z	798	ARG	CA-CB	5.12	1.61	1.53
21	N	726	ASP	C-N	5.12	1.40	1.33
23	P	405	PRO	CA-C	-5.12	1.46	1.52
5	E	73	HIS	CB-CG	5.12	1.57	1.50
12	5	198	LYS	CA-C	-5.12	1.46	1.52
13	6	218	ASP	N-CA	-5.12	1.39	1.46
15	W	35	PHE	CA-CB	5.12	1.61	1.53
27	O	43	GLU	CA-C	-5.12	1.46	1.52
29	I	352	ASN	CA-C	-5.12	1.47	1.53
31	L	144	VAL	CA-C	-5.12	1.46	1.52
31	L	163	THR	CA-C	-5.12	1.46	1.52
9	i	48	ARG	CZ-NH2	5.12	1.40	1.33
10	j	145	GLN	C-N	5.12	1.41	1.34
13	m	196	PHE	CA-C	5.12	1.59	1.52
3	C	32	ALA	N-CA	-5.12	1.39	1.45
3	C	125	HIS	N-CA	-5.12	1.39	1.45
12	l	205	GLY	C-N	5.12	1.41	1.33
21	N	820	GLU	N-CA	-5.12	1.40	1.46
12	l	162	VAL	CA-CB	5.11	1.61	1.54
14	n	107	ASN	CA-CB	-5.11	1.45	1.53
3	C	60	ASP	C-N	5.11	1.41	1.33
22	S	192	GLU	N-CA	-5.11	1.39	1.46
22	S	490	ASN	C-N	5.11	1.39	1.33
27	O	281	ALA	CA-C	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	47	ALA	CA-C	-5.11	1.46	1.52
13	m	223	GLU	CA-C	-5.11	1.46	1.52
1	A	241	ILE	CA-C	-5.11	1.46	1.52
7	G	176	LEU	CA-CB	5.11	1.61	1.53
10	3	187	VAL	N-CA	-5.11	1.40	1.46
20	Z	58	GLU	CA-C	-5.11	1.46	1.52
3	c	98	TYR	C-N	5.11	1.40	1.33
6	f	6	TYR	CA-C	-5.11	1.46	1.52
13	m	72	LEU	C-N	5.11	1.40	1.33
13	m	174	GLY	N-CA	5.11	1.52	1.45
14	n	74	ARG	CZ-NH1	5.11	1.40	1.32
14	7	223	ARG	N-CA	-5.11	1.40	1.46
21	N	295	THR	C-N	5.11	1.40	1.33
21	N	509	GLN	C-N	5.11	1.40	1.33
24	Q	226	HIS	ND1-CE1	5.11	1.37	1.32
27	O	118	GLY	CA-C	5.11	1.58	1.51
31	L	51	GLU	C-N	5.11	1.40	1.33
9	i	89	GLY	N-CA	-5.11	1.39	1.45
8	1	94	LEU	CA-C	-5.11	1.46	1.52
11	4	93	ARG	NE-CZ	5.11	1.38	1.33
11	4	95	ARG	NE-CZ	5.11	1.38	1.33
25	R	96	GLN	CA-CB	5.11	1.62	1.53
26	U	291	LEU	CA-C	-5.11	1.46	1.52
5	e	79	SER	CA-C	-5.11	1.46	1.52
2	B	91	LYS	CA-C	5.11	1.59	1.52
16	V	236	SER	N-CA	-5.11	1.40	1.46
14	n	184	ALA	N-CA	-5.11	1.39	1.46
14	n	237	THR	CA-C	-5.11	1.45	1.52
1	A	11	GLY	C-N	5.11	1.40	1.33
5	E	186	GLU	C-N	5.11	1.40	1.33
6	F	98	VAL	CA-C	-5.11	1.47	1.52
17	T	128	TYR	CA-CB	5.11	1.61	1.53
22	S	82	TYR	CA-CB	5.11	1.60	1.53
33	J	200	ARG	CD-NE	5.11	1.53	1.46
5	e	199	LEU	CA-C	-5.10	1.46	1.52
22	S	145	PHE	N-CA	-5.10	1.40	1.46
22	S	178	LEU	CA-C	-5.10	1.46	1.52
30	K	349	ARG	CD-NE	5.10	1.53	1.46
7	g	93	ARG	NE-CZ	5.10	1.38	1.33
12	l	132	THR	CA-CB	-5.10	1.45	1.53
13	m	229	ARG	NE-CZ	5.10	1.38	1.33
14	n	108	ALA	CA-C	-5.10	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	137	PRO	C-N	5.10	1.40	1.33
22	S	476	LEU	C-N	5.10	1.40	1.33
32	M	171	GLU	CA-C	-5.10	1.46	1.52
32	M	251	LEU	N-CA	-5.10	1.39	1.46
7	G	73	HIS	N-CA	-5.10	1.39	1.46
22	S	34	LEU	CA-CB	5.10	1.61	1.53
24	Q	332	ARG	CA-CB	5.10	1.61	1.53
27	O	368	ASP	CA-CB	5.10	1.61	1.53
28	H	424	THR	N-CA	5.10	1.52	1.46
31	L	194	ARG	CZ-NH2	5.10	1.40	1.33
33	J	232	GLU	C-N	5.10	1.40	1.33
10	j	155	GLU	C-O	-5.10	1.19	1.24
14	n	161	ARG	CZ-NH2	5.10	1.40	1.33
12	5	249	SER	N-CA	-5.10	1.39	1.45
21	N	159	GLU	N-CA	-5.10	1.40	1.46
25	R	43	ARG	CD-NE	5.10	1.53	1.46
27	O	208	ALA	N-CA	-5.10	1.40	1.46
29	I	60	LEU	N-CA	-5.10	1.40	1.46
32	M	154	LEU	C-N	5.10	1.39	1.33
31	L	342	ARG	CZ-NH2	5.10	1.40	1.33
7	G	214	LEU	N-CA	-5.09	1.40	1.46
21	N	528	ARG	CZ-NH2	5.09	1.40	1.33
24	Q	123	GLU	CA-CB	5.09	1.61	1.53
28	H	281	GLN	N-CA	-5.09	1.39	1.46
29	I	120	VAL	C-N	5.09	1.40	1.33
33	J	91	GLU	C-N	5.09	1.41	1.33
14	7	252	TRP	NE1-CE2	-5.09	1.31	1.37
15	W	168	THR	CA-C	-5.09	1.46	1.52
20	Z	158	ALA	C-N	5.09	1.40	1.33
23	P	427	GLU	N-CA	-5.09	1.40	1.46
25	R	344	SER	N-CA	-5.09	1.39	1.46
7	G	218	TRP	N-CA	-5.09	1.39	1.45
8	1	161	VAL	N-CA	-5.09	1.40	1.46
13	6	109	ARG	CZ-NH2	5.09	1.40	1.33
20	Z	924	LYS	C-N	5.09	1.40	1.33
25	R	111	LYS	N-CA	-5.09	1.40	1.46
27	O	327	LEU	CA-CB	5.09	1.61	1.53
28	H	326	ASP	CA-CB	5.09	1.60	1.53
33	J	214	SER	CA-CB	5.09	1.60	1.53
9	i	145	HIS	CA-CB	5.09	1.61	1.53
9	2	102	GLU	C-N	5.09	1.39	1.33
13	6	113	TYR	CZ-OH	5.09	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	135	HIS	CB-CG	5.09	1.57	1.50
24	Q	423	VAL	CA-C	5.09	1.60	1.52
2	B	113	GLU	CA-C	-5.09	1.46	1.52
23	P	36	LEU	CA-C	-5.09	1.46	1.52
32	M	71	ASN	N-CA	-5.09	1.40	1.46
33	J	391	ASN	C-O	-5.09	1.18	1.24
3	c	180	TYR	CA-C	-5.09	1.46	1.52
4	d	12	SER	CA-CB	5.09	1.61	1.53
4	d	166	ARG	C-N	5.09	1.40	1.33
3	C	88	ILE	CA-C	-5.09	1.46	1.52
18	X	98	PHE	C-N	5.09	1.40	1.33
26	U	118	PRO	C-N	5.09	1.40	1.33
17	T	129	LEU	CA-C	-5.08	1.45	1.52
5	E	204	LEU	CA-CB	5.08	1.61	1.53
9	2	59	ASN	N-CA	-5.08	1.40	1.46
11	4	95	ARG	CZ-NH1	5.08	1.39	1.32
16	V	225	LEU	N-CA	5.08	1.52	1.45
22	S	415	SER	N-CA	-5.08	1.39	1.45
25	R	93	LYS	C-N	5.08	1.40	1.33
3	c	210	ARG	CZ-NH1	5.08	1.39	1.32
2	B	4	ARG	NE-CZ	5.08	1.38	1.33
20	Z	183	LYS	CA-C	-5.08	1.46	1.52
22	S	385	SER	CA-C	-5.08	1.46	1.52
24	Q	28	LEU	CA-CB	5.08	1.61	1.53
25	R	411	LEU	CA-C	-5.08	1.46	1.52
26	U	164	GLU	C-N	5.08	1.40	1.33
28	H	462	ARG	C-N	5.08	1.40	1.33
29	I	298	GLY	CA-C	5.08	1.59	1.51
4	D	4	TYR	CZ-OH	5.08	1.48	1.38
11	4	104	ILE	C-N	5.08	1.38	1.33
30	K	87	LYS	N-CA	-5.08	1.40	1.46
8	1	54	ARG	CD-NE	5.08	1.53	1.46
18	X	107	GLY	C-N	5.08	1.41	1.33
20	Z	267	THR	C-N	5.08	1.40	1.33
21	N	662	MET	SD-CE	5.08	1.92	1.79
30	K	77	ARG	C-N	5.08	1.41	1.33
30	K	148	ASP	CA-C	-5.08	1.46	1.52
30	K	306	PHE	CA-C	-5.08	1.46	1.52
13	m	11	ASN	CA-C	-5.08	1.48	1.52
5	E	237	ALA	N-CA	-5.08	1.40	1.46
23	P	276	LEU	N-CA	5.08	1.52	1.46
28	H	411	CYS	CA-C	5.08	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	214	ALA	CA-CB	5.08	1.61	1.53
33	J	286	LYS	CA-CB	5.08	1.61	1.53
4	D	89	ALA	CA-C	-5.08	1.46	1.52
5	E	209	GLU	CA-C	-5.08	1.46	1.52
20	Z	98	ASP	CA-C	5.08	1.59	1.52
22	S	68	LEU	N-CA	-5.08	1.39	1.46
4	d	83	ARG	CZ-NH2	5.07	1.40	1.33
7	g	101	LYS	N-CA	-5.07	1.40	1.46
7	g	180	VAL	C-N	5.07	1.40	1.33
2	B	111	VAL	CA-CB	5.07	1.60	1.54
16	V	160	ASP	CA-CB	5.07	1.61	1.53
17	T	191	LYS	CA-CB	5.07	1.61	1.53
18	X	51	ARG	C-N	-5.07	1.27	1.33
14	7	118	GLU	C-N	5.07	1.40	1.33
15	W	70	GLY	C-N	5.07	1.41	1.33
17	T	99	SER	CA-C	-5.07	1.46	1.52
23	P	235	LEU	N-CA	-5.07	1.40	1.46
29	I	190	GLN	C-N	5.07	1.40	1.33
2	b	204	PHE	C-N	5.07	1.39	1.33
9	2	214	GLU	CA-CB	5.07	1.60	1.53
9	2	217	ARG	NE-CZ	5.07	1.38	1.33
10	3	5	SER	CA-C	-5.07	1.46	1.52
20	Z	539	ASN	CA-CB	5.07	1.60	1.53
21	N	117	TYR	CA-CB	5.07	1.61	1.53
21	N	137	PHE	CA-C	-5.07	1.46	1.52
26	U	143	VAL	C-N	5.07	1.40	1.33
10	3	104	PHE	C-N	5.07	1.40	1.33
30	K	405	SER	CA-C	-5.07	1.46	1.52
2	B	219	PRO	N-CD	-5.07	1.40	1.47
2	B	234	ARG	CZ-NH1	5.07	1.39	1.32
4	D	46	CYS	CA-C	-5.07	1.46	1.52
20	Z	464	ASP	CA-CB	5.07	1.62	1.54
24	Q	126	LYS	CA-CB	5.07	1.62	1.53
6	f	141	GLY	N-CA	-5.07	1.38	1.45
9	i	138	HIS	CA-C	-5.07	1.46	1.52
4	D	99	THR	C-N	5.07	1.40	1.33
18	X	122	TYR	N-CA	-5.07	1.40	1.46
22	S	480	ARG	CD-NE	5.07	1.53	1.46
28	H	114	GLU	CA-C	-5.07	1.46	1.52
30	K	349	ARG	NE-CZ	5.07	1.38	1.33
33	J	46	ALA	C-O	-5.07	1.18	1.24
21	N	87	ASP	CA-CB	5.06	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	323	LYS	C-N	5.06	1.41	1.33
25	R	31	PHE	CA-C	-5.06	1.46	1.52
31	L	160	PRO	CA-C	-5.06	1.46	1.52
7	g	86	ARG	CD-NE	5.06	1.53	1.46
3	C	91	ALA	C-N	5.06	1.40	1.33
14	7	215	ARG	CD-NE	5.06	1.53	1.46
24	Q	382	LEU	N-CA	-5.06	1.39	1.46
30	K	183	GLU	CA-CB	5.06	1.61	1.53
32	M	139	LYS	CA-CB	5.06	1.60	1.53
33	J	304	LEU	C-N	5.06	1.40	1.33
10	j	64	ASN	N-CA	-5.06	1.40	1.46
11	4	173	PRO	C-N	5.06	1.40	1.33
20	Z	553	ARG	CD-NE	5.06	1.53	1.46
21	N	69	TYR	C-N	5.06	1.40	1.33
23	P	12	ASP	N-CA	-5.06	1.40	1.46
29	I	347	LYS	CA-C	-5.06	1.46	1.52
8	h	90	VAL	C-N	5.06	1.40	1.34
12	l	172	MET	CA-C	-5.06	1.46	1.52
11	4	182	LYS	N-CA	-5.06	1.39	1.46
12	5	280	GLY	CA-C	-5.06	1.44	1.51
20	Z	317	GLN	CA-CB	5.06	1.61	1.53
20	Z	754	LYS	N-CA	-5.06	1.40	1.46
23	P	306	ASN	N-CA	-5.06	1.40	1.46
25	R	222	ARG	CZ-NH1	5.06	1.39	1.32
32	M	318	ASP	CA-CB	5.06	1.62	1.53
6	F	209	ASP	CA-C	-5.06	1.45	1.52
21	N	4	THR	C-N	5.06	1.40	1.33
21	N	776	TYR	N-CA	-5.06	1.40	1.46
24	Q	245	SER	CA-C	-5.06	1.46	1.52
26	U	86	LYS	CA-CB	5.06	1.61	1.53
27	O	293	LEU	C-N	5.06	1.40	1.33
28	H	259	CYS	CA-C	-5.06	1.46	1.52
31	L	100	SER	CA-CB	5.06	1.61	1.53
32	M	236	ALA	C-O	-5.06	1.18	1.24
1	a	102	ALA	N-CA	-5.06	1.40	1.46
4	d	70	HIS	CD2-NE2	-5.06	1.32	1.37
20	Z	589	SER	N-CA	-5.05	1.39	1.46
29	I	281	ILE	CA-CB	5.05	1.59	1.53
32	M	237	ALA	N-CA	-5.05	1.40	1.46
7	g	172	ALA	CA-CB	5.05	1.61	1.53
9	i	131	GLY	CA-C	-5.05	1.45	1.51
24	Q	196	ALA	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	36	ARG	C-N	5.05	1.40	1.33
12	l	94	ARG	CD-NE	5.05	1.53	1.46
14	n	149	VAL	N-CA	-5.05	1.40	1.46
20	Z	202	ARG	CZ-NH2	5.05	1.40	1.33
2	b	230	ASP	CA-CB	5.05	1.61	1.53
7	g	127	ASN	CB-CG	5.05	1.64	1.52
5	E	236	THR	C-N	5.05	1.40	1.33
6	F	51	ARG	CZ-NH2	5.05	1.40	1.33
12	5	243	ASP	CA-C	-5.05	1.46	1.52
17	T	178	THR	CA-C	5.05	1.59	1.52
29	I	207	LEU	C-N	5.05	1.40	1.33
21	N	911	LYS	N-CA	5.05	1.52	1.46
7	g	61	PRO	C-O	-5.05	1.18	1.23
12	l	252	LEU	N-CA	-5.05	1.39	1.46
14	n	249	ASN	CA-C	-5.05	1.47	1.53
2	B	197	LYS	CB-CG	5.05	1.67	1.52
12	5	83	PHE	CA-C	-5.05	1.46	1.52
21	N	670	LYS	C-N	5.05	1.40	1.33
5	e	143	LEU	CA-C	-5.04	1.46	1.52
21	N	442	LEU	CA-CB	5.04	1.61	1.53
1	a	108	TYR	N-CA	-5.04	1.39	1.45
4	D	28	LYS	N-CA	-5.04	1.39	1.46
6	F	65	LYS	CA-C	-5.04	1.46	1.52
30	K	326	PRO	N-CA	-5.04	1.41	1.47
33	J	312	ARG	NE-CZ	5.04	1.38	1.33
1	a	117	LEU	CA-CB	5.04	1.61	1.53
9	i	75	ALA	CA-C	-5.04	1.46	1.52
6	F	33	SER	CA-C	5.04	1.59	1.52
10	3	158	LEU	N-CA	-5.04	1.39	1.46
15	W	23	ARG	NE-CZ	5.04	1.38	1.33
22	S	410	LYS	C-N	5.04	1.40	1.33
27	O	387	ARG	C-N	5.04	1.39	1.33
2	b	221	LEU	CA-C	-5.04	1.46	1.52
26	U	243	ASP	C-O	-5.04	1.18	1.24
30	K	54	LEU	C-N	5.04	1.40	1.33
1	A	121	MET	CA-C	-5.04	1.46	1.52
3	C	36	ILE	N-CA	-5.04	1.40	1.46
3	C	235	ILE	C-N	5.04	1.40	1.33
9	2	66	ILE	C-O	-5.04	1.18	1.24
20	Z	912	PHE	CA-C	-5.04	1.46	1.52
22	S	399	TYR	C-N	5.04	1.41	1.33
25	R	288	SER	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	30	THR	C-N	5.04	1.40	1.33
33	J	173	LEU	C-N	5.04	1.40	1.33
14	7	85	GLY	N-CA	-5.04	1.39	1.46
21	N	560	ALA	CA-CB	5.04	1.61	1.53
25	R	142	ALA	CA-CB	5.04	1.61	1.53
3	c	230	PHE	CA-C	-5.04	1.46	1.52
12	l	86	GLY	N-CA	-5.04	1.38	1.45
12	5	115	PHE	CA-C	-5.04	1.46	1.52
21	N	894	ARG	C-N	5.04	1.39	1.33
23	P	171	MET	C-O	5.04	1.30	1.24
32	M	33	ARG	C-N	5.04	1.41	1.34
33	J	213	VAL	N-CA	-5.04	1.40	1.46
10	j	27	LEU	CA-C	-5.03	1.45	1.52
10	j	137	ILE	N-CA	-5.03	1.40	1.46
4	D	162	GLN	N-CA	-5.03	1.39	1.46
14	7	215	ARG	CZ-NH2	5.03	1.40	1.33
24	Q	322	GLU	CA-CB	5.03	1.61	1.53
1	A	12	TYR	C-N	5.03	1.40	1.33
24	Q	212	THR	CA-C	-5.03	1.46	1.52
3	c	34	THR	CA-C	5.03	1.59	1.52
14	n	62	SER	C-N	5.03	1.40	1.33
5	E	188	HIS	ND1-CE1	5.03	1.37	1.32
12	5	222	ASP	CA-CB	5.03	1.59	1.53
14	7	119	ALA	CA-CB	5.03	1.61	1.53
16	V	290	ASN	CA-CB	-5.03	1.45	1.53
21	N	499	HIS	CA-C	-5.03	1.46	1.52
24	Q	342	LEU	C-N	5.03	1.40	1.33
26	U	8	VAL	CA-C	-5.03	1.46	1.52
27	O	166	ARG	CZ-NH1	5.03	1.39	1.32
31	L	110	LYS	N-CA	-5.03	1.39	1.46
21	N	320	SER	CA-CB	5.03	1.61	1.53
22	S	393	ARG	CD-NE	5.03	1.53	1.46
7	g	216	ILE	CA-C	-5.03	1.46	1.52
8	h	147	CYS	C-N	5.03	1.40	1.33
17	T	241	GLU	CA-C	-5.03	1.46	1.52
21	N	591	LEU	C-O	-5.03	1.18	1.24
22	S	482	PRO	CA-CB	5.03	1.60	1.53
23	P	249	ALA	CA-CB	5.03	1.61	1.53
28	H	275	ILE	CA-CB	-5.03	1.47	1.54
33	J	310	ILE	CA-CB	-5.03	1.48	1.54
6	f	21	GLN	CA-C	-5.03	1.46	1.52
1	A	61	ASP	C-N	5.03	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	VAL	CA-CB	5.03	1.60	1.53
12	5	113	ASN	CA-CB	5.03	1.61	1.53
20	Z	287	ARG	NE-CZ	5.03	1.38	1.33
30	K	81	ARG	NE-CZ	5.03	1.38	1.33
14	7	36	GLN	CA-C	-5.02	1.46	1.52
8	1	113	ASP	C-N	5.02	1.40	1.33
10	3	153	LEU	CA-CB	5.02	1.61	1.53
13	6	62	ALA	C-N	5.02	1.40	1.33
20	Z	286	VAL	C-N	5.02	1.40	1.33
21	N	59	GLU	C-N	5.02	1.40	1.33
23	P	308	LEU	C-N	5.02	1.39	1.33
27	O	286	PHE	N-CA	-5.02	1.40	1.46
3	C	45	VAL	CA-CB	-5.02	1.48	1.54
7	G	149	TYR	CA-C	5.02	1.58	1.52
7	G	203	ALA	CA-C	-5.02	1.45	1.52
8	1	47	HIS	C-N	5.02	1.40	1.33
21	N	759	ILE	CA-C	-5.02	1.46	1.52
1	a	82	VAL	C-N	5.02	1.39	1.33
3	c	148	LEU	CA-C	-5.02	1.46	1.52
21	N	532	ALA	N-CA	5.02	1.52	1.46
21	N	761	ILE	C-N	5.02	1.40	1.33
32	M	240	ASN	CA-C	-5.02	1.46	1.52
2	b	95	THR	N-CA	-5.02	1.40	1.46
11	k	33	ASP	CA-CB	5.02	1.60	1.53
2	B	222	LEU	CA-C	-5.02	1.46	1.52
20	Z	94	PRO	C-O	-5.02	1.18	1.24
26	U	208	VAL	CA-CB	-5.02	1.48	1.54
32	M	318	ASP	C-N	-5.02	1.27	1.33
2	b	219	PRO	C-N	5.01	1.41	1.33
3	c	73	ILE	C-N	5.01	1.40	1.33
1	A	214	LEU	CA-C	-5.01	1.46	1.52
7	G	28	VAL	CA-CB	-5.01	1.48	1.54
20	Z	782	ILE	C-N	5.01	1.40	1.33
21	N	708	ALA	CA-C	-5.01	1.46	1.52
23	P	363	LEU	CA-CB	5.01	1.61	1.53
23	P	415	TRP	C-N	5.01	1.40	1.33
24	Q	150	GLN	N-CA	-5.01	1.40	1.46
27	O	387	ARG	CZ-NH1	5.01	1.39	1.32
28	H	370	ARG	C-N	5.01	1.40	1.33
29	I	195	LYS	CA-C	-5.01	1.46	1.52
1	a	188	LYS	C-N	5.01	1.41	1.33
8	h	186	VAL	CA-CB	-5.01	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	68	LYS	CA-C	-5.01	1.46	1.52
16	V	120	SER	CA-C	5.01	1.59	1.52
23	P	100	VAL	CA-CB	-5.01	1.48	1.54
1	a	15	HIS	ND1-CE1	5.01	1.37	1.32
12	l	271	LEU	CA-CB	-5.01	1.45	1.53
12	5	106	VAL	CA-CB	5.01	1.59	1.54
20	Z	718	ASP	CA-C	-5.01	1.46	1.52
21	N	156	ILE	CA-CB	-5.01	1.47	1.54
23	P	259	PRO	N-CA	-5.01	1.40	1.47
28	H	173	ARG	NE-CZ	5.01	1.38	1.33
29	I	246	ARG	NE-CZ	5.01	1.38	1.33
31	L	131	VAL	CA-CB	-5.01	1.47	1.55
33	J	260	GLY	C-N	5.01	1.40	1.33
5	e	73	HIS	ND1-CE1	5.01	1.37	1.32
12	l	140	LEU	CA-C	-5.01	1.46	1.52
1	A	142	THR	CA-C	-5.01	1.46	1.52
15	W	148	GLU	N-CA	5.01	1.52	1.45
16	V	56	GLU	N-CA	-5.01	1.40	1.46
21	N	910	PRO	C-N	5.01	1.40	1.33
24	Q	74	LEU	CA-CB	5.01	1.61	1.53
2	B	103	GLU	N-CA	-5.01	1.39	1.45
20	Z	738	TYR	CA-CB	5.01	1.61	1.53
31	L	405	ASP	CA-CB	5.01	1.62	1.53
4	d	201	GLU	CD-OE2	5.01	1.34	1.25
7	G	228	HIS	N-CA	-5.01	1.39	1.46
14	7	171	SER	N-CA	-5.01	1.40	1.46
22	S	105	PRO	CA-C	-5.01	1.47	1.52
31	L	318	LEU	N-CA	-5.01	1.40	1.46
4	D	83	ARG	NE-CZ	5.00	1.38	1.33
4	D	141	ARG	C-N	5.00	1.40	1.33
13	6	94	ILE	CA-CB	-5.00	1.47	1.54
21	N	606	VAL	CA-C	-5.00	1.47	1.53
24	Q	376	LYS	CA-C	-5.00	1.46	1.52
26	U	295	LYS	CA-CB	5.00	1.61	1.53
12	l	121	ALA	C-O	-5.00	1.17	1.23
14	n	252	TRP	CA-C	-5.00	1.46	1.52
10	3	40	PHE	CA-C	-5.00	1.46	1.52
16	V	132	LEU	N-CA	5.00	1.52	1.46
21	N	222	TYR	CA-CB	5.00	1.62	1.53
21	N	892	PRO	CA-C	-5.00	1.47	1.52
11	k	45	SER	CA-CB	5.00	1.61	1.53
16	V	82	ALA	N-CA	-5.00	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	129	GLU	C-N	5.00	1.40	1.33
26	U	192	ASN	C-O	-5.00	1.18	1.24
32	M	247	ALA	CA-C	-5.00	1.46	1.52
33	J	123	HIS	C-N	5.00	1.40	1.33

All (7767) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	948	TRP	CZ3-CH2-CZ2	-17.62	98.59	121.50
20	Z	776	VAL	CA-C-O	-16.09	107.91	118.69
14	7	209	ALA	CA-C-N	13.94	138.12	120.56
14	7	209	ALA	C-N-CA	13.94	138.12	120.56
16	V	147	VAL	N-CA-C	-13.79	99.72	113.10
30	K	204	ASP	CA-C-N	13.32	129.39	119.66
30	K	204	ASP	C-N-CA	13.32	129.39	119.66
22	S	326	ASP	CA-CB-CG	-13.05	99.55	112.60
10	j	184	GLY	CA-C-O	-12.62	113.53	122.23
7	g	108	PRO	CA-C-N	12.58	128.16	120.24
7	g	108	PRO	C-N-CA	12.58	128.16	120.24
21	N	719	ASN	CA-CB-CG	-12.57	100.03	112.60
22	S	59	ASP	CA-CB-CG	-12.53	100.07	112.60
9	2	67	SER	O-C-N	-12.42	110.98	121.54
22	S	130	VAL	N-CA-C	-11.99	101.69	113.20
20	Z	253	VAL	N-CA-CB	11.92	118.01	110.50
20	Z	632	GLU	CA-C-N	11.85	136.16	120.28
20	Z	632	GLU	C-N-CA	11.85	136.16	120.28
31	L	214	PRO	N-CA-CB	11.74	109.33	103.22
13	m	44	ASN	CA-CB-CG	-11.63	100.97	112.60
1	a	65	ASP	CA-C-N	11.51	131.40	119.19
1	a	65	ASP	C-N-CA	11.51	131.40	119.19
21	N	99	GLU	N-CA-C	-11.46	97.17	113.21
24	Q	225	LEU	N-CA-C	11.45	123.76	111.28
2	B	216	ASP	CA-CB-CG	-11.38	101.22	112.60
7	G	48	PHE	CA-CB-CG	-11.30	102.50	113.80
21	N	717	LEU	N-CA-C	-11.29	100.52	114.75
10	3	127	ILE	O-C-N	-11.17	111.00	122.06
21	N	890	PHE	CA-CB-CG	-11.15	102.65	113.80
17	T	213	ASN	CA-C-N	11.08	135.13	120.28
17	T	213	ASN	C-N-CA	11.08	135.13	120.28
14	n	89	ASP	CA-CB-CG	11.04	123.64	112.60
20	Z	835	ALA	N-CA-C	11.01	123.28	111.28
26	U	82	LYS	CA-C-O	-10.94	109.43	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	132	PHE	CA-CB-CG	-10.86	102.94	113.80
8	h	178	SER	N-CA-C	-10.83	92.39	109.72
20	Z	763	HIS	CE1-NE2-CD2	-10.83	98.17	109.00
12	5	150	SER	N-CA-CB	10.76	125.75	110.36
20	Z	206	ASP	N-CA-C	10.68	123.00	111.36
19	Y	32	ASP	CA-C-N	10.67	134.58	120.28
19	Y	32	ASP	C-N-CA	10.67	134.58	120.28
17	T	220	PHE	CA-CB-CG	-10.63	103.17	113.80
1	A	115	ASP	CA-CB-CG	10.53	123.13	112.60
20	Z	731	GLY	CA-C-N	10.50	134.85	120.46
20	Z	731	GLY	C-N-CA	10.50	134.85	120.46
4	D	185	PRO	CA-C-N	10.49	135.18	120.29
4	D	185	PRO	C-N-CA	10.49	135.18	120.29
10	3	127	ILE	CA-C-O	10.47	128.49	119.38
2	b	59	GLU	N-CA-C	-10.44	99.23	112.90
28	H	164	SER	O-C-N	-10.43	115.03	121.71
11	k	149	ARG	N-CA-C	-10.43	94.57	110.32
18	X	82	LYS	N-CA-C	-10.41	100.88	114.31
7	g	211	ASP	N-CA-C	-10.37	93.94	109.81
13	m	52	PHE	CA-CB-CG	-10.31	103.49	113.80
21	N	96	GLN	CA-C-N	10.30	134.44	120.54
21	N	96	GLN	C-N-CA	10.30	134.44	120.54
4	d	230	ASN	CA-CB-CG	10.30	122.90	112.60
25	R	408	ASP	CA-C-N	10.29	133.29	120.22
25	R	408	ASP	C-N-CA	10.29	133.29	120.22
7	G	183	HIS	CA-C-O	-10.28	111.57	119.59
10	3	162	ASP	CA-CB-CG	-10.22	102.38	112.60
12	l	226	GLU	CA-C-N	10.19	134.76	120.29
12	l	226	GLU	C-N-CA	10.19	134.76	120.29
21	N	417	ARG	NE-CZ-NH1	-10.17	111.33	121.50
9	i	238	THR	N-CA-C	-10.15	100.89	113.38
28	H	467	ASN	CA-CB-CG	10.13	122.73	112.60
4	D	143	ASP	CA-CB-CG	-10.12	102.48	112.60
23	P	384	VAL	N-CA-C	-10.11	100.86	111.58
6	f	41	ASN	CA-CB-CG	-10.10	102.50	112.60
22	S	32	GLN	CA-C-N	10.09	133.80	120.28
22	S	32	GLN	C-N-CA	10.09	133.80	120.28
10	j	12	VAL	N-CA-C	-10.09	94.45	108.27
25	R	274	PRO	N-CA-C	-10.04	100.41	113.57
14	7	51	ASN	CA-CB-CG	-10.03	102.57	112.60
4	D	197	ARG	NE-CZ-NH2	-10.01	110.19	119.20
14	n	249	ASN	CA-CB-CG	-9.99	102.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	157	GLY	CA-C-O	9.95	132.10	122.25
15	W	115	CYS	N-CA-C	-9.94	98.68	114.09
4	d	200	LEU	CA-C-N	9.94	133.60	120.28
4	d	200	LEU	C-N-CA	9.94	133.60	120.28
20	Z	701	ILE	CA-C-N	9.89	133.93	120.38
20	Z	701	ILE	C-N-CA	9.89	133.93	120.38
13	6	143	GLN	N-CA-C	-9.89	100.76	113.12
9	2	96	SER	N-CA-C	9.87	122.04	111.28
24	Q	211	PRO	CA-C-N	9.87	133.50	120.28
24	Q	211	PRO	C-N-CA	9.87	133.50	120.28
24	Q	128	GLU	N-CA-C	-9.85	102.34	114.75
31	L	207	PHE	CA-CB-CG	-9.85	103.95	113.80
4	d	139	ASP	CA-CB-CG	-9.84	102.76	112.60
10	3	8	ASN	CA-CB-CG	-9.84	102.76	112.60
14	n	155	ASN	CA-CB-CG	-9.82	102.78	112.60
5	e	133	LEU	N-CA-C	-9.81	99.73	114.64
21	N	689	LYS	CA-C-O	9.79	129.44	118.97
8	h	197	PHE	CA-CB-CG	-9.76	104.04	113.80
12	l	286	ILE	N-CA-C	-9.76	103.62	113.47
9	i	145	HIS	N-CA-C	-9.74	101.27	113.55
3	C	202	ASP	CA-CB-CG	-9.74	102.86	112.60
2	B	190	HIS	CB-CG-CD2	-9.74	118.54	131.20
10	j	26	ASP	CA-CB-CG	9.73	122.33	112.60
30	K	410	ALA	CA-C-N	9.72	133.30	120.28
30	K	410	ALA	C-N-CA	9.72	133.30	120.28
7	g	161	LYS	N-CA-C	-9.71	101.94	113.88
32	M	216	LYS	O-C-N	9.69	132.05	122.07
20	Z	869	ASP	CA-CB-CG	-9.68	102.92	112.60
24	Q	220	LEU	CA-C-N	9.67	134.03	120.29
24	Q	220	LEU	C-N-CA	9.67	134.03	120.29
12	l	266	HIS	CA-CB-CG	-9.67	104.13	113.80
20	Z	948	TRP	CE2-CD2-CE3	9.62	128.42	118.80
27	O	266	PHE	CA-CB-CG	-9.58	104.22	113.80
17	T	13	ILE	CA-C-N	9.58	134.87	120.31
17	T	13	ILE	C-N-CA	9.58	134.87	120.31
28	H	62	ARG	NE-CZ-NH2	-9.57	110.58	119.20
12	5	225	VAL	CA-C-N	9.56	133.09	120.28
12	5	225	VAL	C-N-CA	9.56	133.09	120.28
21	N	602	VAL	O-C-N	9.56	126.86	120.07
3	c	168	ASN	CA-C-N	9.55	132.86	120.44
3	c	168	ASN	C-N-CA	9.55	132.86	120.44
9	i	181	ILE	CA-C-O	-9.55	110.49	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	272	GLU	CA-C-O	-9.53	110.45	120.55
33	J	378	THR	CA-C-N	9.52	133.40	120.54
33	J	378	THR	C-N-CA	9.52	133.40	120.54
30	K	345	ASP	N-CA-C	-9.52	94.78	108.96
6	f	31	GLN	CA-C-N	9.51	133.42	121.06
6	f	31	GLN	C-N-CA	9.51	133.42	121.06
14	n	178	GLY	CA-C-N	9.46	132.95	120.28
14	n	178	GLY	C-N-CA	9.46	132.95	120.28
4	d	93	ALA	CA-C-O	9.44	130.55	120.55
9	i	95	HIS	CE1-NE2-CD2	-9.43	99.57	109.00
20	Z	602	LEU	N-CA-C	9.41	121.54	111.28
28	H	210	ASP	CA-C-N	9.41	134.94	122.90
28	H	210	ASP	C-N-CA	9.41	134.94	122.90
21	N	65	ALA	CA-C-N	9.40	132.88	120.28
21	N	65	ALA	C-N-CA	9.40	132.88	120.28
22	S	65	ASN	CA-C-O	-9.40	110.46	120.42
12	5	184	GLY	CA-C-N	9.39	129.15	119.76
12	5	184	GLY	C-N-CA	9.39	129.15	119.76
1	a	86	PRO	CA-C-N	9.39	126.15	120.24
1	a	86	PRO	C-N-CA	9.39	126.15	120.24
10	j	137	ILE	N-CA-C	-9.38	94.47	108.17
6	F	78	ALA	CA-C-N	9.38	129.46	119.05
6	F	78	ALA	C-N-CA	9.38	129.46	119.05
27	O	323	ASN	OD1-CG-ND2	-9.38	113.22	122.60
30	K	310	THR	N-CA-C	-9.38	101.36	113.17
28	H	278	GLU	N-CA-C	-9.36	103.94	114.62
8	1	71	HIS	CB-CG-CD2	-9.35	119.04	131.20
22	S	117	SER	N-CA-C	-9.34	100.33	114.16
1	A	99	ALA	N-CA-C	9.33	121.53	111.36
24	Q	80	HIS	CE1-NE2-CD2	-9.32	99.68	109.00
12	l	194	GLY	CA-C-N	9.31	133.98	120.95
12	l	194	GLY	C-N-CA	9.31	133.98	120.95
9	2	115	HIS	CB-CG-CD2	-9.31	119.10	131.20
30	K	420	THR	N-CA-C	-9.30	101.48	112.92
29	I	435	LEU	N-CA-C	-9.29	101.11	111.14
24	Q	305	ALA	CA-C-N	9.28	133.47	120.29
24	Q	305	ALA	C-N-CA	9.28	133.47	120.29
30	K	353	PHE	CA-CB-CG	-9.28	104.52	113.80
32	M	111	THR	N-CA-C	-9.27	102.78	114.56
3	c	94	HIS	CE1-NE2-CD2	-9.27	99.73	109.00
13	m	178	LYS	N-CA-CB	9.26	124.34	109.90
22	S	464	ARG	CA-C-N	9.25	133.13	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	464	ARG	C-N-CA	9.25	133.13	120.46
10	3	127	ILE	N-CA-C	-9.25	104.13	113.10
1	A	206	ALA	CA-C-N	9.25	132.21	120.56
1	A	206	ALA	C-N-CA	9.25	132.21	120.56
32	M	193	LEU	N-CA-CB	9.24	123.70	110.12
14	7	249	ASN	CA-C-N	9.23	133.84	120.82
14	7	249	ASN	C-N-CA	9.23	133.84	120.82
31	L	118	ILE	N-CA-C	-9.23	95.15	108.36
9	2	159	GLY	CA-C-N	9.21	132.62	120.28
9	2	159	GLY	C-N-CA	9.21	132.62	120.28
30	K	173	ASP	N-CA-C	-9.20	101.84	113.43
17	T	93	ASN	CA-C-N	9.19	134.19	121.05
17	T	93	ASN	C-N-CA	9.19	134.19	121.05
30	K	119	VAL	N-CA-C	-9.18	95.31	108.17
4	d	93	ALA	O-C-N	-9.18	112.39	122.12
19	Y	66	ASP	CA-CB-CG	-9.16	103.44	112.60
14	7	122	PRO	CA-C-N	9.15	132.54	120.28
14	7	122	PRO	C-N-CA	9.15	132.54	120.28
7	G	212	PHE	CA-CB-CG	9.14	122.94	113.80
3	C	225	VAL	N-CA-CB	9.12	120.95	110.82
22	S	88	PHE	CA-CB-CG	-9.12	104.68	113.80
21	N	401	LYS	CA-C-N	9.11	129.87	119.94
21	N	401	LYS	C-N-CA	9.11	129.87	119.94
6	f	86	ASN	CA-CB-CG	-9.11	103.49	112.60
9	2	149	ASP	CA-CB-CG	-9.10	103.50	112.60
31	L	164	ASP	CA-C-O	-9.10	110.71	120.17
6	F	222	PHE	CA-CB-CG	-9.09	104.71	113.80
13	m	130	VAL	N-CA-C	-9.09	95.03	108.12
14	7	164	ASN	CA-C-N	9.06	133.33	120.28
14	7	164	ASN	C-N-CA	9.06	133.33	120.28
25	R	325	HIS	CA-CB-CG	-9.05	104.75	113.80
3	C	106	ILE	CA-C-N	9.04	129.09	119.78
3	C	106	ILE	C-N-CA	9.04	129.09	119.78
28	H	307	PHE	CA-CB-CG	9.04	122.84	113.80
20	Z	432	GLY	CA-C-N	9.03	133.56	120.38
20	Z	432	GLY	C-N-CA	9.03	133.56	120.38
31	L	243	PHE	CA-CB-CG	9.02	122.82	113.80
21	N	390	LEU	CA-C-O	-9.02	111.28	119.75
22	S	239	ARG	CA-C-N	9.02	132.16	120.44
22	S	239	ARG	C-N-CA	9.02	132.16	120.44
3	c	20	TYR	CA-C-N	9.01	132.35	120.28
3	c	20	TYR	C-N-CA	9.01	132.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	HIS	CA-CB-CG	-8.99	104.81	113.80
9	i	152	TYR	N-CA-C	-8.99	102.22	113.55
1	A	110	TYR	O-C-N	8.99	133.49	123.33
24	Q	52	ASN	CA-CB-CG	-8.99	103.61	112.60
31	L	281	ASP	CA-CB-CG	-8.98	103.61	112.60
10	j	99	ARG	NE-CZ-NH2	8.98	127.28	119.20
33	J	286	LYS	CG-CD-CE	8.98	131.95	111.30
15	W	116	SER	N-CA-C	8.97	116.29	108.22
11	4	145	ASP	CA-C-O	8.96	130.23	120.82
25	R	318	PRO	N-CA-C	8.96	125.05	114.03
30	K	198	TYR	CA-C-N	8.95	132.27	120.28
30	K	198	TYR	C-N-CA	8.95	132.27	120.28
31	L	53	HIS	CE1-NE2-CD2	-8.95	100.05	109.00
20	Z	625	THR	CA-C-O	-8.95	110.40	118.63
25	R	22	PRO	CA-C-N	8.95	132.07	120.44
25	R	22	PRO	C-N-CA	8.95	132.07	120.44
7	G	127	ASN	N-CA-C	-8.94	100.23	114.09
33	J	285	SER	CA-C-N	8.94	132.06	120.44
33	J	285	SER	C-N-CA	8.94	132.06	120.44
1	A	120	ARG	CA-C-N	8.94	132.25	120.28
1	A	120	ARG	C-N-CA	8.94	132.25	120.28
29	I	59	LEU	CA-C-N	8.93	133.15	120.28
29	I	59	LEU	C-N-CA	8.93	133.15	120.28
7	G	102	LEU	CA-C-O	-8.92	110.97	120.42
21	N	14	ARG	CA-C-N	8.92	133.53	120.87
21	N	14	ARG	C-N-CA	8.92	133.53	120.87
33	J	382	PHE	CA-CB-CG	-8.92	104.88	113.80
20	Z	520	ILE	CA-C-N	8.91	135.60	120.72
20	Z	520	ILE	C-N-CA	8.91	135.60	120.72
32	M	377	GLN	N-CA-C	-8.91	101.52	111.14
12	5	124	ALA	N-CA-C	8.90	120.98	111.28
22	S	370	LEU	CA-C-N	8.90	132.94	120.29
22	S	370	LEU	C-N-CA	8.90	132.94	120.29
15	W	12	ASN	CA-CB-CG	-8.90	103.70	112.60
25	R	187	VAL	CA-C-O	-8.90	111.41	120.85
24	Q	243	PHE	CA-C-O	8.90	129.87	120.70
20	Z	123	ALA	CA-C-N	8.89	132.53	120.44
20	Z	123	ALA	C-N-CA	8.89	132.53	120.44
6	F	191	LYS	CA-C-N	8.89	132.19	120.28
6	F	191	LYS	C-N-CA	8.89	132.19	120.28
31	L	214	PRO	O-C-N	8.89	125.33	121.15
22	S	27	GLU	CA-C-N	8.88	132.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	27	GLU	C-N-CA	8.88	132.19	120.28
9	i	157	GLY	O-C-N	-8.88	114.41	122.85
5	e	247	GLU	CA-C-N	8.87	131.97	120.44
5	e	247	GLU	C-N-CA	8.87	131.97	120.44
20	Z	131	LYS	N-CA-C	-8.87	102.46	113.28
12	5	200	ASP	N-CA-C	-8.86	103.31	114.56
2	b	41	ASN	N-CA-C	-8.85	100.43	112.03
33	J	87	LYS	CA-C-N	8.85	133.20	120.91
33	J	87	LYS	C-N-CA	8.85	133.20	120.91
6	F	190	ILE	CA-C-N	8.84	131.93	120.44
6	F	190	ILE	C-N-CA	8.84	131.93	120.44
20	Z	420	ALA	N-CA-C	8.83	120.91	111.28
32	M	223	PRO	O-C-N	-8.83	117.25	121.31
15	W	58	ASN	CA-C-N	8.82	128.90	119.90
15	W	58	ASN	C-N-CA	8.82	128.90	119.90
25	R	41	GLU	CA-C-N	8.82	132.10	120.28
25	R	41	GLU	C-N-CA	8.82	132.10	120.28
27	O	112	LYS	CA-C-O	-8.82	111.11	120.55
32	M	375	ASN	CA-CB-CG	-8.82	103.78	112.60
12	l	196	ARG	CA-C-O	8.81	129.58	120.24
5	e	35	SER	N-CA-CB	8.81	122.85	110.26
6	f	3	ARG	CA-C-N	8.80	137.55	121.70
6	f	3	ARG	C-N-CA	8.80	137.55	121.70
12	l	263	HIS	CE1-NE2-CD2	-8.79	100.21	109.00
5	E	188	HIS	CA-CB-CG	8.79	122.59	113.80
32	M	202	LYS	CA-C-O	8.78	129.73	120.42
22	S	317	HIS	CA-CB-CG	8.78	122.58	113.80
32	M	270	ALA	CA-C-N	8.77	132.04	120.28
32	M	270	ALA	C-N-CA	8.77	132.04	120.28
9	2	99	THR	N-CA-C	-8.77	102.58	113.28
20	Z	28	LYS	CA-C-N	8.77	131.84	120.44
20	Z	28	LYS	C-N-CA	8.77	131.84	120.44
5	e	205	LYS	CA-C-N	8.76	132.02	120.28
5	e	205	LYS	C-N-CA	8.76	132.02	120.28
21	N	91	ILE	CA-C-N	8.76	132.02	120.28
21	N	91	ILE	C-N-CA	8.76	132.02	120.28
31	L	53	HIS	ND1-CE1-NE2	8.75	117.15	108.40
27	O	323	ASN	CA-C-N	8.75	131.58	120.56
27	O	323	ASN	C-N-CA	8.75	131.58	120.56
29	I	204	HIS	CA-CB-CG	8.75	122.55	113.80
24	Q	51	ARG	CA-C-N	8.74	132.00	120.28
24	Q	51	ARG	C-N-CA	8.74	132.00	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	161	LYS	N-CA-C	-8.74	103.04	114.31
8	1	191	GLY	CA-C-O	8.74	128.30	120.79
25	R	162	ILE	N-CA-C	-8.73	95.35	107.75
21	N	254	SER	CA-C-N	8.73	131.79	120.44
21	N	254	SER	C-N-CA	8.73	131.79	120.44
8	h	21	VAL	N-CA-C	-8.73	96.83	108.35
4	D	42	VAL	O-C-N	-8.73	113.76	123.10
30	K	169	VAL	CA-C-O	-8.73	111.79	119.38
24	Q	360	SER	N-CA-C	8.71	120.78	111.28
22	S	49	ASP	O-C-N	-8.71	113.50	120.38
1	a	204	GLU	CA-C-N	8.71	132.28	120.44
1	a	204	GLU	C-N-CA	8.71	132.28	120.44
32	M	141	LYS	N-CA-C	-8.70	100.33	108.07
29	I	327	ALA	N-CA-CB	8.68	124.20	110.57
30	K	306	PHE	CA-CB-CG	-8.68	105.12	113.80
25	R	35	GLN	N-CA-CB	8.66	122.77	110.04
3	C	120	GLN	CA-C-N	8.65	131.03	120.13
3	C	120	GLN	C-N-CA	8.65	131.03	120.13
21	N	89	PHE	CA-CB-CG	-8.65	105.15	113.80
14	7	44	VAL	N-CA-C	-8.65	96.03	108.48
26	U	73	ILE	CA-C-N	8.64	131.68	120.44
26	U	73	ILE	C-N-CA	8.64	131.68	120.44
9	i	95	HIS	CG-CD2-NE2	8.64	115.84	107.20
32	M	349	PHE	CB-CA-C	-8.64	100.22	110.15
31	L	104	LEU	N-CA-C	-8.63	95.86	109.50
32	M	151	ASP	CA-CB-CG	-8.63	103.97	112.60
9	2	128	ILE	N-CA-C	-8.63	95.15	107.75
12	5	250	VAL	CB-CA-C	-8.62	99.12	110.84
32	M	100	THR	CA-C-N	8.61	135.34	123.11
32	M	100	THR	C-N-CA	8.61	135.34	123.11
26	U	246	GLU	CA-C-N	8.61	132.25	120.46
26	U	246	GLU	C-N-CA	8.61	132.25	120.46
6	F	119	ASN	CA-CB-CG	-8.61	104.00	112.60
10	j	38	ASN	N-CA-C	-8.60	102.10	112.59
12	5	269	GLY	CA-C-N	8.60	132.50	120.29
12	5	269	GLY	C-N-CA	8.60	132.50	120.29
24	Q	275	ILE	N-CA-C	-8.60	104.79	113.47
7	G	182	HIS	CE1-NE2-CD2	-8.60	100.40	109.00
21	N	211	PHE	CA-CB-CG	8.59	122.39	113.80
32	M	177	THR	CA-C-N	8.59	131.79	120.28
32	M	177	THR	C-N-CA	8.59	131.79	120.28
20	Z	389	PHE	CA-CB-CG	-8.56	105.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	394	ILE	O-C-N	8.56	130.17	121.87
31	L	331	ASP	CA-CB-CG	-8.56	104.04	112.60
10	3	68	ARG	NE-CZ-NH2	-8.56	111.50	119.20
25	R	20	ARG	CA-C-N	8.55	125.63	120.24
25	R	20	ARG	C-N-CA	8.55	125.63	120.24
1	a	142	THR	N-CA-CB	8.55	124.16	110.65
25	R	302	ALA	N-CA-C	-8.53	102.89	113.38
28	H	214	CYS	N-CA-C	-8.53	94.42	108.49
4	d	184	PRO	CA-C-O	-8.52	114.77	120.90
14	7	197	ASP	CA-C-N	8.52	127.14	120.33
14	7	197	ASP	C-N-CA	8.52	127.14	120.33
4	d	79	ASN	CA-CB-CG	8.52	121.11	112.60
3	c	173	GLN	N-CA-C	-8.51	101.95	111.14
32	M	192	GLU	CA-C-N	8.51	131.69	120.28
32	M	192	GLU	C-N-CA	8.51	131.69	120.28
30	K	143	SER	CA-C-O	8.51	129.69	120.24
20	Z	398	LYS	N-CA-C	8.50	121.31	111.11
27	O	369	ARG	NE-CZ-NH2	8.50	126.85	119.20
2	B	79	GLY	CA-C-N	8.49	128.11	118.85
2	B	79	GLY	C-N-CA	8.49	128.11	118.85
20	Z	207	ILE	CA-C-N	8.49	127.12	120.33
20	Z	207	ILE	C-N-CA	8.49	127.12	120.33
28	H	185	LEU	CA-C-N	8.49	128.56	119.90
28	H	185	LEU	C-N-CA	8.49	128.56	119.90
6	F	56	LEU	N-CA-C	-8.49	102.94	113.38
8	1	163	PHE	CA-CB-CG	8.49	122.29	113.80
22	S	203	SER	CA-C-N	8.49	131.65	120.28
22	S	203	SER	C-N-CA	8.49	131.65	120.28
13	m	116	HIS	CA-CB-CG	-8.48	105.32	113.80
2	B	243	ILE	CA-C-N	8.48	131.64	120.28
2	B	243	ILE	C-N-CA	8.48	131.64	120.28
13	6	103	HIS	CB-CG-CD2	-8.48	120.18	131.20
1	a	166	TYR	CA-C-N	8.46	131.43	120.44
1	a	166	TYR	C-N-CA	8.46	131.43	120.44
9	2	247	VAL	N-CA-C	-8.46	96.27	108.11
27	O	169	ASN	OD1-CG-ND2	8.45	131.05	122.60
13	6	152	SER	CA-C-N	8.44	131.41	120.44
13	6	152	SER	C-N-CA	8.44	131.41	120.44
16	V	66	VAL	CA-C-O	-8.43	111.92	120.85
20	Z	476	ASP	CA-C-N	8.42	131.56	120.28
20	Z	476	ASP	C-N-CA	8.42	131.56	120.28
21	N	488	CYS	O-C-N	8.41	130.73	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	82	ILE	CA-C-O	-8.41	113.06	118.69
5	e	223	THR	CB-CA-C	8.40	124.91	109.70
1	A	117	LEU	N-CA-C	-8.40	102.20	111.36
29	I	215	PRO	CA-C-N	8.40	130.34	119.84
29	I	215	PRO	C-N-CA	8.40	130.34	119.84
3	C	153	PRO	N-CA-C	-8.40	102.88	114.80
16	V	87	PHE	CA-C-N	8.40	131.36	120.44
16	V	87	PHE	C-N-CA	8.40	131.36	120.44
10	j	113	ASN	CA-CB-CG	-8.38	104.22	112.60
32	M	265	ASP	N-CA-CB	8.38	122.23	110.07
1	A	120	ARG	N-CA-C	8.38	121.54	111.82
20	Z	775	MET	CA-C-N	8.38	127.04	120.33
20	Z	775	MET	C-N-CA	8.38	127.04	120.33
21	N	23	TYR	CA-C-N	8.38	131.51	120.28
21	N	23	TYR	C-N-CA	8.38	131.51	120.28
20	Z	220	ALA	CA-C-N	8.37	131.93	120.46
20	Z	220	ALA	C-N-CA	8.37	131.93	120.46
9	i	103	PRO	CA-C-O	-8.36	111.47	121.67
20	Z	400	ILE	CA-C-N	8.36	131.91	120.46
20	Z	400	ILE	C-N-CA	8.36	131.91	120.46
14	7	36	GLN	CA-C-O	-8.36	112.05	120.66
22	S	54	TRP	CE2-CD2-CE3	8.35	127.15	118.80
19	Y	37	ASP	N-CA-C	-8.35	102.88	113.23
1	A	174	LYS	CA-C-N	8.35	131.81	120.54
1	A	174	LYS	C-N-CA	8.35	131.81	120.54
3	C	46	LEU	N-CA-CB	8.35	125.36	110.83
17	T	123	HIS	CA-CB-CG	-8.35	105.45	113.80
1	a	46	ARG	NE-CZ-NH2	-8.35	111.69	119.20
32	M	206	LYS	N-CA-C	8.34	120.38	111.28
9	2	53	PRO	CA-C-N	8.34	133.94	122.34
9	2	53	PRO	C-N-CA	8.34	133.94	122.34
25	R	248	SER	CA-C-N	8.34	131.36	120.60
25	R	248	SER	C-N-CA	8.34	131.36	120.60
5	E	80	GLY	CA-C-N	8.34	132.63	120.95
5	E	80	GLY	C-N-CA	8.34	132.63	120.95
22	S	118	PHE	CA-CB-CG	-8.34	105.46	113.80
22	S	321	GLN	CA-C-N	8.34	132.98	120.31
22	S	321	GLN	C-N-CA	8.34	132.98	120.31
30	K	45	SER	CA-C-N	8.33	132.11	120.29
30	K	45	SER	C-N-CA	8.33	132.11	120.29
9	i	130	ALA	N-CA-C	-8.32	95.93	108.99
6	f	210	ASN	CA-C-O	8.32	128.20	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	280	ASN	CA-C-N	8.31	131.42	120.28
26	U	280	ASN	C-N-CA	8.31	131.42	120.28
16	V	222	GLN	N-CA-C	-8.31	102.30	111.36
28	H	42	ALA	CA-C-N	8.31	131.55	120.58
28	H	42	ALA	C-N-CA	8.31	131.55	120.58
20	Z	470	ALA	CA-C-N	8.31	131.75	120.54
20	Z	470	ALA	C-N-CA	8.31	131.75	120.54
20	Z	244	ARG	CA-C-O	8.30	129.54	120.82
20	Z	738	TYR	CE1-CZ-CE2	-8.30	103.70	120.30
20	Z	439	TYR	CA-C-N	8.30	132.23	120.28
20	Z	439	TYR	C-N-CA	8.30	132.23	120.28
6	F	6	TYR	N-CA-C	-8.29	102.19	113.30
9	2	115	HIS	CB-CG-ND1	8.29	135.13	122.70
21	N	346	ASN	CA-CB-CG	-8.28	104.32	112.60
7	g	242	PHE	CA-CB-CG	-8.28	105.52	113.80
23	P	78	GLN	CA-C-N	8.28	131.20	120.44
23	P	78	GLN	C-N-CA	8.28	131.20	120.44
32	M	146	VAL	CA-C-N	8.27	128.74	120.31
32	M	146	VAL	C-N-CA	8.27	128.74	120.31
15	W	67	ALA	N-CA-C	-8.27	101.29	112.94
24	Q	409	TYR	N-CA-C	-8.26	102.35	111.36
12	5	229	LEU	N-CA-CB	8.26	122.26	110.12
22	S	105	PRO	CA-C-O	-8.26	112.18	121.43
30	K	301	THR	N-CA-C	-8.26	102.36	111.36
3	c	236	LYS	CA-C-O	-8.25	111.80	120.55
13	m	94	ILE	N-CA-CB	8.25	121.76	110.54
5	E	244	LYS	N-CA-CB	8.25	122.24	110.12
23	P	69	ARG	CA-C-N	8.24	131.16	120.44
23	P	69	ARG	C-N-CA	8.24	131.16	120.44
20	Z	70	ALA	CA-C-N	8.24	131.32	120.28
20	Z	70	ALA	C-N-CA	8.24	131.32	120.28
20	Z	374	LEU	N-CA-CB	8.23	122.14	110.36
18	X	63	PRO	N-CA-C	8.23	123.70	111.03
19	Y	71	ASP	CA-CB-CG	8.22	120.83	112.60
25	R	383	ARG	CA-C-N	8.22	131.09	120.56
25	R	383	ARG	C-N-CA	8.22	131.09	120.56
13	6	116	HIS	CA-CB-CG	8.22	122.02	113.80
8	h	196	ILE	N-CA-C	-8.22	97.50	108.35
12	l	236	ILE	CA-C-O	-8.22	112.41	120.95
13	m	217	LYS	N-CA-C	-8.22	102.29	113.30
7	G	224	THR	N-CA-C	-8.22	102.00	114.16
29	I	259	ASP	CA-CB-CG	-8.22	104.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	118	ASN	OD1-CG-ND2	8.21	130.81	122.60
20	Z	352	LYS	N-CA-C	8.21	120.31	111.36
1	a	92	ASN	CA-CB-CG	8.21	120.81	112.60
21	N	365	PHE	CA-C-N	8.21	131.95	120.29
21	N	365	PHE	C-N-CA	8.21	131.95	120.29
24	Q	406	ASP	CA-C-N	8.21	131.28	120.28
24	Q	406	ASP	C-N-CA	8.21	131.28	120.28
32	M	342	ARG	N-CA-C	-8.21	104.41	114.75
8	1	43	LEU	N-CA-C	-8.21	95.36	108.73
17	T	138	ASP	CA-CB-CG	-8.21	104.39	112.60
17	T	122	PHE	CA-C-N	8.19	132.76	120.31
17	T	122	PHE	C-N-CA	8.19	132.76	120.31
30	K	104	ASP	N-CA-C	-8.19	97.63	108.19
6	F	150	SER	N-CA-C	-8.19	102.30	111.14
21	N	436	ASP	CA-CB-CG	-8.19	104.41	112.60
5	e	118	ASP	N-CA-CB	8.18	122.27	110.16
4	D	230	ASN	CA-CB-CG	-8.18	104.42	112.60
15	W	175	THR	N-CA-C	-8.18	99.50	109.72
33	J	32	LEU	CA-C-N	8.18	131.24	120.28
33	J	32	LEU	C-N-CA	8.18	131.24	120.28
1	a	205	PHE	CA-CB-CG	-8.17	105.63	113.80
28	H	321	ASP	CA-CB-CG	-8.17	104.43	112.60
29	I	305	THR	N-CA-CB	8.16	122.12	110.12
2	B	124	SER	CA-C-N	8.16	128.63	120.31
2	B	124	SER	C-N-CA	8.16	128.63	120.31
21	N	509	GLN	N-CA-C	-8.16	101.43	112.94
10	j	100	PHE	CA-CB-CG	-8.16	105.64	113.80
11	k	120	ASP	CA-CB-CG	-8.16	104.44	112.60
16	V	129	PHE	CA-CB-CG	-8.16	105.64	113.80
8	h	14	ALA	N-CA-C	-8.15	94.81	108.75
31	L	378	ALA	CA-C-N	8.15	131.20	120.28
31	L	378	ALA	C-N-CA	8.15	131.20	120.28
20	Z	958	ASN	CA-CB-CG	-8.15	104.45	112.60
1	A	209	HIS	CE1-NE2-CD2	-8.15	100.85	109.00
5	E	67	ILE	N-CA-C	-8.15	96.70	108.11
25	R	382	ASP	N-CA-C	-8.14	96.69	109.72
29	I	151	HIS	CB-CG-ND1	8.14	134.91	122.70
3	c	65	LYS	N-CA-C	-8.14	100.25	112.54
13	m	27	ASP	N-CA-C	-8.13	101.82	113.21
14	7	104	VAL	CA-C-N	8.13	131.18	120.28
14	7	104	VAL	C-N-CA	8.13	131.18	120.28
31	L	213	LYS	CA-C-O	-8.13	112.09	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	180	ASN	CA-C-N	8.13	131.84	120.29
2	b	180	ASN	C-N-CA	8.13	131.84	120.29
9	2	81	THR	CA-C-N	8.13	131.18	120.28
9	2	81	THR	C-N-CA	8.13	131.18	120.28
19	Y	75	ASN	CA-C-N	8.13	131.52	120.54
19	Y	75	ASN	C-N-CA	8.13	131.52	120.54
5	e	157	HIS	CE1-NE2-CD2	-8.13	100.87	109.00
26	U	195	LYS	CA-C-N	8.12	131.17	120.28
26	U	195	LYS	C-N-CA	8.12	131.17	120.28
5	e	215	ASN	OD1-CG-ND2	8.12	130.72	122.60
14	7	203	VAL	CA-C-N	8.12	131.00	120.44
14	7	203	VAL	C-N-CA	8.12	131.00	120.44
32	M	387	ASN	CA-C-N	8.12	129.12	120.03
32	M	387	ASN	C-N-CA	8.12	129.12	120.03
12	l	185	PRO	N-CA-CB	8.12	110.89	103.34
12	5	208	GLN	CA-C-N	8.12	131.81	120.29
12	5	208	GLN	C-N-CA	8.12	131.81	120.29
17	T	133	ILE	CA-C-N	8.11	131.50	120.38
17	T	133	ILE	C-N-CA	8.11	131.50	120.38
4	d	117	GLN	O-C-N	-8.11	113.52	122.12
24	Q	379	GLN	CA-C-O	-8.11	111.95	120.55
5	e	23	GLN	N-CA-C	-8.11	101.51	111.40
12	5	202	PHE	CA-CB-CG	-8.11	105.69	113.80
21	N	580	ASN	CA-CB-CG	8.11	120.71	112.60
10	j	83	GLU	CA-C-N	8.10	128.19	119.28
10	j	83	GLU	C-N-CA	8.10	128.19	119.28
23	P	142	ASP	CA-CB-CG	8.10	120.70	112.60
28	H	205	ASP	N-CA-C	-8.10	99.34	111.81
23	P	132	VAL	CA-C-N	8.09	131.78	120.29
23	P	132	VAL	C-N-CA	8.09	131.78	120.29
6	f	190	ILE	O-C-N	-8.09	113.98	121.91
26	U	5	HIS	CA-C-N	8.09	131.12	120.28
26	U	5	HIS	C-N-CA	8.09	131.12	120.28
11	4	113	LYS	CA-C-O	-8.09	110.97	119.22
20	Z	614	VAL	CA-C-N	8.08	131.11	120.28
20	Z	614	VAL	C-N-CA	8.08	131.11	120.28
20	Z	809	MET	CA-C-N	8.08	131.76	120.29
20	Z	809	MET	C-N-CA	8.08	131.76	120.29
2	b	83	ARG	CA-C-N	8.08	131.89	120.42
2	b	83	ARG	C-N-CA	8.08	131.89	120.42
17	T	68	ALA	CA-C-N	8.07	131.10	120.28
17	T	68	ALA	C-N-CA	8.07	131.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	217	MET	CA-C-O	-8.07	111.78	120.17
15	W	58	ASN	O-C-N	-8.07	116.20	121.85
4	d	108	TYR	O-C-N	8.07	131.35	122.15
9	i	177	LYS	N-CA-C	8.06	119.70	111.07
20	Z	146	PHE	CA-CB-CG	8.06	121.86	113.80
25	R	388	VAL	N-CA-C	-8.05	96.12	107.80
33	J	211	ILE	N-CA-CB	8.05	124.52	111.23
33	J	131	ASP	CA-CB-CG	-8.05	104.55	112.60
15	W	175	THR	CA-C-O	-8.05	113.06	119.66
14	n	190	LYS	O-C-N	8.04	130.36	122.07
33	J	8	SER	N-CA-C	-8.04	102.50	112.88
29	I	285	ASP	N-CA-C	8.04	120.04	111.28
11	4	83	PHE	CA-CB-CG	-8.03	105.77	113.80
29	I	235	ALA	CA-C-N	8.03	131.45	120.46
29	I	235	ALA	C-N-CA	8.03	131.45	120.46
11	k	187	ASP	CA-CB-CG	-8.02	104.58	112.60
26	U	182	ALA	N-CA-C	-8.02	105.48	114.62
28	H	52	THR	N-CA-CB	8.02	121.63	110.01
9	i	89	GLY	CA-C-N	8.01	131.02	120.28
9	i	89	GLY	C-N-CA	8.01	131.02	120.28
14	n	209	ALA	CA-C-N	8.01	131.80	120.42
14	n	209	ALA	C-N-CA	8.01	131.80	120.42
28	H	76	LEU	N-CA-C	-8.01	95.05	108.75
11	k	165	VAL	CA-C-N	8.01	131.01	120.28
11	k	165	VAL	C-N-CA	8.01	131.01	120.28
23	P	144	VAL	CA-C-O	-8.01	112.36	120.85
26	U	238	ASN	OD1-CG-ND2	-8.00	114.60	122.60
20	Z	210	TYR	CA-CB-CG	-7.99	99.51	113.90
7	G	184	PRO	N-CA-C	-7.99	105.41	114.92
13	6	87	HIS	CE1-NE2-CD2	-7.99	101.01	109.00
1	a	230	LYS	CA-C-N	7.98	133.44	122.19
1	a	230	LYS	C-N-CA	7.98	133.44	122.19
33	J	124	LYS	CA-C-N	7.98	131.44	120.35
33	J	124	LYS	C-N-CA	7.98	131.44	120.35
1	A	12	TYR	CA-C-N	7.98	136.77	121.54
1	A	12	TYR	C-N-CA	7.98	136.77	121.54
5	E	100	ASN	OD1-CG-ND2	7.98	130.58	122.60
23	P	289	ASN	N-CA-C	-7.97	101.65	113.61
26	U	252	HIS	CE1-NE2-CD2	-7.97	101.03	109.00
4	d	53	LYS	CA-C-N	7.97	131.30	120.54
4	d	53	LYS	C-N-CA	7.97	131.30	120.54
5	e	223	THR	N-CA-C	-7.97	95.29	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	290	ILE	N-CA-C	-7.97	96.78	108.89
23	P	88	GLN	O-C-N	7.97	133.09	122.41
4	D	17	ILE	N-CA-C	-7.96	94.62	107.28
14	n	107	ASN	CA-C-N	7.96	131.60	120.29
14	n	107	ASN	C-N-CA	7.96	131.60	120.29
7	G	220	SER	CA-C-N	7.96	131.28	120.38
7	G	220	SER	C-N-CA	7.96	131.28	120.38
20	Z	495	ILE	CA-C-N	7.96	130.79	120.44
20	Z	495	ILE	C-N-CA	7.96	130.79	120.44
12	l	128	GLN	CA-C-N	7.95	130.78	120.44
12	l	128	GLN	C-N-CA	7.95	130.78	120.44
29	I	418	GLN	CA-C-N	7.95	131.58	120.29
29	I	418	GLN	C-N-CA	7.95	131.58	120.29
14	7	69	PHE	CA-CB-CG	-7.95	105.85	113.80
21	N	446	ALA	CA-C-N	7.95	130.93	120.28
21	N	446	ALA	C-N-CA	7.95	130.93	120.28
23	P	239	GLN	CA-C-N	7.95	131.58	120.29
23	P	239	GLN	C-N-CA	7.95	131.58	120.29
7	g	182	HIS	N-CA-CB	7.95	121.92	110.16
1	A	127	ILE	CA-C-O	-7.95	112.69	120.95
20	Z	574	TYR	CA-C-N	7.95	132.02	120.82
20	Z	574	TYR	C-N-CA	7.95	132.02	120.82
16	V	239	ALA	CA-C-N	7.94	130.92	120.28
16	V	239	ALA	C-N-CA	7.94	130.92	120.28
20	Z	945	ILE	N-CA-CB	7.94	120.52	110.99
4	d	98	LEU	O-C-N	-7.93	113.52	122.09
26	U	157	LEU	CA-C-N	7.93	127.99	119.90
26	U	157	LEU	C-N-CA	7.93	127.99	119.90
33	J	253	ILE	N-CA-C	-7.93	102.71	110.72
27	O	263	PHE	CA-CB-CG	-7.93	105.87	113.80
32	M	414	ASP	CA-CB-CG	-7.93	104.67	112.60
27	O	129	ILE	CA-C-O	-7.92	112.71	120.95
20	Z	267	THR	N-CA-CB	7.92	121.88	110.16
28	H	113	ASP	CA-C-O	-7.92	112.55	120.70
2	B	187	ASP	CA-CB-CG	-7.91	104.69	112.60
26	U	22	TYR	CA-C-O	7.91	128.81	120.42
3	C	71	ASP	CA-CB-CG	-7.91	104.69	112.60
2	B	101	TYR	N-CA-C	-7.91	102.92	114.39
13	6	130	VAL	CA-C-O	7.91	129.10	120.64
22	S	28	GLU	N-CA-CB	7.91	121.75	110.12
21	N	836	GLU	CA-C-N	7.91	134.05	121.08
21	N	836	GLU	C-N-CA	7.91	134.05	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	113	ASN	CA-C-O	-7.91	113.37	120.56
3	c	215	THR	N-CA-C	-7.90	96.05	109.24
25	R	311	THR	CA-C-O	-7.90	112.53	120.82
12	l	271	LEU	CA-C-N	7.89	131.19	120.38
12	l	271	LEU	C-N-CA	7.89	131.19	120.38
17	T	214	GLU	CA-C-N	7.89	131.49	120.29
17	T	214	GLU	C-N-CA	7.89	131.49	120.29
10	3	34	LEU	CA-C-N	7.88	129.99	120.92
10	3	34	LEU	C-N-CA	7.88	129.99	120.92
14	7	211	VAL	N-CA-C	7.88	118.66	110.62
21	N	707	ASN	CA-CB-CG	-7.88	104.72	112.60
17	T	153	MET	N-CA-C	7.88	119.86	111.28
14	n	39	VAL	N-CA-CB	7.87	123.54	112.52
1	a	221	ASN	CA-CB-CG	-7.87	104.73	112.60
13	m	63	ASN	OD1-CG-ND2	7.87	130.47	122.60
9	i	45	ALA	O-C-N	-7.87	115.67	123.46
25	R	267	LYS	CA-C-N	7.86	130.66	120.44
25	R	267	LYS	C-N-CA	7.86	130.66	120.44
17	T	31	LYS	O-C-N	7.86	131.94	122.27
32	M	106	VAL	CB-CA-C	7.86	120.27	111.08
21	N	736	PHE	CA-CB-CG	-7.86	105.94	113.80
29	I	266	GLN	CA-C-N	7.86	130.46	120.56
29	I	266	GLN	C-N-CA	7.86	130.46	120.56
4	d	91	VAL	N-CA-CB	7.85	120.62	110.57
29	I	259	ASP	CA-C-N	7.85	126.86	121.13
29	I	259	ASP	C-N-CA	7.85	126.86	121.13
11	k	166	GLN	CA-C-N	7.85	130.80	120.28
11	k	166	GLN	C-N-CA	7.85	130.80	120.28
33	J	298	ASP	CA-CB-CG	-7.85	104.75	112.60
32	M	89	ASN	CA-C-N	7.84	133.00	121.31
32	M	89	ASN	C-N-CA	7.84	133.00	121.31
22	S	472	HIS	CE1-NE2-CD2	-7.84	101.16	109.00
33	J	282	PHE	CA-CB-CG	-7.84	105.96	113.80
2	B	214	ILE	N-CA-C	-7.84	94.07	107.24
27	O	117	ASN	CA-C-O	7.84	128.99	119.97
10	3	60	VAL	O-C-N	7.83	129.90	121.83
15	W	14	GLU	N-CA-C	-7.83	104.67	112.97
21	N	234	ASP	CA-CB-CG	7.83	120.43	112.60
14	n	39	VAL	O-C-N	-7.83	114.39	123.00
29	I	149	LEU	CA-C-N	7.83	133.23	122.19
29	I	149	LEU	C-N-CA	7.83	133.23	122.19
4	D	139	ASP	CA-C-O	-7.83	113.30	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	242	SER	CA-C-N	7.83	131.09	120.44
24	Q	242	SER	C-N-CA	7.83	131.09	120.44
31	L	313	ASP	N-CA-C	-7.83	102.64	112.90
23	P	280	LEU	CA-C-O	7.83	128.93	120.24
24	Q	210	CYS	CA-C-O	-7.83	112.43	120.96
9	2	59	ASN	CA-CB-CG	-7.82	104.78	112.60
9	2	212	ASP	CA-CB-CG	-7.82	104.78	112.60
2	B	214	ILE	N-CA-CB	7.82	122.10	112.10
16	V	109	HIS	CB-CG-CD2	-7.82	121.04	131.20
22	S	413	LEU	N-CA-C	-7.81	97.45	109.24
25	R	35	GLN	CA-C-N	7.81	133.27	120.23
25	R	35	GLN	C-N-CA	7.81	133.27	120.23
27	O	379	LYS	CA-C-N	7.80	130.58	120.44
27	O	379	LYS	C-N-CA	7.80	130.58	120.44
30	K	244	HIS	O-C-N	-7.80	115.07	123.26
29	I	317	ASP	CA-CB-CG	-7.80	104.80	112.60
10	j	66	MET	N-CA-C	7.79	119.78	111.28
25	R	296	LEU	CB-CA-C	-7.79	98.64	110.88
26	U	248	ASP	CA-CB-CG	-7.79	104.81	112.60
4	D	159	TRP	CA-C-N	7.79	130.56	120.44
4	D	159	TRP	C-N-CA	7.79	130.56	120.44
22	S	472	HIS	ND1-CE1-NE2	7.78	116.18	108.40
8	h	152	ARG	N-CA-C	-7.77	97.59	109.95
10	3	68	ARG	NH1-CZ-NH2	7.77	129.41	119.30
2	b	18	LEU	CA-C-N	7.77	129.86	120.14
2	b	18	LEU	C-N-CA	7.77	129.86	120.14
20	Z	429	ASN	N-CA-C	-7.77	96.49	108.76
6	F	98	VAL	N-CA-C	-7.76	105.13	111.81
32	M	210	MET	O-C-N	7.76	130.35	122.12
14	n	141	ASN	CA-C-N	7.76	127.71	120.03
14	n	141	ASN	C-N-CA	7.76	127.71	120.03
5	E	148	ASP	CA-CB-CG	7.76	120.36	112.60
17	T	78	PHE	CA-CB-CG	7.76	121.56	113.80
14	7	98	ARG	NE-CZ-NH2	7.75	126.18	119.20
29	I	161	GLN	CA-C-N	7.75	133.79	122.63
29	I	161	GLN	C-N-CA	7.75	133.79	122.63
31	L	298	ASP	N-CA-C	-7.75	102.16	111.69
10	3	50	PHE	CA-CB-CG	-7.75	106.05	113.80
20	Z	968	ASP	CA-C-N	7.75	134.19	122.65
20	Z	968	ASP	C-N-CA	7.75	134.19	122.65
20	Z	763	HIS	CG-CD2-NE2	7.74	114.94	107.20
21	N	731	VAL	CA-C-N	7.74	128.74	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	731	VAL	C-N-CA	7.74	128.74	119.99
7	g	86	ARG	N-CA-C	-7.74	102.79	111.07
5	E	89	ILE	N-CA-C	-7.74	101.07	111.44
15	W	92	GLN	OE1-CD-NE2	7.74	130.34	122.60
24	Q	195	LYS	CA-C-N	7.74	130.50	120.44
24	Q	195	LYS	C-N-CA	7.74	130.50	120.44
14	7	242	LYS	N-CA-CB	7.74	122.72	110.65
21	N	835	LYS	N-CA-C	-7.74	97.61	109.14
23	P	91	LEU	N-CA-C	-7.74	103.42	113.17
4	d	183	GLU	CA-C-N	7.73	125.30	119.66
4	d	183	GLU	C-N-CA	7.73	125.30	119.66
13	6	221	ARG	N-CA-C	-7.73	98.44	110.42
11	4	145	ASP	O-C-N	-7.72	114.12	122.07
24	Q	30	LEU	N-CA-C	7.72	119.70	111.28
20	Z	846	PHE	N-CA-C	-7.72	97.34	109.07
9	2	214	GLU	CA-C-O	7.72	129.50	120.70
23	P	97	ILE	CA-C-N	7.72	130.95	120.38
23	P	97	ILE	C-N-CA	7.72	130.95	120.38
7	G	182	HIS	CG-CD2-NE2	7.71	114.92	107.20
17	T	49	ASP	CA-C-N	7.71	130.28	120.56
17	T	49	ASP	C-N-CA	7.71	130.28	120.56
19	Y	48	THR	N-CA-C	-7.71	96.66	109.24
32	M	415	PHE	O-C-N	7.71	130.30	122.12
20	Z	917	ASN	N-CA-C	-7.71	97.56	109.52
9	2	97	LEU	CA-C-N	7.71	130.61	120.28
9	2	97	LEU	C-N-CA	7.71	130.61	120.28
7	g	201	TYR	N-CA-C	7.71	119.68	111.28
23	P	350	LEU	CA-C-N	7.71	130.61	120.28
23	P	350	LEU	C-N-CA	7.71	130.61	120.28
25	R	128	LEU	CA-C-N	7.71	130.61	120.28
25	R	128	LEU	C-N-CA	7.71	130.61	120.28
20	Z	808	SER	O-C-N	-7.71	110.99	122.39
25	R	204	TRP	N-CA-C	-7.70	103.69	113.23
3	c	94	HIS	ND1-CE1-NE2	7.70	116.10	108.40
8	1	40	THR	N-CA-CB	7.70	123.50	110.49
17	T	149	ASP	CA-C-N	7.70	130.59	120.28
17	T	149	ASP	C-N-CA	7.70	130.59	120.28
2	b	66	LEU	CB-CA-C	7.69	122.38	109.84
8	h	35	ILE	N-CA-C	-7.69	97.36	108.36
1	a	229	THR	N-CA-CB	7.69	122.48	110.87
1	A	218	PHE	CA-CB-CG	-7.69	106.11	113.80
5	E	48	LEU	CA-C-N	7.69	127.48	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	48	LEU	C-N-CA	7.69	127.48	122.18
7	G	189	ALA	CA-C-N	7.69	130.43	120.44
7	G	189	ALA	C-N-CA	7.69	130.43	120.44
11	4	158	LEU	N-CA-C	-7.69	102.23	111.69
29	I	151	HIS	CB-CG-CD2	-7.69	121.21	131.20
20	Z	474	LEU	CA-C-N	7.69	130.58	120.28
20	Z	474	LEU	C-N-CA	7.69	130.58	120.28
32	M	129	LEU	CA-C-O	-7.68	110.82	120.04
16	V	141	VAL	N-CA-CB	7.68	122.01	111.41
3	c	87	LEU	CA-C-N	7.68	130.98	120.46
3	c	87	LEU	C-N-CA	7.68	130.98	120.46
10	j	158	LEU	CA-C-N	7.68	133.31	121.03
10	j	158	LEU	C-N-CA	7.68	133.31	121.03
6	f	138	ASP	CA-CB-CG	7.67	120.27	112.60
23	P	199	LEU	CA-C-N	7.67	130.56	120.28
23	P	199	LEU	C-N-CA	7.67	130.56	120.28
5	e	18	GLU	N-CA-C	-7.67	103.95	113.38
3	c	207	THR	CA-C-N	7.67	131.96	120.31
3	c	207	THR	C-N-CA	7.67	131.96	120.31
20	Z	565	PHE	CA-C-N	7.67	130.55	120.28
20	Z	565	PHE	C-N-CA	7.67	130.55	120.28
27	O	56	PRO	N-CA-CB	7.66	108.27	101.83
5	e	197	GLU	N-CA-C	7.66	119.27	111.07
23	P	101	MET	N-CA-C	7.66	119.71	111.36
24	Q	175	VAL	N-CA-C	-7.66	102.99	110.72
3	c	100	LYS	CA-C-N	7.65	133.49	120.71
3	c	100	LYS	C-N-CA	7.65	133.49	120.71
22	S	429	ASP	CA-CB-CG	-7.65	104.95	112.60
30	K	168	ASP	CA-CB-CG	-7.65	104.95	112.60
23	P	188	ILE	CA-C-N	7.64	131.93	120.31
23	P	188	ILE	C-N-CA	7.64	131.93	120.31
26	U	20	ASP	CA-CB-CG	7.64	120.24	112.60
4	d	45	GLY	CA-C-O	-7.64	114.92	121.57
22	S	329	GLU	CA-C-N	7.64	131.93	120.31
22	S	329	GLU	C-N-CA	7.64	131.93	120.31
29	I	317	ASP	N-CA-C	-7.64	94.52	110.80
20	Z	258	PRO	N-CA-C	7.64	120.02	110.70
24	Q	377	LEU	CA-C-N	7.64	130.51	120.28
24	Q	377	LEU	C-N-CA	7.64	130.51	120.28
17	T	151	TRP	CA-C-O	-7.63	112.46	120.55
22	S	65	ASN	O-C-N	7.63	130.85	122.15
4	D	218	ASP	CA-CB-CG	-7.63	104.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	180	ILE	CA-C-N	7.63	133.25	123.10
11	4	180	ILE	C-N-CA	7.63	133.25	123.10
17	T	211	PHE	CA-CB-CG	-7.63	106.17	113.80
24	Q	405	GLN	N-CA-C	-7.63	97.77	109.14
20	Z	464	ASP	CA-CB-CG	-7.63	104.97	112.60
27	O	23	HIS	CA-CB-CG	7.63	121.43	113.80
11	k	104	ILE	N-CA-C	-7.62	97.43	108.11
5	E	73	HIS	ND1-CE1-NE2	7.62	116.02	108.40
24	Q	80	HIS	ND1-CE1-NE2	7.62	116.02	108.40
9	i	60	CYS	N-CA-C	-7.62	96.94	108.52
24	Q	24	GLU	N-CA-C	7.62	119.58	111.28
3	c	204	SER	N-CA-C	-7.61	104.14	113.50
21	N	671	LEU	N-CA-C	-7.61	103.58	113.17
31	L	325	MET	CA-C-N	7.61	134.36	122.94
31	L	325	MET	C-N-CA	7.61	134.36	122.94
7	g	98	SER	CA-C-N	7.61	130.48	120.28
7	g	98	SER	C-N-CA	7.61	130.48	120.28
22	S	208	ILE	N-CA-C	-7.61	103.04	110.72
1	a	104	PHE	CA-C-N	7.60	130.47	120.28
1	a	104	PHE	C-N-CA	7.60	130.47	120.28
28	H	85	MET	N-CA-C	-7.60	102.94	112.90
31	L	80	ASN	CA-CB-CG	-7.60	105.00	112.60
6	f	83	VAL	N-CA-C	-7.60	103.05	110.72
1	A	14	ARG	CA-C-O	7.60	128.47	119.28
20	Z	562	TRP	CD2-CE2-CZ2	-7.60	114.80	122.40
32	M	218	ALA	N-CA-C	-7.60	97.50	109.50
7	g	94	GLU	CA-C-N	7.59	130.46	120.28
7	g	94	GLU	C-N-CA	7.59	130.46	120.28
22	S	348	LEU	N-CA-CB	7.59	121.40	110.16
16	V	261	LEU	CA-C-N	7.59	136.04	121.54
16	V	261	LEU	C-N-CA	7.59	136.04	121.54
18	X	38	ASN	CA-CB-CG	-7.59	105.01	112.60
31	L	290	ARG	N-CA-C	-7.59	94.63	110.80
7	g	224	THR	N-CA-C	-7.59	102.93	114.16
12	5	133	TRP	CB-CG-CD2	-7.59	116.17	126.80
20	Z	272	TYR	N-CA-C	7.59	119.55	111.28
11	k	146	HIS	O-C-N	-7.59	113.89	122.09
9	2	40	GLY	O-C-N	-7.59	117.50	123.80
24	Q	43	GLY	CA-C-N	7.59	136.03	121.54
24	Q	43	GLY	C-N-CA	7.59	136.03	121.54
14	n	135	GLN	OE1-CD-NE2	7.59	130.19	122.60
26	U	128	GLN	N-CA-C	-7.58	104.05	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	265	ASP	CA-CB-CG	-7.58	105.02	112.60
4	d	117	GLN	CA-C-N	7.58	130.44	120.28
4	d	117	GLN	C-N-CA	7.58	130.44	120.28
27	O	8	ASP	CA-C-N	7.58	130.44	120.28
27	O	8	ASP	C-N-CA	7.58	130.44	120.28
22	S	323	LEU	CA-C-O	-7.58	112.39	120.42
22	S	397	LEU	N-CA-C	7.58	119.54	111.28
20	Z	553	ARG	NE-CZ-NH2	-7.57	112.38	119.20
23	P	44	LYS	N-CA-C	-7.57	102.25	113.61
6	f	28	ALA	CA-C-N	7.57	130.10	120.56
6	f	28	ALA	C-N-CA	7.57	130.10	120.56
7	g	87	HIS	CA-CB-CG	7.57	121.37	113.80
23	P	65	LEU	CA-C-O	7.57	128.44	120.42
18	X	37	PRO	N-CA-CB	7.57	111.19	103.25
21	N	302	PHE	CA-CB-CG	-7.57	106.23	113.80
33	J	210	PHE	CA-CB-CG	7.56	121.36	113.80
30	K	150	LEU	O-C-N	-7.56	115.65	121.55
8	h	148	ASP	CA-CB-CG	7.56	120.16	112.60
8	h	162	ASP	CA-CB-CG	-7.56	105.04	112.60
16	V	68	VAL	N-CA-C	-7.55	97.70	108.65
22	S	320	ILE	CA-C-N	7.55	131.02	120.29
22	S	320	ILE	C-N-CA	7.55	131.02	120.29
32	M	180	TYR	N-CA-C	-7.55	104.11	112.72
21	N	51	ASP	CB-CA-C	-7.55	98.01	110.85
14	n	236	ASN	CA-CB-CG	-7.55	105.05	112.60
27	O	104	ALA	CA-C-N	7.55	130.71	120.44
27	O	104	ALA	C-N-CA	7.55	130.71	120.44
2	b	124	SER	CA-C-N	7.54	127.27	120.10
2	b	124	SER	C-N-CA	7.54	127.27	120.10
11	4	100	VAL	N-CA-CB	7.54	122.08	111.82
16	V	96	LYS	N-CA-C	7.54	119.50	111.28
11	4	11	ASP	CA-CB-CG	7.54	120.14	112.60
25	R	95	ASP	CA-CB-CG	-7.54	105.06	112.60
20	Z	738	TYR	OH-CZ-CE2	7.54	142.50	119.90
10	3	23	ILE	N-CA-C	-7.53	98.41	108.35
20	Z	247	GLN	N-CA-CB	7.53	121.19	110.12
32	M	416	VAL	N-CA-CB	7.53	120.78	110.54
31	L	206	ILE	CA-C-O	7.53	128.60	120.47
3	C	97	ASN	N-CA-C	-7.53	103.16	111.36
14	7	172	SER	N-CA-C	-7.53	98.40	108.11
8	1	156	SER	N-CA-C	-7.53	99.38	110.52
21	N	748	PHE	CA-CB-CG	-7.53	106.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	284	GLU	CB-CG-CD	-7.53	99.81	112.60
7	G	114	ASP	CA-CB-CG	-7.52	105.08	112.60
21	N	57	ASP	CA-C-N	7.52	130.36	120.28
21	N	57	ASP	C-N-CA	7.52	130.36	120.28
27	O	81	TYR	CA-C-N	7.52	130.36	120.28
27	O	81	TYR	C-N-CA	7.52	130.36	120.28
31	L	157	ARG	NE-CZ-NH2	7.52	125.97	119.20
9	i	152	TYR	CB-CA-C	7.52	121.00	109.34
7	g	9	ASP	N-CA-CB	7.52	123.20	110.49
23	P	210	ASN	CA-C-N	7.52	127.23	119.64
23	P	210	ASN	C-N-CA	7.52	127.23	119.64
29	I	224	ALA	CA-C-N	7.52	128.11	120.14
29	I	224	ALA	C-N-CA	7.52	128.11	120.14
3	c	215	THR	CA-C-N	7.51	133.09	123.10
3	c	215	THR	C-N-CA	7.51	133.09	123.10
7	g	223	GLU	N-CA-C	-7.50	102.03	113.89
21	N	602	VAL	CA-C-O	-7.50	112.47	118.85
5	e	80	GLY	N-CA-C	-7.50	103.98	111.56
9	i	88	ILE	CA-C-N	7.50	129.75	120.22
9	i	88	ILE	C-N-CA	7.50	129.75	120.22
11	k	176	PHE	N-CA-C	-7.50	103.69	114.12
26	U	14	VAL	CA-C-O	-7.50	113.22	121.17
27	O	148	ASP	CA-C-O	-7.50	112.47	120.42
32	M	421	GLU	N-CA-CB	7.50	121.41	110.47
33	J	116	ARG	NE-CZ-NH2	7.50	125.95	119.20
21	N	141	ILE	CA-C-N	7.49	130.32	120.28
21	N	141	ILE	C-N-CA	7.49	130.32	120.28
22	S	144	LEU	N-CA-CB	7.49	121.14	110.12
9	i	104	ARG	CA-C-N	7.49	132.93	120.64
9	i	104	ARG	C-N-CA	7.49	132.93	120.64
4	D	151	GLU	CA-C-N	7.49	128.43	120.12
4	D	151	GLU	C-N-CA	7.49	128.43	120.12
16	V	29	ILE	N-CA-C	-7.49	96.94	107.80
31	L	428	LEU	CA-C-O	-7.49	112.48	120.42
7	g	220	SER	CA-C-N	7.49	130.65	120.54
7	g	220	SER	C-N-CA	7.49	130.65	120.54
1	a	110	TYR	CB-CG-CD1	-7.48	109.57	120.80
1	a	160	ALA	CB-CA-C	-7.48	97.02	110.70
6	F	22	VAL	CB-CA-C	-7.48	102.22	112.24
12	l	273	TRP	CA-C-O	-7.47	113.00	120.70
10	3	124	PHE	CA-CB-CG	-7.47	106.33	113.80
13	6	153	LEU	CA-C-N	7.47	132.51	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	153	LEU	C-N-CA	7.47	132.51	120.55
21	N	776	TYR	N-CA-CB	7.47	120.99	109.85
4	d	189	GLU	N-CA-C	7.47	120.30	111.71
5	E	176	SER	N-CA-C	7.47	119.42	111.28
7	G	219	CYS	N-CA-C	-7.47	95.60	107.93
6	F	230	VAL	N-CA-C	-7.47	105.56	112.43
2	b	85	LEU	CA-C-N	7.46	132.26	120.47
2	b	85	LEU	C-N-CA	7.46	132.26	120.47
21	N	795	GLU	CA-C-N	7.46	129.96	120.56
21	N	795	GLU	C-N-CA	7.46	129.96	120.56
3	c	161	LYS	N-CA-C	-7.46	105.08	114.56
12	l	82	ARG	NE-CZ-NH1	7.46	128.96	121.50
20	Z	915	ALA	N-CA-C	-7.46	101.71	111.71
14	7	37	PRO	CA-C-O	-7.46	113.25	121.23
3	c	113	ARG	CA-C-N	7.45	130.13	120.44
3	c	113	ARG	C-N-CA	7.45	130.13	120.44
6	f	191	LYS	CA-C-N	7.45	130.26	120.28
6	f	191	LYS	C-N-CA	7.45	130.26	120.28
33	J	106	ASP	N-CA-C	-7.45	104.43	113.97
18	X	51	ARG	CA-C-O	-7.45	111.98	120.03
21	N	203	ARG	N-CA-C	-7.45	103.16	111.28
4	D	103	PRO	CA-C-N	7.45	130.54	120.63
4	D	103	PRO	C-N-CA	7.45	130.54	120.63
7	G	81	LEU	CA-C-N	7.45	127.58	120.43
7	G	81	LEU	C-N-CA	7.45	127.58	120.43
27	O	81	TYR	N-CA-CB	7.45	121.18	110.16
5	e	216	ASN	CA-CB-CG	-7.45	105.15	112.60
28	H	228	PRO	N-CA-CB	7.45	110.27	103.20
8	h	156	SER	CA-C-N	7.44	130.25	120.28
8	h	156	SER	C-N-CA	7.44	130.25	120.28
11	k	70	ARG	CA-C-O	7.44	128.50	120.24
2	b	109	LEU	N-CA-C	7.44	119.39	111.28
20	Z	185	ASP	CA-C-N	7.44	132.41	120.07
20	Z	185	ASP	C-N-CA	7.44	132.41	120.07
21	N	693	GLY	CA-C-N	7.44	130.85	120.29
21	N	693	GLY	C-N-CA	7.44	130.85	120.29
17	T	142	LEU	CA-C-N	7.44	130.85	120.29
17	T	142	LEU	C-N-CA	7.44	130.85	120.29
3	c	20	TYR	N-CA-CB	7.43	121.67	110.22
10	3	81	ALA	CA-C-N	7.43	131.09	120.98
10	3	81	ALA	C-N-CA	7.43	131.09	120.98
5	E	160	PRO	CA-C-N	7.43	130.55	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	160	PRO	C-N-CA	7.43	130.55	120.44
6	F	122	SER	CA-C-N	7.43	132.98	122.72
6	F	122	SER	C-N-CA	7.43	132.98	122.72
13	6	201	GLU	N-CA-CB	7.43	120.79	110.01
18	X	112	ASN	CA-C-N	7.43	133.28	122.36
18	X	112	ASN	C-N-CA	7.43	133.28	122.36
5	E	148	ASP	N-CA-C	-7.43	98.11	109.85
16	V	32	ILE	CA-C-N	7.43	130.84	120.29
16	V	32	ILE	C-N-CA	7.43	130.84	120.29
4	d	242	GLU	CA-C-N	7.43	130.24	120.28
4	d	242	GLU	C-N-CA	7.43	130.24	120.28
10	j	44	PHE	CA-C-O	-7.43	113.15	121.40
23	P	183	GLN	CA-C-N	7.43	130.24	120.28
23	P	183	GLN	C-N-CA	7.43	130.24	120.28
31	L	50	GLN	OE1-CD-NE2	7.43	130.03	122.60
11	4	76	SER	CA-C-N	7.42	128.08	119.47
11	4	76	SER	C-N-CA	7.42	128.08	119.47
11	k	23	ARG	NH1-CZ-NH2	-7.42	109.65	119.30
12	5	144	ARG	O-C-N	-7.42	113.69	122.15
24	Q	56	THR	CA-C-N	7.42	130.53	120.44
24	Q	56	THR	C-N-CA	7.42	130.53	120.44
31	L	232	ALA	CA-C-N	7.42	130.22	120.28
31	L	232	ALA	C-N-CA	7.42	130.22	120.28
21	N	614	ASN	OD1-CG-ND2	7.42	130.02	122.60
7	g	19	GLY	CA-C-O	7.42	125.74	118.77
14	n	95	HIS	ND1-CE1-NE2	7.42	115.81	108.40
17	T	180	ILE	N-CA-C	-7.42	103.23	110.72
32	M	284	ASP	CA-CB-CG	7.42	120.02	112.60
21	N	409	GLY	N-CA-C	7.41	123.30	113.37
30	K	244	HIS	CE1-NE2-CD2	-7.41	101.59	109.00
7	g	21	ASN	CA-CB-CG	7.41	120.01	112.60
9	2	194	ASN	N-CA-CB	-7.41	99.76	110.65
20	Z	367	SER	N-CA-CB	7.41	122.85	110.77
22	S	49	ASP	CA-CB-CG	7.41	120.01	112.60
24	Q	229	ASP	N-CA-CB	7.41	122.48	110.40
27	O	288	ARG	CA-C-O	-7.41	113.04	120.82
21	N	877	GLN	CA-C-N	7.41	131.57	120.31
21	N	877	GLN	C-N-CA	7.41	131.57	120.31
20	Z	856	HIS	CE1-NE2-CD2	-7.41	101.59	109.00
29	I	196	GLU	N-CA-CB	7.41	121.12	110.16
5	E	188	HIS	CG-CD2-NE2	7.40	114.60	107.20
28	H	192	ASP	N-CA-C	7.40	122.88	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	154	ASN	CA-CB-CG	-7.40	105.20	112.60
16	V	134	SER	O-C-N	-7.40	113.46	122.34
33	J	272	MET	CA-C-N	7.40	130.80	120.29
33	J	272	MET	C-N-CA	7.40	130.80	120.29
2	b	168	SER	CA-C-N	7.40	130.93	120.42
2	b	168	SER	C-N-CA	7.40	130.93	120.42
8	1	77	SER	N-CA-CB	7.40	121.11	110.16
28	H	191	ILE	N-CA-C	-7.40	105.36	113.43
8	h	155	MET	N-CA-C	-7.40	98.95	110.42
10	j	164	PHE	CA-C-N	7.40	130.19	120.28
10	j	164	PHE	C-N-CA	7.40	130.19	120.28
20	Z	630	LYS	CA-C-N	7.40	128.35	119.99
20	Z	630	LYS	C-N-CA	7.40	128.35	119.99
28	H	90	ARG	NE-CZ-NH2	7.40	125.86	119.20
30	K	409	GLU	CA-C-N	7.40	130.79	120.29
30	K	409	GLU	C-N-CA	7.40	130.79	120.29
33	J	316	PHE	CA-CB-CG	-7.40	106.40	113.80
31	L	316	ASP	N-CA-CB	7.40	123.07	110.50
20	Z	201	LEU	CA-C-N	7.39	130.19	120.28
20	Z	201	LEU	C-N-CA	7.39	130.19	120.28
20	Z	398	LYS	CA-C-N	7.39	130.19	120.28
20	Z	398	LYS	C-N-CA	7.39	130.19	120.28
29	I	138	LYS	N-CA-C	-7.39	103.24	111.82
5	E	27	SER	N-CA-C	-7.39	103.52	112.54
20	Z	176	GLU	N-CA-C	-7.39	103.86	113.17
20	Z	247	GLN	OE1-CD-NE2	-7.39	115.21	122.60
30	K	213	GLY	N-CA-C	-7.39	97.27	112.34
30	K	307	ASP	CA-C-N	7.39	135.65	121.54
30	K	307	ASP	C-N-CA	7.39	135.65	121.54
7	g	91	ARG	NE-CZ-NH2	7.39	125.85	119.20
10	j	124	PHE	CA-CB-CG	-7.39	106.41	113.80
29	I	60	LEU	N-CA-CB	7.39	121.59	110.22
9	i	102	GLU	CA-C-N	7.38	127.31	119.85
9	i	102	GLU	C-N-CA	7.38	127.31	119.85
1	A	209	HIS	ND1-CE1-NE2	7.38	115.78	108.40
8	1	91	PHE	CA-C-N	7.38	130.17	120.28
8	1	91	PHE	C-N-CA	7.38	130.17	120.28
32	M	182	ASP	N-CA-C	-7.38	102.53	112.94
33	J	238	ARG	N-CA-C	7.38	119.11	111.14
9	2	145	HIS	ND1-CE1-NE2	7.38	115.78	108.40
24	Q	71	LYS	CA-C-N	7.38	130.77	120.29
24	Q	71	LYS	C-N-CA	7.38	130.77	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	16	LEU	N-CA-C	-7.38	98.19	109.41
33	J	49	ASN	CA-CB-CG	-7.38	105.22	112.60
20	Z	181	GLY	CA-C-O	7.38	127.55	119.06
20	Z	505	VAL	CA-C-N	7.38	130.17	120.28
20	Z	505	VAL	C-N-CA	7.38	130.17	120.28
3	C	31	HIS	ND1-CE1-NE2	7.37	115.77	108.40
14	n	205	VAL	N-CA-C	-7.37	103.28	110.72
26	U	230	GLN	CA-C-N	7.37	130.15	120.28
26	U	230	GLN	C-N-CA	7.37	130.15	120.28
8	1	26	ASP	CA-CB-CG	-7.37	105.23	112.60
21	N	469	VAL	CA-C-N	7.37	130.75	120.29
21	N	469	VAL	C-N-CA	7.37	130.75	120.29
21	N	83	LEU	N-CA-C	-7.36	103.89	113.17
9	2	172	LYS	CA-C-N	7.36	131.28	120.90
9	2	172	LYS	C-N-CA	7.36	131.28	120.90
21	N	204	SER	CA-C-N	7.36	130.01	120.44
21	N	204	SER	C-N-CA	7.36	130.01	120.44
5	e	202	LYS	CA-C-N	7.36	130.87	120.42
5	e	202	LYS	C-N-CA	7.36	130.87	120.42
2	B	100	ILE	N-CA-C	-7.36	105.94	112.12
21	N	884	PHE	CA-CB-CG	-7.36	106.44	113.80
26	U	155	LEU	CA-C-O	-7.36	112.36	120.38
10	3	31	SER	CB-CA-C	-7.36	100.56	110.79
4	D	178	ASN	CA-C-N	7.36	131.94	121.42
4	D	178	ASN	C-N-CA	7.36	131.94	121.42
26	U	90	ILE	N-CA-C	-7.36	106.14	113.20
31	L	363	ILE	CA-C-N	7.35	130.73	120.29
31	L	363	ILE	C-N-CA	7.35	130.73	120.29
2	B	103	GLU	N-CA-CB	7.35	123.94	111.66
3	C	125	HIS	ND1-CE1-NE2	7.35	115.75	108.40
17	T	139	ASP	CA-CB-CG	-7.35	105.25	112.60
2	B	127	VAL	N-CA-C	-7.35	97.90	108.48
13	6	111	PHE	N-CA-C	-7.35	98.18	108.76
20	Z	141	SER	N-CA-CB	-7.35	99.62	110.49
26	U	116	ASN	CA-C-O	-7.34	113.38	121.23
22	S	74	LEU	CA-C-N	7.34	130.11	120.28
22	S	74	LEU	C-N-CA	7.34	130.11	120.28
2	B	126	GLY	N-CA-C	-7.34	105.67	115.21
2	b	230	ASP	CA-CB-CG	7.33	119.93	112.60
4	d	106	VAL	N-CA-C	7.33	118.10	110.62
4	D	217	PRO	CA-C-N	7.33	133.05	122.35
4	D	217	PRO	C-N-CA	7.33	133.05	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	40	SER	N-CA-C	-7.33	98.22	109.14
7	g	73	HIS	ND1-CE1-NE2	7.33	115.73	108.40
3	C	97	ASN	CA-CB-CG	7.33	119.93	112.60
10	j	73	LEU	CA-C-N	7.33	129.97	120.44
10	j	73	LEU	C-N-CA	7.33	129.97	120.44
20	Z	164	VAL	O-C-N	7.33	128.98	121.87
31	L	213	LYS	CA-C-N	7.33	124.93	119.66
31	L	213	LYS	C-N-CA	7.33	124.93	119.66
3	C	92	ARG	CA-C-N	7.32	130.82	120.42
3	C	92	ARG	C-N-CA	7.32	130.82	120.42
1	A	16	ILE	CB-CA-C	-7.32	102.88	110.93
15	W	166	GLU	N-CA-C	-7.32	103.32	114.16
30	K	180	GLN	CA-C-N	7.32	130.82	120.28
30	K	180	GLN	C-N-CA	7.32	130.82	120.28
29	I	340	ARG	N-CA-CB	7.32	123.40	110.37
2	b	105	PRO	CA-C-N	7.32	127.35	119.89
2	b	105	PRO	C-N-CA	7.32	127.35	119.89
7	g	82	ILE	N-CA-CB	7.32	116.16	110.45
22	S	143	GLN	CA-C-O	7.32	128.31	120.55
29	I	432	LEU	N-CA-C	-7.32	103.24	111.14
14	7	234	ASP	CA-C-O	7.31	129.66	121.11
23	P	73	ASP	CA-C-N	7.31	130.08	120.28
23	P	73	ASP	C-N-CA	7.31	130.08	120.28
33	J	118	ASP	CA-CB-CG	7.31	119.91	112.60
20	Z	543	THR	O-C-N	-7.31	112.37	122.46
29	I	409	MET	CA-C-O	7.31	128.26	119.78
32	M	207	PHE	CA-CB-CG	-7.31	106.49	113.80
26	U	295	LYS	CA-C-N	7.30	130.79	120.42
26	U	295	LYS	C-N-CA	7.30	130.79	120.42
2	b	212	ALA	O-C-N	-7.30	115.59	123.26
11	k	132	ALA	N-CA-CB	7.30	122.83	110.49
7	G	138	PHE	CA-C-O	-7.30	113.64	121.38
4	D	233	VAL	CA-C-N	7.30	131.40	120.31
4	D	233	VAL	C-N-CA	7.30	131.40	120.31
28	H	393	SER	CA-C-N	7.30	130.06	120.28
28	H	393	SER	C-N-CA	7.30	130.06	120.28
5	e	73	HIS	CB-CG-CD2	-7.30	121.72	131.20
33	J	204	HIS	N-CA-C	7.30	119.23	111.28
24	Q	131	VAL	CA-C-N	7.29	130.39	120.54
24	Q	131	VAL	C-N-CA	7.29	130.39	120.54
25	R	91	TRP	N-CA-C	-7.29	103.84	112.89
33	J	229	MET	CA-C-N	7.29	130.78	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	229	MET	C-N-CA	7.29	130.78	120.42
9	i	195	ASP	CA-CB-CG	-7.29	105.31	112.60
5	E	14	THR	CA-C-O	-7.29	112.30	120.32
15	W	105	VAL	N-CA-C	-7.29	105.73	112.43
22	S	387	VAL	CA-C-N	7.29	129.89	120.56
22	S	387	VAL	C-N-CA	7.29	129.89	120.56
1	a	125	SER	N-CA-CB	7.28	120.83	110.12
6	f	219	ASP	N-CA-C	-7.28	105.57	114.75
13	m	203	HIS	CG-CD2-NE2	7.28	114.48	107.20
5	E	173	GLY	CA-C-N	7.28	130.04	120.28
5	E	173	GLY	C-N-CA	7.28	130.04	120.28
7	G	152	GLU	CA-C-O	-7.28	113.32	120.97
29	I	117	HIS	ND1-CE1-NE2	7.28	115.68	108.40
29	I	142	GLU	O-C-N	-7.28	116.71	121.88
30	K	258	PHE	CA-CB-CG	-7.28	106.52	113.80
21	N	787	MET	CA-C-O	7.28	128.76	120.54
22	S	461	PHE	CA-C-O	-7.28	112.71	120.42
3	C	67	TYR	CA-C-O	-7.28	112.29	120.66
21	N	778	LYS	N-CA-C	-7.28	95.30	110.80
29	I	224	ALA	CA-C-O	-7.28	112.60	120.17
22	S	108	ALA	O-C-N	7.27	132.26	122.59
13	6	159	ASP	N-CA-C	-7.27	104.29	113.02
32	M	228	LYS	CA-C-N	7.27	130.35	120.54
32	M	228	LYS	C-N-CA	7.27	130.35	120.54
2	b	177	LYS	CA-C-O	-7.27	113.19	120.82
5	e	87	SER	CA-C-N	7.27	130.02	120.28
5	e	87	SER	C-N-CA	7.27	130.02	120.28
25	R	229	LYS	CA-C-N	7.27	130.32	120.44
25	R	229	LYS	C-N-CA	7.27	130.32	120.44
32	M	292	ASP	CA-C-N	7.27	132.84	122.09
32	M	292	ASP	C-N-CA	7.27	132.84	122.09
10	j	35	GLY	CA-C-O	-7.27	114.79	121.18
21	N	287	LEU	N-CA-CB	7.26	120.80	110.12
22	S	314	ASN	OD1-CG-ND2	-7.26	115.34	122.60
31	L	187	THR	CA-C-N	7.26	130.35	120.54
31	L	187	THR	C-N-CA	7.26	130.35	120.54
13	m	110	PHE	CA-CB-CG	-7.26	106.54	113.80
20	Z	320	SER	CA-C-N	7.26	130.33	120.38
20	Z	320	SER	C-N-CA	7.26	130.33	120.38
1	a	151	GLY	CA-C-N	7.26	127.70	119.93
1	a	151	GLY	C-N-CA	7.26	127.70	119.93
16	V	83	VAL	N-CA-C	-7.26	97.71	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	934	GLU	N-CA-C	7.26	120.22	110.35
28	H	377	PHE	CA-CB-CG	-7.26	106.54	113.80
6	f	52	ASN	CA-C-O	-7.26	113.49	121.33
20	Z	503	ASP	CA-C-N	7.26	130.01	120.28
20	Z	503	ASP	C-N-CA	7.26	130.01	120.28
31	L	74	LEU	CA-C-O	-7.26	112.85	120.55
2	B	186	GLU	CA-C-O	7.26	128.24	120.55
16	V	134	SER	N-CA-C	-7.26	103.99	112.92
20	Z	491	LEU	N-CA-CB	7.26	120.90	110.16
5	E	189	SER	N-CA-C	-7.25	103.52	112.88
9	2	211	LYS	CA-C-N	7.25	133.13	120.87
9	2	211	LYS	C-N-CA	7.25	133.13	120.87
11	4	191	GLN	CA-C-N	7.25	132.97	123.11
11	4	191	GLN	C-N-CA	7.25	132.97	123.11
27	O	286	PHE	CA-C-N	7.25	130.59	120.29
27	O	286	PHE	C-N-CA	7.25	130.59	120.29
17	T	165	GLN	N-CA-C	7.25	119.27	111.36
22	S	71	ALA	CA-C-N	7.25	130.00	120.28
22	S	71	ALA	C-N-CA	7.25	130.00	120.28
21	N	125	THR	N-CA-C	-7.25	105.35	114.56
33	J	376	HIS	ND1-CE1-NE2	7.25	115.65	108.40
21	N	864	LYS	O-C-N	-7.25	113.90	120.71
23	P	21	PHE	CA-C-O	-7.25	111.96	118.63
20	Z	84	ALA	N-CA-C	-7.25	102.54	112.03
21	N	55	PHE	CA-CB-CG	-7.25	106.55	113.80
20	Z	453	LEU	CA-C-N	7.25	129.42	120.22
20	Z	453	LEU	C-N-CA	7.25	129.42	120.22
20	Z	315	ALA	CA-C-O	-7.24	112.81	120.63
27	O	327	LEU	N-CA-CB	7.24	120.88	110.16
20	Z	898	HIS	CE1-NE2-CD2	-7.24	101.76	109.00
21	N	400	ILE	CA-C-O	7.24	128.29	120.47
28	H	353	PHE	CA-CB-CG	-7.24	106.56	113.80
6	f	207	THR	CA-C-N	7.24	129.68	120.56
6	f	207	THR	C-N-CA	7.24	129.68	120.56
27	O	71	ASP	N-CA-C	-7.23	105.64	114.75
14	7	87	SER	N-CA-CB	7.23	122.64	111.22
13	6	172	THR	CA-CB-OG1	7.23	120.44	109.60
14	7	125	ILE	CA-C-N	7.23	129.84	120.44
14	7	125	ILE	C-N-CA	7.23	129.84	120.44
22	S	300	ALA	N-CA-C	7.23	118.82	109.64
28	H	394	LYS	O-C-N	-7.23	114.46	122.12
7	g	108	PRO	CA-C-O	-7.22	113.11	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	88	PHE	O-C-N	7.22	129.78	122.12
12	5	111	GLU	CA-C-N	7.22	129.81	120.56
12	5	111	GLU	C-N-CA	7.22	129.81	120.56
24	Q	427	PHE	CA-C-N	7.22	130.54	120.29
24	Q	427	PHE	C-N-CA	7.22	130.54	120.29
31	L	392	ARG	NE-CZ-NH2	-7.22	112.70	119.20
13	m	27	ASP	CA-CB-CG	7.22	119.82	112.60
25	R	73	ASN	N-CA-C	-7.22	103.58	113.18
1	a	54	ILE	N-CA-C	-7.21	97.64	108.17
7	g	183	HIS	CE1-NE2-CD2	-7.21	101.78	109.00
1	A	123	ASN	CA-C-N	7.21	129.95	120.28
1	A	123	ASN	C-N-CA	7.21	129.95	120.28
12	5	254	HIS	CE1-NE2-CD2	-7.21	101.79	109.00
5	e	42	THR	N-CA-C	-7.21	98.69	108.86
20	Z	293	MET	CA-C-N	7.21	129.65	120.56
20	Z	293	MET	C-N-CA	7.21	129.65	120.56
31	L	73	GLN	CA-C-O	-7.21	112.91	120.55
15	W	136	ASN	CA-CB-CG	-7.21	105.39	112.60
30	K	172	ALA	N-CA-C	-7.21	102.05	111.71
22	S	344	PRO	N-CA-CB	7.21	111.17	103.39
1	A	187	LYS	O-C-N	7.21	129.76	122.12
20	Z	385	PHE	CA-C-N	7.20	131.85	120.47
20	Z	385	PHE	C-N-CA	7.20	131.85	120.47
23	P	23	LYS	CA-C-N	7.20	129.64	120.56
23	P	23	LYS	C-N-CA	7.20	129.64	120.56
3	c	85	GLU	CA-C-N	7.20	129.63	120.56
3	c	85	GLU	C-N-CA	7.20	129.63	120.56
21	N	585	ARG	CA-C-N	7.20	129.93	120.28
21	N	585	ARG	C-N-CA	7.20	129.93	120.28
24	Q	24	GLU	CA-C-N	7.20	129.80	120.44
24	Q	24	GLU	C-N-CA	7.20	129.80	120.44
18	X	121	ILE	CA-C-N	7.20	129.93	120.28
18	X	121	ILE	C-N-CA	7.20	129.93	120.28
9	2	129	VAL	N-CA-C	-7.20	98.09	108.17
21	N	382	GLY	CA-C-N	7.20	130.51	120.29
21	N	382	GLY	C-N-CA	7.20	130.51	120.29
5	E	105	GLU	N-CA-C	-7.20	97.39	108.76
11	4	118	GLN	OE1-CD-NE2	7.19	129.79	122.60
9	2	94	LEU	CB-CA-C	-7.19	99.59	110.88
21	N	680	LYS	N-CA-C	-7.19	104.31	113.23
17	T	169	GLN	N-CA-C	-7.19	103.67	113.30
7	g	101	LYS	N-CA-C	-7.19	103.14	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	129	GLU	N-CA-C	-7.18	105.14	114.04
4	d	180	ASP	CA-CB-CG	-7.18	105.42	112.60
20	Z	949	ILE	N-CA-C	7.18	120.06	111.09
5	E	188	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
15	W	9	VAL	N-CA-C	-7.17	95.19	107.24
21	N	639	ASP	CA-CB-CG	-7.17	105.43	112.60
33	J	31	GLU	CA-C-N	7.17	130.48	120.29
33	J	31	GLU	C-N-CA	7.17	130.48	120.29
31	L	382	MET	CA-C-O	7.17	128.15	120.55
5	E	61	SER	CA-C-N	7.17	133.60	122.49
5	E	61	SER	C-N-CA	7.17	133.60	122.49
3	C	113	ARG	CA-C-N	7.17	129.76	120.44
3	C	113	ARG	C-N-CA	7.17	129.76	120.44
14	7	39	VAL	N-CA-CB	7.17	118.53	110.72
28	H	230	LEU	CA-C-N	-7.17	114.38	122.26
28	H	230	LEU	C-N-CA	-7.17	114.38	122.26
2	B	32	VAL	CA-C-O	-7.16	114.18	122.13
21	N	7	ALA	CA-C-O	-7.16	111.74	118.33
31	L	405	ASP	CA-CB-CG	7.16	119.76	112.60
33	J	322	ALA	N-CA-CB	7.16	120.76	110.16
10	3	150	CYS	CA-C-O	7.16	128.14	120.55
21	N	617	VAL	CA-C-O	-7.16	113.26	120.85
7	G	159	GLY	N-CA-C	-7.16	103.38	112.54
5	e	73	HIS	CA-CB-CG	7.16	120.96	113.80
21	N	703	GLN	CA-C-N	7.15	127.88	119.94
21	N	703	GLN	C-N-CA	7.15	127.88	119.94
30	K	204	ASP	CA-C-O	-7.15	110.94	121.46
18	X	79	LYS	N-CA-C	-7.15	103.77	114.64
20	Z	130	GLY	CA-C-O	-7.15	111.07	119.01
29	I	83	LYS	CA-C-O	-7.15	110.36	120.16
16	V	186	GLN	CA-C-N	7.15	130.58	120.28
16	V	186	GLN	C-N-CA	7.15	130.58	120.28
26	U	258	SER	CA-C-N	7.15	129.73	120.44
26	U	258	SER	C-N-CA	7.15	129.73	120.44
22	S	129	GLU	CA-C-N	7.15	130.65	122.36
22	S	129	GLU	C-N-CA	7.15	130.65	122.36
5	e	23	GLN	CA-C-N	7.15	130.57	120.42
5	e	23	GLN	C-N-CA	7.15	130.57	120.42
8	h	86	THR	N-CA-C	-7.15	103.42	111.14
23	P	230	HIS	ND1-CE1-NE2	7.15	115.55	108.40
16	V	199	LEU	CA-C-N	7.14	130.85	120.71
16	V	199	LEU	C-N-CA	7.14	130.85	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	181	ASP	CA-CB-CG	-7.14	105.46	112.60
9	i	68	PRO	N-CA-CB	-7.14	96.05	103.19
14	n	198	ILE	N-CA-CB	7.14	115.31	110.52
5	E	192	THR	CA-C-O	-7.14	112.92	121.56
17	T	128	TYR	CA-C-N	7.14	130.56	120.28
17	T	128	TYR	C-N-CA	7.14	130.56	120.28
14	7	117	GLU	N-CA-C	-7.14	103.79	114.64
20	Z	118	VAL	CA-C-N	7.14	130.56	120.28
20	Z	118	VAL	C-N-CA	7.14	130.56	120.28
20	Z	539	ASN	CA-CB-CG	-7.13	105.47	112.60
24	Q	141	LEU	CA-C-N	7.13	129.84	120.28
24	Q	141	LEU	C-N-CA	7.13	129.84	120.28
25	R	187	VAL	CA-C-N	7.13	129.84	120.28
25	R	187	VAL	C-N-CA	7.13	129.84	120.28
1	a	46	ARG	NE-CZ-NH1	7.13	128.63	121.50
14	7	172	SER	CA-C-N	7.13	128.10	120.47
14	7	172	SER	C-N-CA	7.13	128.10	120.47
20	Z	108	ASP	O-C-N	7.13	129.52	121.32
32	M	269	LEU	CA-C-N	7.13	129.83	120.28
32	M	269	LEU	C-N-CA	7.13	129.83	120.28
10	j	81	ALA	CA-C-O	7.13	129.91	121.36
12	5	149	ILE	N-CA-CB	7.13	118.30	110.53
23	P	323	ASN	OD1-CG-ND2	7.13	129.73	122.60
4	D	28	LYS	CA-C-N	7.12	129.70	120.44
4	D	28	LYS	C-N-CA	7.12	129.70	120.44
21	N	129	ILE	CA-C-N	7.12	131.50	120.60
21	N	129	ILE	C-N-CA	7.12	131.50	120.60
17	T	206	LYS	CA-C-N	7.12	129.82	120.28
17	T	206	LYS	C-N-CA	7.12	129.82	120.28
11	4	164	CYS	CB-CA-C	-7.12	98.75	110.85
19	Y	74	THR	CA-C-O	-7.12	113.01	120.55
24	Q	154	SER	CA-C-N	7.12	129.81	120.28
24	Q	154	SER	C-N-CA	7.12	129.81	120.28
8	h	156	SER	CA-C-O	-7.11	114.05	121.87
28	H	305	ILE	N-CA-C	-7.11	97.88	108.12
9	2	104	ARG	CD-NE-CZ	-7.11	114.44	124.40
3	c	143	ARG	N-CA-C	-7.11	104.47	113.43
2	b	242	GLU	CA-C-N	7.11	130.20	120.46
2	b	242	GLU	C-N-CA	7.11	130.20	120.46
7	G	40	ILE	N-CA-C	-7.11	97.37	107.75
21	N	749	LEU	CA-C-O	7.11	128.21	119.11
21	N	821	LYS	N-CA-C	7.11	118.81	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	150	HIS	CA-C-N	7.11	129.80	120.28
29	I	150	HIS	C-N-CA	7.11	129.80	120.28
30	K	66	ASP	CA-CB-CG	-7.11	105.49	112.60
5	e	215	ASN	N-CA-C	-7.10	104.62	113.28
21	N	663	ILE	CB-CA-C	-7.10	102.42	112.22
28	H	306	ILE	CB-CA-C	7.10	120.22	110.99
11	4	141	PHE	CA-C-N	7.10	131.10	120.31
11	4	141	PHE	C-N-CA	7.10	131.10	120.31
5	e	138	PHE	CA-CB-CG	-7.09	106.71	113.80
12	5	86	GLY	N-CA-C	-7.09	101.00	110.58
7	g	196	ALA	N-CA-CB	7.09	120.55	110.12
6	F	47	VAL	N-CA-C	-7.09	97.91	108.12
20	Z	546	ILE	CA-C-N	7.09	129.78	120.28
20	Z	546	ILE	C-N-CA	7.09	129.78	120.28
29	I	330	LYS	O-C-N	-7.09	115.40	122.99
14	7	125	ILE	O-C-N	7.09	128.75	121.87
29	I	364	ILE	N-CA-CB	7.09	118.84	110.55
2	B	118	MET	CA-C-N	7.08	130.35	120.29
2	B	118	MET	C-N-CA	7.08	130.35	120.29
6	F	149	PRO	N-CA-C	-7.08	104.71	114.27
24	Q	232	TYR	N-CA-C	-7.08	104.51	113.72
7	g	50	VAL	CA-C-O	7.08	126.91	120.96
8	h	129	HIS	CA-CB-CG	7.08	120.88	113.80
6	F	9	ASP	CA-CB-CG	7.08	119.68	112.60
22	S	150	LYS	N-CA-CB	7.08	122.45	110.49
33	J	5	VAL	CA-C-N	7.08	131.50	122.16
33	J	5	VAL	C-N-CA	7.08	131.50	122.16
21	N	69	TYR	CA-C-O	-7.07	112.92	120.42
22	S	306	SER	CA-C-N	7.07	130.06	120.44
22	S	306	SER	C-N-CA	7.07	130.06	120.44
6	f	107	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	103	GLU	CA-C-N	7.07	129.63	120.44
1	A	103	GLU	C-N-CA	7.07	129.63	120.44
16	V	133	ASN	N-CA-C	-7.07	97.78	108.52
33	J	288	ILE	O-C-N	-7.07	115.73	122.09
2	B	187	ASP	N-CA-CB	7.07	120.25	110.01
13	6	81	LYS	O-C-N	-7.07	114.79	122.07
16	V	38	LEU	N-CA-C	7.06	119.83	111.71
31	L	206	ILE	N-CA-C	7.06	119.92	111.09
31	L	397	GLU	CA-C-N	7.06	129.74	120.28
31	L	397	GLU	C-N-CA	7.06	129.74	120.28
33	J	200	ARG	N-CA-C	-7.06	103.66	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	10	ARG	NE-CZ-NH2	-7.06	112.85	119.20
8	1	199	PRO	N-CA-C	7.06	124.05	113.81
23	P	10	ASP	CA-CB-CG	-7.06	105.54	112.60
3	c	130	PRO	CB-CA-C	7.06	120.72	110.63
27	O	230	PHE	CA-CB-CG	-7.06	106.74	113.80
32	M	190	ILE	N-CA-C	-7.06	103.59	110.72
9	i	128	ILE	N-CA-C	-7.05	97.69	107.99
22	S	53	ILE	O-C-N	7.05	129.10	121.83
12	5	80	ALA	N-CA-C	-7.05	97.92	108.99
32	M	271	LYS	CB-CA-C	-7.05	99.08	110.79
21	N	225	LEU	CA-C-N	7.05	130.43	120.28
21	N	225	LEU	C-N-CA	7.05	130.43	120.28
30	K	342	SER	N-CA-C	-7.05	105.30	114.04
33	J	10	ILE	CA-C-N	7.05	134.66	121.97
33	J	10	ILE	C-N-CA	7.05	134.66	121.97
5	E	48	LEU	CB-CA-C	-7.05	99.39	110.74
14	7	256	LYS	CA-C-N	7.05	130.05	120.54
14	7	256	LYS	C-N-CA	7.05	130.05	120.54
2	b	187	ASP	CA-CB-CG	7.04	119.64	112.60
18	X	34	GLU	N-CA-C	-7.04	96.93	108.41
20	Z	291	GLU	CA-C-N	7.04	129.60	120.44
20	Z	291	GLU	C-N-CA	7.04	129.60	120.44
12	5	268	VAL	N-CA-C	7.04	117.80	110.62
33	J	96	VAL	N-CA-C	-7.04	98.35	108.42
4	d	215	VAL	CB-CA-C	7.04	121.04	110.63
2	B	190	HIS	CB-CG-ND1	7.04	133.25	122.70
10	3	147	PHE	CA-C-N	7.04	127.75	119.94
10	3	147	PHE	C-N-CA	7.04	127.75	119.94
21	N	364	LYS	CG-CD-CE	7.04	127.48	111.30
26	U	64	ASP	CA-C-N	7.04	133.47	122.70
26	U	64	ASP	C-N-CA	7.04	133.47	122.70
20	Z	187	SER	N-CA-C	-7.03	104.34	114.12
21	N	747	HIS	CG-CD2-NE2	7.03	114.23	107.20
10	j	75	LYS	CA-C-N	7.03	130.00	120.44
10	j	75	LYS	C-N-CA	7.03	130.00	120.44
22	S	422	MET	CG-SD-CE	-7.03	85.43	100.90
5	E	198	LEU	CA-C-N	7.03	130.00	120.44
5	E	198	LEU	C-N-CA	7.03	130.00	120.44
20	Z	342	LEU	CA-C-N	7.03	129.70	120.28
20	Z	342	LEU	C-N-CA	7.03	129.70	120.28
24	Q	210	CYS	CA-C-N	7.03	128.62	119.84
24	Q	210	CYS	C-N-CA	7.03	128.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	237	THR	CA-CB-OG1	7.03	120.14	109.60
6	F	11	VAL	N-CA-C	-7.03	105.97	112.43
32	M	129	LEU	CA-C-N	7.03	127.07	119.90
32	M	129	LEU	C-N-CA	7.03	127.07	119.90
11	4	141	PHE	N-CA-CB	7.02	120.56	110.16
20	Z	742	GLY	CA-C-N	7.02	130.39	120.42
20	Z	742	GLY	C-N-CA	7.02	130.39	120.42
17	T	17	ASN	N-CA-C	-7.02	104.86	113.50
24	Q	334	HIS	ND1-CE1-NE2	7.02	115.42	108.40
20	Z	603	VAL	CA-C-N	7.02	128.92	120.14
20	Z	603	VAL	C-N-CA	7.02	128.92	120.14
29	I	414	GLU	CA-C-O	-7.02	113.45	120.82
32	M	179	THR	N-CA-CB	7.02	122.36	110.49
21	N	286	LEU	CA-C-N	7.02	129.69	120.28
21	N	286	LEU	C-N-CA	7.02	129.69	120.28
33	J	20	LYS	CA-C-O	-7.02	111.85	118.73
20	Z	71	LEU	CA-C-N	7.02	129.68	120.28
20	Z	71	LEU	C-N-CA	7.02	129.68	120.28
22	S	248	ASP	N-CA-C	7.02	118.93	111.28
31	L	149	ASP	CA-CB-CG	-7.02	105.58	112.60
12	5	159	SER	N-CA-CB	7.02	120.54	110.16
23	P	440	HIS	CA-CB-CG	7.01	120.81	113.80
5	e	199	LEU	CA-C-O	-7.01	113.48	120.70
5	e	224	LYS	CA-C-N	7.01	129.99	120.38
5	e	224	LYS	C-N-CA	7.01	129.99	120.38
3	c	22	VAL	N-CA-C	-7.01	103.47	110.62
13	m	148	GLY	CA-C-N	7.01	129.55	120.44
13	m	148	GLY	C-N-CA	7.01	129.55	120.44
13	6	57	ASN	CA-CB-CG	-7.01	105.59	112.60
23	P	179	PHE	N-CA-CB	7.01	120.53	110.16
14	7	95	HIS	CA-CB-CG	7.01	120.81	113.80
21	N	422	TYR	CA-C-N	7.01	130.96	120.31
21	N	422	TYR	C-N-CA	7.01	130.96	120.31
22	S	79	ASN	CA-C-O	7.01	127.98	120.55
27	O	56	PRO	CA-C-O	7.01	125.02	118.29
5	e	12	VAL	N-CA-C	-7.00	106.18	112.90
8	h	195	LEU	N-CA-C	-7.00	98.67	109.24
20	Z	952	SER	N-CA-C	-7.00	98.00	108.99
32	M	223	PRO	N-CA-C	7.00	117.19	110.47
32	M	427	SER	CA-C-O	7.00	127.84	120.42
6	f	204	GLU	N-CA-C	-7.00	98.53	108.96
23	P	50	SER	CA-C-N	7.00	130.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	50	SER	C-N-CA	7.00	130.36	120.28
8	h	53	CYS	N-CA-C	-7.00	98.83	109.95
9	2	108	ALA	N-CA-C	-7.00	103.73	111.36
29	I	207	LEU	CA-C-N	7.00	129.65	120.28
29	I	207	LEU	C-N-CA	7.00	129.65	120.28
4	D	109	LEU	CA-C-O	-6.99	113.50	120.70
5	E	42	THR	CA-CB-OG1	6.99	120.09	109.60
20	Z	242	PHE	CA-CB-CG	6.99	120.79	113.80
28	H	326	ASP	CA-CB-CG	-6.99	105.61	112.60
16	V	221	TRP	N-CA-C	-6.99	104.22	112.89
17	T	157	TYR	CA-C-N	6.99	129.98	120.54
17	T	157	TYR	C-N-CA	6.99	129.98	120.54
20	Z	627	LYS	CA-C-N	6.99	129.95	120.44
20	Z	627	LYS	C-N-CA	6.99	129.95	120.44
25	R	217	HIS	ND1-CE1-NE2	6.99	115.39	108.40
32	M	154	LEU	N-CA-C	-6.99	98.46	109.50
11	k	8	ARG	CA-C-N	6.99	130.38	122.48
11	k	8	ARG	C-N-CA	6.99	130.38	122.48
2	B	204	PHE	CA-CB-CG	-6.99	106.81	113.80
28	H	76	LEU	CA-C-N	6.99	128.82	120.09
28	H	76	LEU	C-N-CA	6.99	128.82	120.09
8	h	142	PHE	N-CA-C	6.99	118.89	111.28
24	Q	140	LYS	CA-C-N	6.99	129.64	120.28
24	Q	140	LYS	C-N-CA	6.99	129.64	120.28
10	j	129	CYS	O-C-N	-6.98	115.29	123.25
26	U	173	HIS	CA-CB-CG	6.98	120.78	113.80
28	H	466	TYR	CA-C-O	6.98	126.12	118.65
32	M	105	ASN	CA-CB-CG	6.98	119.58	112.60
4	d	31	THR	CA-C-N	6.98	131.90	120.94
4	d	31	THR	C-N-CA	6.98	131.90	120.94
17	T	23	CYS	CB-CA-C	-6.98	99.21	110.79
20	Z	547	MET	N-CA-C	6.98	118.89	111.28
26	U	89	LEU	CA-C-N	-6.98	114.27	122.36
26	U	89	LEU	C-N-CA	-6.98	114.27	122.36
24	Q	248	ASN	CA-CB-CG	6.97	119.57	112.60
1	a	241	ILE	CA-C-N	6.97	129.62	120.28
1	a	241	ILE	C-N-CA	6.97	129.62	120.28
12	5	217	SER	N-CA-C	-6.97	104.58	113.23
20	Z	135	LEU	CA-C-N	6.97	129.62	120.28
20	Z	135	LEU	C-N-CA	6.97	129.62	120.28
1	a	113	PRO	N-CD-CG	6.97	113.65	103.20
4	d	20	VAL	CA-C-O	-6.97	113.31	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	VAL	O-C-N	6.97	128.63	121.87
13	6	59	VAL	N-CA-C	-6.97	98.12	108.85
20	Z	129	ASN	CB-CA-C	-6.97	99.23	110.79
1	a	65	ASP	CA-C-O	-6.96	113.13	120.23
16	V	221	TRP	CA-C-N	6.96	130.18	120.29
16	V	221	TRP	C-N-CA	6.96	130.18	120.29
20	Z	948	TRP	CG-CD2-CE3	-6.96	126.94	133.90
22	S	183	LEU	N-CA-CB	6.96	121.02	110.30
20	Z	136	ARG	CA-C-N	6.96	129.61	120.28
20	Z	136	ARG	C-N-CA	6.96	129.61	120.28
1	a	221	ASN	CB-CA-C	-6.96	99.93	111.13
8	1	153	GLU	CA-C-N	6.96	134.83	121.54
8	1	153	GLU	C-N-CA	6.96	134.83	121.54
30	K	382	VAL	CA-C-O	6.96	128.19	120.95
30	K	411	TYR	CA-C-N	6.96	130.30	120.28
30	K	411	TYR	C-N-CA	6.96	130.30	120.28
31	L	348	GLU	N-CA-C	-6.96	97.90	109.24
2	B	98	LYS	N-CA-C	-6.96	104.79	112.72
5	E	73	HIS	CE1-NE2-CD2	-6.96	102.04	109.00
14	n	187	LEU	N-CA-C	-6.95	103.14	111.69
3	C	228	LYS	CA-C-O	6.95	127.61	120.24
16	V	202	ASP	CA-CB-CG	-6.95	105.65	112.60
20	Z	197	LYS	CA-C-O	-6.95	113.52	120.82
11	4	139	TYR	N-CA-C	-6.95	105.33	113.88
14	7	121	GLU	N-CA-C	-6.95	100.70	110.29
16	V	64	ASN	CA-CB-CG	-6.95	105.65	112.60
5	e	111	SER	O-C-N	-6.95	113.02	122.33
21	N	140	MET	CA-C-N	6.95	129.45	120.56
21	N	140	MET	C-N-CA	6.95	129.45	120.56
28	H	71	GLU	CA-C-N	6.95	131.85	120.94
28	H	71	GLU	C-N-CA	6.95	131.85	120.94
28	H	450	VAL	CA-C-N	6.95	129.98	120.46
28	H	450	VAL	C-N-CA	6.95	129.98	120.46
3	c	56	LEU	N-CA-C	-6.95	103.92	112.88
6	F	82	ARG	N-CA-C	6.95	118.85	111.28
13	6	31	LEU	N-CA-C	-6.95	97.02	108.76
17	T	237	ASN	CA-C-O	-6.95	113.55	120.70
21	N	823	PRO	N-CA-C	6.95	123.03	113.65
22	S	156	VAL	N-CA-CB	-6.95	102.42	110.55
1	a	193	HIS	ND1-CE1-NE2	6.95	115.34	108.40
1	A	111	ASP	CA-CB-CG	-6.95	105.65	112.60
16	V	57	PHE	O-C-N	6.95	131.12	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	276	LEU	CA-C-N	6.95	129.47	120.44
23	P	276	LEU	C-N-CA	6.95	129.47	120.44
9	2	191	GLY	CA-C-N	6.94	129.31	120.56
9	2	191	GLY	C-N-CA	6.94	129.31	120.56
1	A	147	ASP	CA-CB-CG	6.94	119.54	112.60
26	U	62	ASN	N-CA-C	-6.94	98.08	109.40
10	j	89	GLN	CA-C-O	6.94	127.91	120.55
21	N	168	SER	CA-C-N	6.94	130.15	120.29
21	N	168	SER	C-N-CA	6.94	130.15	120.29
28	H	355	THR	CA-C-N	6.94	130.14	120.29
28	H	355	THR	C-N-CA	6.94	130.14	120.29
22	S	298	ARG	N-CA-C	6.94	118.84	111.28
6	f	119	ASN	CB-CG-ND2	6.94	126.81	116.40
6	f	210	ASN	O-C-N	-6.94	113.82	122.35
24	Q	352	GLU	O-C-N	-6.94	114.19	120.71
30	K	144	ASN	OD1-CG-ND2	6.94	129.54	122.60
31	L	346	LYS	N-CA-CB	6.94	121.24	110.21
19	Y	74	THR	CA-CB-OG1	6.94	120.00	109.60
23	P	195	GLN	CA-C-N	6.94	130.27	120.28
23	P	195	GLN	C-N-CA	6.94	130.27	120.28
2	B	18	LEU	CA-C-N	6.93	128.81	120.14
2	B	18	LEU	C-N-CA	6.93	128.81	120.14
20	Z	348	LEU	CA-C-N	6.93	129.87	120.44
20	Z	348	LEU	C-N-CA	6.93	129.87	120.44
21	N	89	PHE	CA-C-N	6.93	130.13	120.29
21	N	89	PHE	C-N-CA	6.93	130.13	120.29
31	L	209	ARG	NE-CZ-NH1	-6.93	114.57	121.50
31	L	146	VAL	CA-C-O	6.93	128.95	121.67
21	N	532	ALA	N-CA-C	-6.93	104.02	113.30
22	S	47	THR	CA-C-N	6.93	129.56	120.28
22	S	47	THR	C-N-CA	6.93	129.56	120.28
33	J	152	GLY	CA-C-O	-6.93	115.95	122.39
4	d	223	ALA	N-CA-C	-6.92	97.61	108.90
21	N	276	GLU	CA-C-O	-6.92	113.21	120.55
22	S	184	TRP	CB-CG-CD1	6.92	137.29	126.90
21	N	392	GLY	N-CA-C	-6.92	106.21	115.21
21	N	721	ASP	CB-CA-C	-6.92	97.60	109.65
22	S	93	LEU	N-CA-C	6.92	118.83	111.28
33	J	89	GLN	O-C-N	-6.92	113.36	121.32
4	d	65	SER	N-CA-C	-6.92	98.12	109.40
7	g	183	HIS	ND1-CE1-NE2	6.92	115.32	108.40
20	Z	262	VAL	N-CA-CB	6.92	119.95	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	763	HIS	ND1-CE1-NE2	6.92	115.32	108.40
21	N	112	GLU	O-C-N	6.92	129.50	122.03
8	h	141	THR	CA-C-N	6.92	129.55	120.28
8	h	141	THR	C-N-CA	6.92	129.55	120.28
9	i	157	GLY	CA-C-N	6.92	130.12	120.29
9	i	157	GLY	C-N-CA	6.92	130.12	120.29
1	a	174	LYS	CA-C-N	6.92	129.88	120.54
1	a	174	LYS	C-N-CA	6.92	129.88	120.54
2	B	92	VAL	CA-C-N	6.92	129.55	120.28
2	B	92	VAL	C-N-CA	6.92	129.55	120.28
25	R	266	LEU	CA-C-N	6.92	129.43	120.44
25	R	266	LEU	C-N-CA	6.92	129.43	120.44
27	O	288	ARG	O-C-N	6.91	129.19	122.07
25	R	94	PHE	CB-CG-CD1	-6.91	108.95	120.70
24	Q	226	HIS	ND1-CE1-NE2	6.91	115.31	108.40
9	i	192	ILE	N-CA-CB	6.91	120.94	110.58
7	G	147	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	97	ALA	CA-C-N	6.91	129.83	120.44
1	A	97	ALA	C-N-CA	6.91	129.83	120.44
5	E	121	LEU	N-CA-CB	6.91	120.27	110.12
20	Z	49	LEU	O-C-N	-6.91	114.96	122.07
20	Z	187	SER	O-C-N	-6.91	114.26	122.27
22	S	201	ILE	CA-C-N	6.91	130.10	120.29
22	S	201	ILE	C-N-CA	6.91	130.10	120.29
31	L	107	GLU	N-CA-C	-6.91	96.94	108.75
29	I	272	GLY	CA-C-N	6.90	129.53	120.28
29	I	272	GLY	C-N-CA	6.90	129.53	120.28
13	m	33	GLY	CA-C-N	6.90	132.54	120.87
13	m	33	GLY	C-N-CA	6.90	132.54	120.87
4	d	29	ARG	N-CA-C	6.90	118.45	111.07
25	R	354	ALA	N-CA-C	-6.90	103.69	111.14
12	5	284	ASN	N-CA-C	-6.90	103.54	112.23
31	L	95	ILE	CA-C-N	6.90	129.52	120.28
31	L	95	ILE	C-N-CA	6.90	129.52	120.28
14	n	121	GLU	CA-C-N	6.89	126.86	119.28
14	n	121	GLU	C-N-CA	6.89	126.86	119.28
28	H	243	PRO	N-CA-CB	6.89	109.45	103.31
22	S	432	ILE	CA-C-O	-6.89	112.76	120.96
31	L	85	GLU	CA-C-N	6.89	129.51	120.28
31	L	85	GLU	C-N-CA	6.89	129.51	120.28
31	L	199	LEU	O-C-N	-6.89	113.39	121.32
6	f	71	GLY	N-CA-C	-6.89	99.43	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	274	GLN	CA-C-N	6.89	130.68	120.83
16	V	274	GLN	C-N-CA	6.89	130.68	120.83
29	I	54	ARG	N-CA-C	6.89	119.81	111.82
12	l	265	ASN	N-CA-C	-6.89	97.67	108.90
8	1	35	ILE	CA-C-N	6.89	129.81	120.44
8	1	35	ILE	C-N-CA	6.89	129.81	120.44
20	Z	85	VAL	CA-C-O	-6.89	110.72	119.95
27	O	287	LEU	CA-C-N	6.89	129.39	120.44
27	O	287	LEU	C-N-CA	6.89	129.39	120.44
30	K	126	LEU	CA-C-N	6.89	130.61	120.90
30	K	126	LEU	C-N-CA	6.89	130.61	120.90
9	2	152	TYR	N-CA-C	-6.88	106.08	114.75
12	5	176	ILE	CA-C-O	-6.88	112.75	120.74
28	H	349	ILE	N-CA-C	-6.88	98.47	108.11
9	i	66	ILE	N-CA-C	-6.88	105.05	111.45
20	Z	715	ALA	N-CA-C	6.88	118.78	111.28
20	Z	829	GLN	N-CA-C	6.88	118.78	111.28
12	l	97	ALA	N-CA-C	-6.88	96.84	108.26
23	P	279	ASP	N-CA-C	6.88	119.62	111.71
25	R	361	VAL	O-C-N	-6.88	114.74	121.83
33	J	320	SER	O-C-N	6.88	130.75	121.74
27	O	172	TYR	N-CA-C	-6.88	103.84	111.82
11	4	190	ARG	N-CA-C	-6.88	98.86	109.24
24	Q	107	VAL	N-CA-C	-6.88	102.63	109.02
3	C	19	LEU	CA-C-N	6.87	130.18	120.28
3	C	19	LEU	C-N-CA	6.87	130.18	120.28
24	Q	311	LEU	N-CA-C	-6.87	103.85	111.82
2	b	32	VAL	CB-CA-C	-6.87	100.02	111.29
8	1	185	VAL	N-CA-CB	6.87	120.56	111.90
15	W	36	ILE	CA-C-N	6.87	129.37	120.44
15	W	36	ILE	C-N-CA	6.87	129.37	120.44
29	I	117	HIS	CE1-NE2-CD2	-6.87	102.13	109.00
1	a	149	GLU	N-CA-C	-6.87	104.57	114.12
27	O	162	SER	CB-CA-C	-6.87	102.70	111.70
15	W	163	ASN	CA-CB-CG	6.87	119.47	112.60
15	W	178	PRO	N-CA-CB	6.87	107.83	103.23
22	S	372	LEU	CA-C-N	6.87	129.48	120.28
22	S	372	LEU	C-N-CA	6.87	129.48	120.28
28	H	299	ARG	NE-CZ-NH2	-6.86	113.02	119.20
21	N	495	PRO	CA-C-N	6.86	129.36	120.44
21	N	495	PRO	C-N-CA	6.86	129.36	120.44
31	L	369	LYS	N-CA-C	-6.86	98.51	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	250	VAL	O-C-N	-6.86	114.77	121.83
21	N	716	GLN	N-CA-C	-6.86	100.05	110.14
22	S	255	SER	N-CA-C	-6.86	104.82	112.57
8	h	201	GLU	CA-C-N	6.86	130.03	120.29
8	h	201	GLU	C-N-CA	6.86	130.03	120.29
28	H	404	TRP	CG-CD2-CE3	-6.86	127.04	133.90
31	L	387	ASN	CA-CB-CG	-6.86	105.74	112.60
7	g	116	LEU	N-CA-C	6.86	118.75	111.28
7	G	77	VAL	N-CA-C	-6.86	99.30	108.35
33	J	235	VAL	N-CA-CB	6.86	118.57	110.55
29	I	65	ILE	N-CA-CB	6.85	119.34	110.57
6	F	69	HIS	CG-CD2-NE2	6.85	114.05	107.20
20	Z	421	SER	CA-C-N	6.85	129.84	120.46
20	Z	421	SER	C-N-CA	6.85	129.84	120.46
5	e	90	GLU	O-C-N	6.85	129.38	122.12
14	n	218	TYR	CA-CB-CG	-6.85	101.57	113.90
18	X	126	ILE	CA-C-N	6.85	128.91	120.22
18	X	126	ILE	C-N-CA	6.85	128.91	120.22
21	N	309	ILE	N-CA-C	-6.85	98.57	108.36
31	L	279	PHE	CA-CB-CG	-6.85	106.95	113.80
12	5	104	GLN	N-CA-C	-6.84	103.29	112.94
13	m	130	VAL	CA-CB-CG2	-6.84	98.77	110.40
24	Q	102	GLU	N-CA-C	6.84	118.74	111.28
10	3	163	LEU	CA-C-N	6.84	129.33	120.44
10	3	163	LEU	C-N-CA	6.84	129.33	120.44
21	N	920	VAL	CA-C-N	6.84	129.44	120.28
21	N	920	VAL	C-N-CA	6.84	129.44	120.28
5	e	10	ARG	CD-NE-CZ	-6.84	114.83	124.40
32	M	175	LYS	CA-C-N	6.84	127.25	119.93
32	M	175	LYS	C-N-CA	6.84	127.25	119.93
2	b	45	ILE	N-CA-C	-6.84	98.19	108.17
5	E	12	VAL	CB-CA-C	-6.84	103.17	111.85
19	Y	35	PHE	CA-CB-CG	6.84	120.64	113.80
27	O	124	ASP	CA-CB-CG	6.84	119.44	112.60
10	j	178	ASP	CA-C-N	6.83	129.32	120.44
10	j	178	ASP	C-N-CA	6.83	129.32	120.44
30	K	414	GLN	N-CA-C	-6.83	102.06	111.28
5	e	192	THR	CA-C-N	6.83	129.99	120.29
5	e	192	THR	C-N-CA	6.83	129.99	120.29
5	E	54	ALA	N-CA-CB	6.83	123.80	111.37
17	T	225	ASN	CA-CB-CG	-6.83	105.77	112.60
13	6	84	HIS	ND1-CE1-NE2	6.83	115.23	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	142	VAL	CA-C-N	6.83	129.43	120.28
22	S	142	VAL	C-N-CA	6.83	129.43	120.28
33	J	393	ASN	CA-C-N	6.83	129.43	120.28
33	J	393	ASN	C-N-CA	6.83	129.43	120.28
3	C	129	ARG	CA-C-O	-6.82	113.26	120.70
6	F	185	ASN	CA-C-O	-6.82	113.29	121.00
16	V	245	VAL	CA-C-N	6.82	129.98	120.29
16	V	245	VAL	C-N-CA	6.82	129.98	120.29
20	Z	968	ASP	N-CA-C	-6.82	97.29	108.41
32	M	148	VAL	N-CA-C	-6.82	98.29	108.46
33	J	279	LEU	CA-C-N	6.82	129.73	120.38
33	J	279	LEU	C-N-CA	6.82	129.73	120.38
13	6	84	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
1	A	200	GLU	CB-CG-CD	-6.82	101.00	112.60
25	R	235	LEU	CA-C-N	6.82	129.72	120.44
25	R	235	LEU	C-N-CA	6.82	129.72	120.44
26	U	223	HIS	CA-CB-CG	-6.82	106.98	113.80
21	N	743	PHE	CA-CB-CG	-6.82	106.98	113.80
33	J	331	HIS	ND1-CE1-NE2	6.82	115.22	108.40
2	B	226	GLY	CA-C-O	-6.82	111.22	119.06
31	L	395	ALA	CA-C-N	6.82	129.97	120.29
31	L	395	ALA	C-N-CA	6.82	129.97	120.29
24	Q	17	GLU	N-CA-C	-6.82	104.78	113.23
25	R	254	SER	N-CA-C	6.82	118.36	111.07
13	6	76	PHE	CA-C-N	6.81	129.41	120.28
13	6	76	PHE	C-N-CA	6.81	129.41	120.28
14	7	155	ASN	N-CA-C	-6.81	105.25	113.97
15	W	46	GLU	CA-C-N	6.81	131.49	122.30
15	W	46	GLU	C-N-CA	6.81	131.49	122.30
25	R	98	LEU	CA-C-O	6.81	128.18	120.90
30	K	105	GLN	N-CA-C	-6.81	104.10	112.88
5	e	249	ALA	N-CA-C	6.80	119.71	111.82
7	G	152	GLU	O-C-N	6.80	129.44	121.21
20	Z	158	ALA	CA-C-N	6.80	129.40	120.28
20	Z	158	ALA	C-N-CA	6.80	129.40	120.28
33	J	375	ILE	N-CA-C	6.80	116.95	110.42
22	S	256	LYS	N-CA-C	-6.80	104.88	113.72
5	e	71	ASP	CA-C-O	6.80	125.09	120.19
21	N	282	TYR	CA-C-N	6.80	130.15	120.49
21	N	282	TYR	C-N-CA	6.80	130.15	120.49
23	P	15	GLN	CA-C-N	6.80	129.78	120.46
23	P	15	GLN	C-N-CA	6.80	129.78	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	394	LYS	CA-C-N	6.80	130.65	120.31
28	H	394	LYS	C-N-CA	6.80	130.65	120.31
12	l	215	LEU	CA-C-O	-6.80	113.21	120.42
20	Z	75	ILE	CA-C-O	-6.80	114.20	121.27
12	l	210	PHE	CA-C-N	6.80	129.39	120.28
12	l	210	PHE	C-N-CA	6.80	129.39	120.28
8	1	45	ARG	NE-CZ-NH1	-6.80	114.70	121.50
26	U	100	ARG	N-CA-C	-6.80	100.16	109.95
26	U	179	ARG	CA-C-N	6.80	129.72	120.54
26	U	179	ARG	C-N-CA	6.80	129.72	120.54
32	M	176	PRO	O-C-N	6.80	131.14	122.85
4	d	205	THR	CA-C-O	6.80	127.92	120.71
13	6	151	ALA	N-CA-C	6.80	119.53	111.71
20	Z	52	LEU	O-C-N	-6.80	115.07	122.07
20	Z	53	VAL	CA-C-N	6.80	129.39	120.28
20	Z	53	VAL	C-N-CA	6.80	129.39	120.28
14	n	173	PRO	N-CA-C	-6.79	104.73	114.18
3	c	56	LEU	CB-CA-C	-6.79	99.24	110.72
10	j	173	ASN	CA-C-O	6.79	127.08	119.41
7	G	11	SER	N-CA-C	-6.79	98.75	109.07
20	Z	153	TYR	N-CA-C	-6.79	103.67	112.23
24	Q	77	PHE	N-CA-C	6.79	118.68	111.28
24	Q	272	LEU	N-CA-C	-6.79	104.47	112.89
29	I	340	ARG	O-C-N	-6.79	113.51	121.32
30	K	64	GLN	N-CA-CB	6.79	120.10	110.12
22	S	98	SER	N-CA-CB	6.79	120.08	109.83
3	C	165	VAL	N-CA-C	-6.79	95.23	109.34
4	D	229	ILE	CA-C-N	6.79	130.62	120.31
4	D	229	ILE	C-N-CA	6.79	130.62	120.31
21	N	185	ILE	CB-CG1-CD1	6.79	128.05	113.80
20	Z	593	HIS	CE1-NE2-CD2	-6.78	102.22	109.00
21	N	127	ASP	CA-C-N	6.78	129.24	120.56
21	N	127	ASP	C-N-CA	6.78	129.24	120.56
27	O	385	GLU	CA-C-N	6.78	129.36	120.28
27	O	385	GLU	C-N-CA	6.78	129.36	120.28
10	3	183	TRP	CA-C-N	6.78	134.69	121.41
10	3	183	TRP	C-N-CA	6.78	134.69	121.41
6	f	218	LYS	N-CA-C	-6.78	104.70	114.12
17	T	24	GLU	N-CA-CB	6.78	120.78	110.28
29	I	412	THR	CA-C-N	6.78	129.36	120.28
29	I	412	THR	C-N-CA	6.78	129.36	120.28
3	C	53	THR	N-CA-CB	6.77	121.94	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	252	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
26	U	294	ASN	CA-CB-CG	-6.77	105.83	112.60
3	c	187	ASP	CA-CB-CG	-6.77	105.83	112.60
14	n	115	ASP	CA-CB-CG	-6.77	105.83	112.60
3	C	191	GLU	CA-C-O	6.77	127.72	120.55
4	D	210	ILE	N-CA-CB	6.77	120.75	111.41
25	R	366	ASN	CA-CB-CG	-6.77	105.83	112.60
29	I	262	ARG	CA-C-N	6.77	129.90	120.29
29	I	262	ARG	C-N-CA	6.77	129.90	120.29
6	f	19	LEU	N-CA-C	-6.76	98.81	109.50
7	G	161	LYS	N-CA-C	-6.76	104.50	112.89
3	C	9	ARG	CA-C-N	6.76	130.02	120.28
3	C	9	ARG	C-N-CA	6.76	130.02	120.28
21	N	525	ASN	CA-CB-CG	-6.76	105.84	112.60
23	P	315	GLN	CA-C-N	6.76	129.23	120.44
23	P	315	GLN	C-N-CA	6.76	129.23	120.44
30	K	88	ARG	N-CA-C	6.76	119.51	111.33
1	A	172	GLY	CA-C-N	6.76	126.36	119.19
1	A	172	GLY	C-N-CA	6.76	126.36	119.19
23	P	6	PRO	N-CA-CB	6.76	110.35	103.25
25	R	236	ALA	O-C-N	6.76	129.39	122.09
27	O	290	LYS	CA-C-N	6.76	129.72	120.46
27	O	290	LYS	C-N-CA	6.76	129.72	120.46
13	6	151	ALA	CA-C-N	6.76	129.23	120.44
13	6	151	ALA	C-N-CA	6.76	129.23	120.44
17	T	130	ASP	CA-CB-CG	6.76	119.36	112.60
22	S	111	ARG	NE-CZ-NH2	-6.76	113.12	119.20
24	Q	420	ASN	N-CA-CB	6.76	120.06	110.12
30	K	142	HIS	ND1-CE1-NE2	6.76	115.16	108.40
4	D	208	LYS	N-CA-C	-6.76	105.07	113.38
20	Z	224	LEU	O-C-N	-6.76	114.96	122.12
20	Z	844	ALA	CA-C-N	6.76	129.64	120.38
20	Z	844	ALA	C-N-CA	6.76	129.64	120.38
21	N	710	GLY	N-CA-C	-6.76	104.93	115.67
24	Q	377	LEU	N-CA-CB	6.75	120.75	110.28
9	i	211	LYS	CA-C-O	-6.75	113.21	121.11
14	n	180	GLY	N-CA-C	-6.75	105.99	114.16
11	4	181	VAL	N-CA-C	-6.75	97.89	107.75
15	W	18	ASN	CA-CB-CG	-6.75	105.85	112.60
22	S	38	LEU	CA-C-N	6.75	129.88	120.29
22	S	38	LEU	C-N-CA	6.75	129.88	120.29
24	Q	19	GLN	CB-CG-CD	-6.75	101.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	269	LYS	CA-C-N	6.75	130.01	120.42
29	I	269	LYS	C-N-CA	6.75	130.01	120.42
13	6	50	LYS	CB-CA-C	-6.75	96.99	110.42
18	X	100	TRP	N-CA-CB	6.75	121.10	110.84
20	Z	781	GLY	N-CA-C	6.75	120.83	112.73
1	a	111	ASP	CA-CB-CG	-6.75	105.85	112.60
4	d	131	VAL	N-CA-C	-6.75	98.46	108.45
19	Y	80	GLU	CA-C-N	6.75	129.88	120.29
19	Y	80	GLU	C-N-CA	6.75	129.88	120.29
20	Z	837	TYR	CA-C-N	6.75	129.32	120.28
20	Z	837	TYR	C-N-CA	6.75	129.32	120.28
28	H	429	PHE	CB-CG-CD1	6.75	132.17	120.70
29	I	68	HIS	ND1-CE1-NE2	6.75	115.15	108.40
29	I	424	MET	CA-C-N	6.75	134.61	122.06
29	I	424	MET	C-N-CA	6.75	134.61	122.06
14	n	49	TYR	N-CA-C	-6.75	99.35	108.86
20	Z	396	ASN	CA-CB-CG	-6.75	105.85	112.60
25	R	311	THR	N-CA-CB	6.75	119.80	110.01
22	S	196	ARG	NE-CZ-NH2	-6.75	113.13	119.20
14	n	228	PHE	CA-C-O	-6.75	114.01	121.23
10	3	87	PHE	CA-C-N	6.75	129.21	120.44
10	3	87	PHE	C-N-CA	6.75	129.21	120.44
22	S	360	PHE	CA-CB-CG	-6.75	107.06	113.80
1	a	202	VAL	CA-C-N	6.74	129.70	120.46
1	a	202	VAL	C-N-CA	6.74	129.70	120.46
13	m	118	ILE	CA-C-O	6.74	127.51	120.36
2	B	205	ASN	N-CA-C	-6.74	98.11	108.76
11	4	151	ASP	N-CA-C	-6.74	99.09	109.14
15	W	141	ILE	N-CA-C	-6.74	98.67	108.11
10	j	43	ILE	N-CA-CB	6.74	118.07	110.72
20	Z	587	THR	O-C-N	6.74	129.01	122.07
29	I	197	SER	N-CA-C	6.74	119.97	111.69
30	K	400	TYR	N-CA-C	-6.74	103.78	113.21
32	M	345	ARG	N-CA-C	-6.74	97.92	108.90
9	i	170	HIS	CG-CD2-NE2	6.73	113.93	107.20
3	C	96	GLN	CB-CG-CD	6.73	124.05	112.60
9	2	74	GLY	CA-C-O	6.73	127.17	121.11
26	U	43	SER	CA-C-N	6.73	129.19	120.44
26	U	43	SER	C-N-CA	6.73	129.19	120.44
3	c	109	GLU	N-CA-CB	6.73	120.01	110.12
10	3	99	ARG	CB-CA-C	-6.73	97.71	109.02
23	P	30	ASN	CB-CA-C	-6.73	100.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	157	PHE	CA-C-O	-6.73	113.60	119.72
12	5	272	PHE	CA-C-N	6.73	129.84	120.29
12	5	272	PHE	C-N-CA	6.73	129.84	120.29
20	Z	801	HIS	CB-CG-ND1	6.73	132.79	122.70
21	N	428	VAL	CA-C-N	6.73	129.19	120.44
21	N	428	VAL	C-N-CA	6.73	129.19	120.44
33	J	252	SER	N-CA-C	-6.73	104.95	113.02
4	d	78	LEU	N-CA-CB	6.73	119.87	109.85
7	G	98	SER	CA-C-N	6.72	129.18	120.44
7	G	98	SER	C-N-CA	6.72	129.18	120.44
7	g	114	ASP	CA-C-N	6.72	129.84	120.29
7	g	114	ASP	C-N-CA	6.72	129.84	120.29
3	C	91	ALA	N-CA-C	6.72	118.69	111.36
17	T	8	THR	N-CA-C	-6.72	104.70	113.17
20	Z	718	ASP	N-CA-C	-6.72	103.88	111.07
26	U	198	LYS	N-CA-CB	6.72	120.65	110.30
5	e	195	GLU	CA-C-N	6.72	129.18	120.44
5	e	195	GLU	C-N-CA	6.72	129.18	120.44
17	T	237	ASN	CA-CB-CG	-6.72	105.88	112.60
23	P	207	THR	N-CA-CB	6.72	121.01	110.46
26	U	231	ASP	CA-C-N	6.72	129.27	120.60
26	U	231	ASP	C-N-CA	6.72	129.27	120.60
33	J	324	ARG	CA-C-N	6.72	129.28	120.28
33	J	324	ARG	C-N-CA	6.72	129.28	120.28
20	Z	542	ILE	O-C-N	6.72	129.93	122.61
22	S	480	ARG	NE-CZ-NH2	6.72	125.25	119.20
2	B	232	GLY	CA-C-O	-6.71	115.95	122.46
21	N	230	VAL	CA-C-N	6.71	129.17	120.44
21	N	230	VAL	C-N-CA	6.71	129.17	120.44
22	S	361	THR	O-C-N	6.71	128.99	122.07
29	I	203	THR	N-CA-C	6.71	118.60	111.28
30	K	244	HIS	ND1-CE1-NE2	6.71	115.11	108.40
28	H	52	THR	CA-C-N	6.71	129.28	120.28
28	H	52	THR	C-N-CA	6.71	129.28	120.28
2	b	114	VAL	N-CA-CB	6.71	119.67	110.54
21	N	650	ASP	N-CA-C	6.71	118.25	111.07
23	P	134	VAL	CA-C-N	6.71	130.51	120.31
23	P	134	VAL	C-N-CA	6.71	130.51	120.31
26	U	199	GLY	CA-C-N	6.71	129.27	120.28
26	U	199	GLY	C-N-CA	6.71	129.27	120.28
31	L	251	ILE	CB-CA-C	6.71	117.87	110.62
9	2	194	ASN	CA-CB-CG	-6.71	105.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	198	GLU	O-C-N	6.71	128.98	122.07
30	K	114	THR	O-C-N	-6.71	113.34	122.33
1	A	113	PRO	CA-C-N	6.71	129.57	120.38
1	A	113	PRO	C-N-CA	6.71	129.57	120.38
25	R	354	ALA	CA-C-N	6.71	129.27	120.28
25	R	354	ALA	C-N-CA	6.71	129.27	120.28
31	L	114	GLU	N-CA-C	-6.71	105.10	113.28
21	N	275	THR	CA-C-N	6.71	129.26	120.28
21	N	275	THR	C-N-CA	6.71	129.26	120.28
21	N	536	ILE	CA-C-N	6.71	129.16	120.44
21	N	536	ILE	C-N-CA	6.71	129.16	120.44
4	D	70	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
27	O	373	TRP	CB-CG-CD2	-6.70	117.42	126.80
3	C	181	LYS	N-CA-C	-6.70	97.67	109.06
6	f	212	SER	N-CA-C	-6.70	97.14	108.26
14	n	185	ASN	CA-C-O	-6.70	110.98	120.16
32	M	93	ASP	N-CA-C	-6.70	96.53	110.80
13	m	96	SER	CA-C-N	6.70	129.25	120.28
13	m	96	SER	C-N-CA	6.70	129.25	120.28
15	W	170	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
30	K	240	SER	N-CA-C	-6.70	104.58	112.89
6	f	43	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
2	b	137	ALA	CA-C-O	6.70	127.93	120.70
16	V	253	LYS	CA-C-N	6.70	129.14	120.44
16	V	253	LYS	C-N-CA	6.70	129.14	120.44
27	O	321	LYS	N-CA-C	-6.69	104.37	112.54
28	H	261	ARG	CA-C-O	-6.69	112.53	120.10
8	h	186	VAL	N-CA-C	-6.69	98.09	107.80
21	N	896	PHE	CA-C-O	6.69	128.55	121.19
8	1	70	TYR	N-CA-C	-6.69	104.07	111.36
1	a	15	HIS	ND1-CE1-NE2	6.69	115.09	108.40
13	m	16	ASN	CA-CB-CG	6.69	119.29	112.60
20	Z	415	MET	CA-C-N	6.69	129.13	120.44
20	Z	415	MET	C-N-CA	6.69	129.13	120.44
9	i	67	SER	N-CA-C	-6.69	100.45	108.14
21	N	910	PRO	CA-C-N	6.68	129.78	120.29
21	N	910	PRO	C-N-CA	6.68	129.78	120.29
7	g	73	HIS	CE1-NE2-CD2	-6.68	102.32	109.00
22	S	263	ASP	CA-C-N	6.68	129.59	122.11
22	S	263	ASP	C-N-CA	6.68	129.59	122.11
1	a	235	THR	CA-C-O	-6.68	113.10	120.38
2	B	9	LEU	N-CA-C	-6.68	104.26	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	247	GLY	N-CA-C	-6.68	101.56	110.58
16	V	297	THR	CA-C-N	6.68	129.23	120.28
16	V	297	THR	C-N-CA	6.68	129.23	120.28
27	O	100	ASP	CA-C-N	6.68	129.23	120.28
27	O	100	ASP	C-N-CA	6.68	129.23	120.28
31	L	100	SER	O-C-N	6.68	129.30	122.09
21	N	370	SER	N-CA-C	6.68	119.39	111.71
21	N	663	ILE	O-C-N	6.68	128.71	121.83
27	O	246	SER	N-CA-CB	6.68	119.69	110.01
10	j	3	ASP	CA-CB-CG	-6.67	105.93	112.60
17	T	115	SER	N-CA-C	6.67	119.39	111.71
23	P	30	ASN	OD1-CG-ND2	6.67	129.28	122.60
28	H	188	PRO	CA-C-N	6.67	127.04	119.83
28	H	188	PRO	C-N-CA	6.67	127.04	119.83
10	j	67	PHE	CA-CB-CG	-6.67	107.13	113.80
9	2	181	ILE	N-CA-C	-6.67	104.26	110.53
12	5	223	LEU	N-CA-C	-6.67	99.18	109.52
23	P	246	GLN	N-CA-C	6.67	120.68	112.54
32	M	377	GLN	CA-C-N	6.67	130.45	120.31
32	M	377	GLN	C-N-CA	6.67	130.45	120.31
14	n	95	HIS	CE1-NE2-CD2	-6.67	102.33	109.00
21	N	417	ARG	NH1-CZ-NH2	6.67	127.97	119.30
5	e	147	HIS	ND1-CE1-NE2	6.66	115.06	108.40
14	n	173	PRO	O-C-N	6.66	131.64	122.38
2	B	205	ASN	N-CA-CB	6.66	123.05	111.39
4	D	113	VAL	CA-CB-CG1	6.66	121.73	110.40
21	N	444	HIS	CG-CD2-NE2	6.66	113.86	107.20
27	O	169	ASN	N-CA-C	-6.66	103.94	111.14
30	K	67	TYR	N-CA-C	-6.66	104.10	111.36
30	K	201	ILE	N-CA-C	-6.66	104.27	110.53
14	n	139	LYS	CA-CB-CG	6.66	127.42	114.10
6	F	123	TYR	N-CA-C	-6.66	98.38	109.24
20	Z	250	VAL	CA-C-N	6.66	129.21	120.28
20	Z	250	VAL	C-N-CA	6.66	129.21	120.28
8	1	40	THR	N-CA-C	-6.66	96.61	110.80
21	N	531	LEU	N-CA-C	-6.66	104.38	113.30
28	H	232	PRO	CA-C-N	6.66	129.75	120.29
28	H	232	PRO	C-N-CA	6.66	129.75	120.29
1	a	41	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	a	100	GLU	CA-C-O	-6.66	113.36	120.42
4	d	43	VAL	N-CA-C	-6.66	98.85	108.17
5	E	177	GLU	CA-C-N	-6.66	111.95	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	177	GLU	C-N-CA	-6.66	111.95	120.34
12	5	84	GLN	CA-C-N	6.66	128.68	120.22
12	5	84	GLN	C-N-CA	6.66	128.68	120.22
22	S	142	VAL	O-C-N	-6.66	115.39	121.91
6	F	85	SER	N-CA-CB	6.66	120.01	110.16
8	1	166	HIS	CB-CA-C	-6.66	100.43	110.88
20	Z	718	ASP	CA-C-N	6.66	127.51	119.99
20	Z	718	ASP	C-N-CA	6.66	127.51	119.99
33	J	183	LYS	N-CA-C	-6.66	105.19	113.38
29	I	150	HIS	CA-CB-CG	-6.65	107.15	113.80
30	K	230	THR	N-CA-C	-6.65	103.95	111.14
5	E	23	GLN	CA-C-N	6.65	129.87	120.42
5	E	23	GLN	C-N-CA	6.65	129.87	120.42
9	2	54	ILE	CA-CB-CG1	6.65	121.71	110.40
21	N	543	ASP	N-CA-CB	6.65	120.82	110.44
3	C	44	ILE	N-CA-C	-6.65	98.80	108.11
21	N	548	ARG	N-CA-CB	6.65	120.54	110.30
24	Q	9	GLU	CB-CG-CD	-6.65	101.30	112.60
24	Q	416	VAL	CA-C-O	-6.65	113.80	120.85
13	m	103	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
22	S	103	SER	CA-C-O	-6.65	112.10	119.08
28	H	386	ALA	N-CA-CB	6.65	119.89	110.12
7	G	229	LYS	N-CA-C	-6.64	98.97	109.07
32	M	223	PRO	CA-C-N	6.64	126.61	120.03
32	M	223	PRO	C-N-CA	6.64	126.61	120.03
2	B	146	SER	CA-C-N	6.64	133.61	121.85
2	B	146	SER	C-N-CA	6.64	133.61	121.85
10	3	155	GLU	CA-C-O	-6.64	113.17	119.55
15	W	173	THR	CA-C-N	6.64	132.65	122.68
15	W	173	THR	C-N-CA	6.64	132.65	122.68
21	N	210	SER	CA-C-N	6.64	129.18	120.28
21	N	210	SER	C-N-CA	6.64	129.18	120.28
27	O	30	GLU	CA-C-N	6.64	129.07	120.44
27	O	30	GLU	C-N-CA	6.64	129.07	120.44
33	J	395	GLU	CA-C-N	6.64	129.18	120.28
33	J	395	GLU	C-N-CA	6.64	129.18	120.28
24	Q	407	ALA	CA-C-N	6.64	129.18	120.28
24	Q	407	ALA	C-N-CA	6.64	129.18	120.28
9	i	64	HIS	CA-C-O	6.64	128.17	120.80
12	l	233	LYS	O-C-N	6.64	129.72	122.15
12	l	278	GLU	CA-C-O	6.64	127.46	120.42
20	Z	771	HIS	CE1-NE2-CD2	-6.64	102.36	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	232	GLU	N-CA-C	-6.64	105.22	113.38
30	K	320	ARG	NE-CZ-NH2	6.64	125.17	119.20
32	M	173	ASP	CA-C-N	6.64	130.18	120.82
32	M	173	ASP	C-N-CA	6.64	130.18	120.82
13	m	155	MET	N-CA-CB	6.63	120.72	110.43
8	1	94	LEU	CA-C-O	-6.63	113.87	120.70
20	Z	361	HIS	CA-CB-CG	-6.63	107.17	113.80
21	N	439	VAL	CA-C-N	6.63	129.47	120.38
21	N	439	VAL	C-N-CA	6.63	129.47	120.38
23	P	369	LEU	O-C-N	6.63	130.63	122.34
28	H	152	ILE	CB-CA-C	6.63	122.17	111.29
28	H	436	LYS	N-CA-C	-6.63	104.32	112.88
3	c	229	ILE	N-CA-C	-6.63	100.14	108.89
5	e	73	HIS	ND1-CE1-NE2	6.63	115.03	108.40
23	P	59	LEU	CA-C-O	6.63	127.59	120.10
31	L	429	GLU	N-CA-C	-6.63	104.81	113.17
2	B	233	PRO	CA-C-O	-6.63	114.14	121.23
27	O	23	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
29	I	68	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
3	C	123	THR	CA-C-N	6.63	129.70	120.29
3	C	123	THR	C-N-CA	6.63	129.70	120.29
20	Z	108	ASP	CA-C-N	6.63	126.41	119.05
20	Z	108	ASP	C-N-CA	6.63	126.41	119.05
13	m	30	VAL	N-CA-C	-6.62	98.02	108.95
21	N	704	GLY	CA-C-N	6.62	129.83	120.42
21	N	704	GLY	C-N-CA	6.62	129.83	120.42
4	D	44	LEU	N-CA-C	-6.62	96.23	108.02
20	Z	781	GLY	O-C-N	-6.62	115.83	122.19
25	R	300	ASP	CA-CB-CG	-6.62	105.98	112.60
28	H	424	THR	CA-C-N	6.62	129.15	120.28
28	H	424	THR	C-N-CA	6.62	129.15	120.28
1	a	214	LEU	N-CA-CB	6.62	120.50	110.30
4	d	98	LEU	CA-C-O	6.62	127.52	120.70
21	N	398	ARG	CA-C-N	6.62	129.15	120.28
21	N	398	ARG	C-N-CA	6.62	129.15	120.28
27	O	182	LYS	CA-C-N	6.62	132.02	122.35
27	O	182	LYS	C-N-CA	6.62	132.02	122.35
29	I	431	ASN	CA-CB-CG	-6.62	105.98	112.60
28	H	133	SER	N-CA-C	-6.62	102.42	111.56
11	k	116	LEU	N-CA-C	-6.62	98.41	109.07
14	n	111	ASN	CA-CB-CG	6.62	119.22	112.60
25	R	112	GLU	CA-C-O	-6.62	113.41	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	236	ALA	CA-C-O	-6.62	113.89	120.70
12	l	105	THR	CA-C-O	6.62	127.47	120.33
10	3	36	VAL	O-C-N	-6.62	114.30	122.57
24	Q	92	LYS	N-CA-C	-6.62	104.78	112.92
6	F	67	ASP	CA-CB-CG	6.61	119.21	112.60
21	N	885	ILE	N-CA-C	-6.61	98.82	108.87
24	Q	361	HIS	ND1-CE1-NE2	6.61	115.01	108.40
5	e	26	TYR	CA-C-N	6.61	131.76	120.72
5	e	26	TYR	C-N-CA	6.61	131.76	120.72
14	7	141	ASN	CA-C-O	-6.61	115.13	121.34
24	Q	361	HIS	CE1-NE2-CD2	-6.61	102.39	109.00
8	h	123	PRO	CA-C-N	6.61	129.03	120.44
8	h	123	PRO	C-N-CA	6.61	129.03	120.44
20	Z	257	PRO	CB-CA-C	6.61	118.98	110.92
23	P	400	VAL	CB-CA-C	6.61	119.34	110.42
32	M	79	VAL	N-CA-C	-6.61	98.95	108.53
20	Z	492	GLY	CA-C-N	6.61	129.13	120.28
20	Z	492	GLY	C-N-CA	6.61	129.13	120.28
33	J	13	GLU	N-CA-CB	6.61	120.39	110.22
14	n	170	TYR	CA-C-N	6.60	132.11	123.00
14	n	170	TYR	C-N-CA	6.60	132.11	123.00
24	Q	120	LYS	N-CA-C	-6.60	104.01	111.14
8	h	79	TYR	N-CA-C	-6.60	103.83	112.41
23	P	19	GLU	N-CA-C	-6.60	105.26	113.38
21	N	224	THR	CA-C-N	6.60	129.12	120.28
21	N	224	THR	C-N-CA	6.60	129.12	120.28
24	Q	13	ARG	O-C-N	6.60	129.12	122.12
24	Q	256	GLU	CA-C-O	6.60	127.55	120.55
28	H	224	VAL	CA-C-O	-6.60	113.73	121.05
4	d	234	THR	N-CA-C	6.59	118.47	111.28
15	W	24	THR	N-CA-C	-6.59	99.39	109.41
9	i	119	TYR	CB-CA-C	-6.59	99.08	110.09
11	k	17	SER	CA-C-O	-6.59	112.43	120.54
21	N	232	LEU	N-CA-CB	6.59	120.45	110.30
29	I	418	GLN	N-CA-C	6.59	118.47	111.28
25	R	164	THR	N-CA-C	-6.59	104.18	111.36
1	a	186	PHE	CA-C-N	6.59	129.40	120.44
1	a	186	PHE	C-N-CA	6.59	129.40	120.44
7	g	222	SER	CA-C-O	-6.59	112.30	119.08
2	B	128	ARG	CA-C-O	-6.59	114.66	120.19
5	E	92	ALA	CA-C-N	6.59	129.00	120.44
5	E	92	ALA	C-N-CA	6.59	129.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	223	GLY	CA-C-N	6.59	129.55	120.39
29	I	223	GLY	C-N-CA	6.59	129.55	120.39
30	K	63	LEU	CA-C-N	6.59	129.10	120.28
30	K	63	LEU	C-N-CA	6.59	129.10	120.28
10	3	190	ILE	N-CA-C	-6.58	98.89	108.11
12	5	134	LEU	N-CA-C	-6.58	104.18	111.36
25	R	363	PHE	N-CA-C	-6.58	104.18	111.36
30	K	88	ARG	CA-C-N	6.58	129.48	120.46
30	K	88	ARG	C-N-CA	6.58	129.48	120.46
22	S	172	ASN	CA-CB-CG	6.58	119.18	112.60
22	S	470	GLN	O-C-N	-6.58	114.65	122.15
1	A	186	PHE	CA-CB-CG	-6.58	107.22	113.80
2	b	103	GLU	N-CA-C	-6.58	99.07	109.07
1	A	96	ARG	NE-CZ-NH2	-6.58	113.28	119.20
28	H	111	GLU	O-C-N	6.58	129.65	122.15
2	b	30	GLN	OE1-CD-NE2	6.58	129.18	122.60
6	F	110	HIS	CG-CD2-NE2	6.58	113.78	107.20
8	1	112	ASP	CA-C-N	6.58	133.13	122.67
8	1	112	ASP	C-N-CA	6.58	133.13	122.67
20	Z	377	ALA	CA-C-N	6.58	131.12	120.60
20	Z	377	ALA	C-N-CA	6.58	131.12	120.60
12	l	159	SER	CA-C-N	6.57	129.38	120.44
12	l	159	SER	C-N-CA	6.57	129.38	120.44
3	C	225	VAL	O-C-N	6.57	130.22	122.66
28	H	215	LYS	CA-C-N	6.57	129.09	120.28
28	H	215	LYS	C-N-CA	6.57	129.09	120.28
16	V	173	THR	N-CA-C	-6.57	104.89	113.17
20	Z	611	THR	O-C-N	6.57	130.98	121.78
10	j	134	LYS	CA-C-O	6.57	126.34	119.51
4	d	229	ILE	O-C-N	6.57	129.22	121.80
12	5	141	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
21	N	76	GLU	N-CA-C	6.57	118.44	111.28
24	Q	67	THR	CA-C-N	6.57	133.52	121.70
24	Q	67	THR	C-N-CA	6.57	133.52	121.70
13	m	189	ILE	CA-C-O	-6.57	114.27	121.29
1	A	194	ILE	O-C-N	-6.57	115.45	122.61
7	G	85	GLY	N-CA-C	-6.57	104.57	113.37
15	W	112	ALA	CA-C-O	6.57	127.54	120.32
22	S	137	PHE	CA-CB-CG	6.57	120.36	113.80
6	f	36	VAL	CA-C-O	6.56	127.28	120.39
7	g	247	ILE	N-CA-CB	6.56	120.43	110.58
19	Y	60	TRP	CA-C-N	6.56	130.03	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	60	TRP	C-N-CA	6.56	130.03	120.71
20	Z	221	VAL	N-CA-CB	6.56	119.47	110.54
29	I	382	THR	CA-C-N	6.56	129.07	120.28
29	I	382	THR	C-N-CA	6.56	129.07	120.28
1	a	184	ASN	N-CA-CB	6.56	119.76	110.12
25	R	272	ASP	N-CA-CB	6.56	120.85	110.55
27	O	124	ASP	CA-C-N	6.56	128.55	120.22
27	O	124	ASP	C-N-CA	6.56	128.55	120.22
30	K	396	ARG	N-CA-C	6.56	118.43	111.28
20	Z	326	VAL	O-C-N	6.56	128.72	121.90
30	K	291	GLU	N-CA-C	6.56	119.27	111.33
20	Z	311	ALA	N-CA-C	6.56	118.43	111.28
29	I	252	LEU	CA-C-O	6.56	126.26	119.05
2	b	94	HIS	CA-CB-CG	-6.55	107.25	113.80
14	n	115	ASP	N-CA-C	-6.55	103.53	113.89
3	C	244	ILE	N-CA-C	6.55	116.69	110.53
10	3	173	ASN	CA-C-N	6.55	129.60	120.29
10	3	173	ASN	C-N-CA	6.55	129.60	120.29
32	M	410	VAL	CB-CA-C	6.55	120.54	111.49
5	E	182	GLU	CA-C-N	6.55	131.66	120.72
5	E	182	GLU	C-N-CA	6.55	131.66	120.72
4	d	160	SER	CB-CA-C	-6.55	100.59	110.88
20	Z	104	ASP	CA-CB-CG	6.55	119.15	112.60
16	V	23	THR	CA-C-O	6.55	127.31	120.30
22	S	68	LEU	N-CA-C	6.55	120.28	111.24
31	L	382	MET	O-C-N	-6.55	115.18	122.12
14	n	125	ILE	CA-C-O	-6.55	114.14	120.95
31	L	144	VAL	N-CA-CB	6.55	117.86	110.72
2	b	171	ALA	CA-C-O	-6.54	113.61	120.55
21	N	367	ALA	CA-C-N	6.54	129.34	120.44
21	N	367	ALA	C-N-CA	6.54	129.34	120.44
32	M	239	THR	CA-CB-OG1	6.54	119.42	109.60
3	c	102	TYR	N-CA-C	-6.54	105.22	113.72
3	c	221	ASN	O-C-N	6.54	131.29	122.59
10	j	193	ASP	N-CA-C	-6.54	104.70	114.64
2	B	190	HIS	ND1-CE1-NE2	6.54	114.94	108.40
21	N	247	GLU	CA-C-O	-6.54	113.62	120.55
29	I	85	PHE	CA-CB-CG	6.54	120.34	113.80
21	N	566	SER	CA-C-O	6.54	127.48	120.55
13	m	159	ASP	CA-C-N	6.54	129.04	120.28
13	m	159	ASP	C-N-CA	6.54	129.04	120.28
1	A	67	THR	CA-CB-OG1	6.54	119.41	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	264	GLY	CA-C-N	6.54	129.69	120.28
33	J	264	GLY	C-N-CA	6.54	129.69	120.28
16	V	184	ASN	CA-CB-CG	6.54	119.14	112.60
21	N	77	SER	CA-C-N	6.54	129.36	120.54
21	N	77	SER	C-N-CA	6.54	129.36	120.54
6	f	130	VAL	CA-C-N	6.53	128.70	122.36
6	f	130	VAL	C-N-CA	6.53	128.70	122.36
20	Z	735	GLU	CA-C-N	6.53	129.03	120.28
20	Z	735	GLU	C-N-CA	6.53	129.03	120.28
24	Q	309	ARG	NE-CZ-NH2	-6.53	113.32	119.20
29	I	268	PHE	N-CA-C	-6.53	104.00	112.23
20	Z	111	LEU	CA-C-N	6.53	129.03	120.28
20	Z	111	LEU	C-N-CA	6.53	129.03	120.28
32	M	271	LYS	N-CA-C	6.53	118.40	111.28
7	G	126	TYR	N-CA-C	-6.53	99.91	109.18
14	7	191	VAL	CA-C-O	-6.53	114.31	121.29
7	g	10	LEU	N-CA-C	-6.53	104.80	112.89
8	h	83	SER	CA-C-N	6.53	129.03	120.28
8	h	83	SER	C-N-CA	6.53	129.03	120.28
8	h	186	VAL	N-CA-CB	-6.53	103.24	111.46
8	1	80	GLY	CA-C-N	6.53	129.46	120.39
8	1	80	GLY	C-N-CA	6.53	129.46	120.39
28	H	74	THR	N-CA-C	-6.53	104.50	114.16
29	I	104	LEU	CA-C-O	6.53	127.41	120.36
33	J	61	GLU	CA-C-N	6.53	129.03	120.28
33	J	61	GLU	C-N-CA	6.53	129.03	120.28
33	J	97	ASP	CA-C-O	6.53	128.47	121.55
22	S	112	ASN	N-CA-C	-6.52	99.41	109.52
23	P	108	LYS	CA-C-N	6.52	129.31	120.44
23	P	108	LYS	C-N-CA	6.52	129.31	120.44
16	V	243	SER	N-CA-CB	6.52	119.71	110.12
21	N	555	ILE	N-CA-CB	6.52	119.41	110.54
23	P	284	ILE	N-CA-C	-6.52	104.13	110.72
13	6	69	GLY	CA-C-O	-6.52	113.75	120.66
16	V	173	THR	N-CA-CB	6.52	120.14	110.49
21	N	90	ASP	CA-CB-CG	-6.52	106.08	112.60
10	j	126	LEU	CA-C-O	-6.52	113.93	120.90
5	E	189	SER	CA-C-N	6.52	132.41	122.37
5	E	189	SER	C-N-CA	6.52	132.41	122.37
10	3	173	ASN	CA-C-O	6.52	127.41	120.70
20	Z	48	ASP	CA-C-O	-6.52	113.64	120.55
22	S	399	TYR	CB-CA-C	-6.52	97.90	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	31	GLN	O-C-N	6.52	129.58	122.15
20	Z	904	LEU	N-CA-C	-6.51	103.39	112.12
5	E	35	SER	CA-C-N	6.51	131.01	121.31
5	E	35	SER	C-N-CA	6.51	131.01	121.31
24	Q	334	HIS	CE1-NE2-CD2	-6.51	102.49	109.00
26	U	110	PHE	CA-CB-CG	-6.51	107.29	113.80
27	O	23	HIS	ND1-CE1-NE2	6.51	114.91	108.40
29	I	132	ILE	N-CA-C	-6.51	98.36	107.80
31	L	286	ILE	O-C-N	-6.51	114.43	122.57
4	d	231	GLN	OE1-CD-NE2	6.51	129.11	122.60
3	C	97	ASN	N-CA-CB	6.51	119.80	110.16
22	S	399	TYR	CB-CG-CD2	-6.51	111.04	120.80
23	P	278	ASN	CB-CA-C	-6.51	100.66	110.88
27	O	46	THR	CA-C-N	6.51	129.33	120.54
27	O	46	THR	C-N-CA	6.51	129.33	120.54
1	A	97	ALA	N-CA-C	6.51	118.45	111.36
15	W	20	ASP	N-CA-C	-6.51	106.30	114.56
16	V	245	VAL	CB-CA-C	-6.51	103.50	112.02
20	Z	159	LEU	CA-C-N	6.51	129.29	120.44
20	Z	159	LEU	C-N-CA	6.51	129.29	120.44
30	K	260	LEU	CA-C-N	6.51	129.00	120.28
30	K	260	LEU	C-N-CA	6.51	129.00	120.28
2	b	232	GLY	CA-C-N	6.50	127.97	119.84
2	b	232	GLY	C-N-CA	6.50	127.97	119.84
22	S	269	GLU	CB-CA-C	-6.50	99.79	110.85
22	S	472	HIS	CG-CD2-NE2	6.50	113.70	107.20
24	Q	210	CYS	N-CA-C	-6.50	101.65	110.36
31	L	59	GLN	CA-C-N	6.50	130.19	120.31
31	L	59	GLN	C-N-CA	6.50	130.19	120.31
17	T	35	ILE	CA-CB-CG2	6.50	121.55	110.50
5	e	236	THR	N-CA-C	-6.50	104.28	111.36
11	k	32	ASP	CA-CB-CG	-6.50	106.10	112.60
1	A	243	GLU	N-CA-CB	6.50	119.67	110.12
20	Z	239	GLU	CA-C-N	6.50	128.99	120.28
20	Z	239	GLU	C-N-CA	6.50	128.99	120.28
7	G	207	ASN	OD1-CG-ND2	-6.50	116.10	122.60
24	Q	432	VAL	N-CA-C	-6.50	105.23	113.22
30	K	72	GLN	CB-CG-CD	-6.50	101.56	112.60
13	m	35	THR	N-CA-C	-6.49	104.99	113.17
22	S	286	TYR	CA-C-N	6.49	129.51	120.29
22	S	286	TYR	C-N-CA	6.49	129.51	120.29
28	H	45	TYR	CA-C-N	6.49	128.88	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	45	TYR	C-N-CA	6.49	128.88	120.44
11	4	116	LEU	N-CA-C	-6.49	98.32	108.90
17	T	11	LEU	CA-C-N	6.49	129.51	120.29
17	T	11	LEU	C-N-CA	6.49	129.51	120.29
20	Z	16	SER	CA-C-N	6.49	130.18	120.31
20	Z	16	SER	C-N-CA	6.49	130.18	120.31
20	Z	98	ASP	CA-C-N	6.49	128.98	120.28
20	Z	98	ASP	C-N-CA	6.49	128.98	120.28
8	1	172	ILE	CB-CA-C	-6.49	103.26	112.22
20	Z	780	MET	N-CA-C	-6.49	104.28	111.36
33	J	226	GLY	CA-C-N	6.49	130.18	120.31
33	J	226	GLY	C-N-CA	6.49	130.18	120.31
13	6	187	GLU	N-CA-C	-6.49	104.29	111.36
20	Z	47	THR	N-CA-C	-6.49	104.13	111.07
1	A	36	ASN	N-CA-C	-6.49	104.68	112.59
21	N	151	LYS	N-CA-C	-6.49	104.06	112.23
29	I	321	ASP	CA-CB-CG	6.49	119.09	112.60
11	k	106	GLY	N-CA-C	-6.49	101.67	111.14
23	P	90	LYS	N-CA-C	-6.49	105.24	113.02
10	3	13	VAL	N-CA-C	-6.48	98.70	108.17
21	N	20	VAL	N-CA-C	6.48	116.64	110.42
21	N	545	SER	CA-C-N	6.48	129.50	120.29
21	N	545	SER	C-N-CA	6.48	129.50	120.29
3	c	123	THR	CA-C-N	6.48	129.26	120.44
3	c	123	THR	C-N-CA	6.48	129.26	120.44
18	X	77	PRO	N-CA-C	6.48	123.19	114.18
31	L	162	GLU	N-CA-CB	6.48	120.41	110.49
10	j	62	THR	N-CA-C	6.48	118.14	111.14
23	P	337	HIS	N-CA-C	-6.48	105.68	113.97
21	N	820	GLU	CA-C-N	6.48	129.25	120.44
21	N	820	GLU	C-N-CA	6.48	129.25	120.44
25	R	204	TRP	CA-C-N	6.48	130.16	120.31
25	R	204	TRP	C-N-CA	6.48	130.16	120.31
21	N	16	ASN	CA-C-N	6.48	133.91	121.54
21	N	16	ASN	C-N-CA	6.48	133.91	121.54
27	O	153	LEU	O-C-N	6.47	129.53	122.15
14	n	107	ASN	OD1-CG-ND2	6.47	129.07	122.60
10	3	44	PHE	N-CA-C	-6.47	99.50	109.14
7	G	201	TYR	CB-CA-C	-6.47	100.05	110.79
8	1	46	VAL	N-CA-C	-6.47	106.94	113.47
28	H	311	ILE	O-C-N	-6.47	114.48	122.57
30	K	202	GLY	N-CA-C	-6.47	105.99	115.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	171	VAL	CA-C-N	6.47	128.85	120.44
4	d	171	VAL	C-N-CA	6.47	128.85	120.44
7	g	76	CYS	N-CA-C	-6.47	98.84	108.99
3	C	200	THR	CA-C-N	6.47	130.67	121.42
3	C	200	THR	C-N-CA	6.47	130.67	121.42
3	C	207	THR	N-CA-C	-6.47	99.92	109.81
9	2	249	ILE	CA-CB-CG2	-6.47	99.50	110.50
11	4	86	GLN	OE1-CD-NE2	6.47	129.07	122.60
13	6	68	ASP	CA-C-N	6.47	127.11	120.00
13	6	68	ASP	C-N-CA	6.47	127.11	120.00
17	T	50	ILE	N-CA-C	-6.47	104.21	110.42
6	f	185	ASN	CB-CA-C	-6.46	101.94	110.34
2	B	174	PHE	CB-CG-CD1	6.46	131.69	120.70
20	Z	841	GLU	N-CA-C	-6.46	98.84	108.99
1	a	206	ALA	CA-C-N	6.46	128.70	120.56
1	a	206	ALA	C-N-CA	6.46	128.70	120.56
13	6	44	ASN	O-C-N	6.46	129.07	122.09
20	Z	774	ARG	N-CA-CB	6.46	119.69	110.13
7	g	100	LYS	CA-C-N	6.46	129.18	120.65
7	g	100	LYS	C-N-CA	6.46	129.18	120.65
8	1	16	THR	CA-CB-OG1	6.46	119.29	109.60
4	d	9	SER	N-CA-C	-6.46	104.98	112.92
20	Z	713	LYS	CA-C-O	6.46	127.35	120.70
20	Z	794	ASP	CA-CB-CG	-6.46	106.14	112.60
23	P	282	HIS	O-C-N	-6.46	114.33	122.27
24	Q	173	SER	N-CA-C	-6.46	104.32	111.36
27	O	298	GLU	CA-C-N	6.46	129.46	120.29
27	O	298	GLU	C-N-CA	6.46	129.46	120.29
2	b	200	VAL	CB-CA-C	6.46	119.75	110.33
6	f	138	ASP	CA-C-N	6.46	130.93	120.60
6	f	138	ASP	C-N-CA	6.46	130.93	120.60
27	O	44	SER	CA-C-N	6.46	128.93	120.28
27	O	44	SER	C-N-CA	6.46	128.93	120.28
27	O	383	LYS	N-CA-CB	6.46	119.71	110.16
2	B	111	VAL	N-CA-CB	-6.45	102.31	110.57
4	D	150	THR	N-CA-C	-6.45	99.52	109.52
8	1	163	PHE	CA-C-N	6.45	129.58	120.42
8	1	163	PHE	C-N-CA	6.45	129.58	120.42
20	Z	613	ASP	CA-C-N	6.45	131.79	121.34
20	Z	613	ASP	C-N-CA	6.45	131.79	121.34
22	S	128	ILE	N-CA-C	6.45	118.38	109.80
22	S	307	LEU	N-CA-C	-6.45	104.17	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	385	ARG	N-CA-C	-6.45	105.23	113.23
33	J	318	PRO	CA-C-N	6.45	126.41	119.76
33	J	318	PRO	C-N-CA	6.45	126.41	119.76
22	S	399	TYR	N-CA-CB	6.45	121.96	110.80
24	Q	412	ALA	CA-C-N	6.45	129.45	120.29
24	Q	412	ALA	C-N-CA	6.45	129.45	120.29
30	K	142	HIS	CE1-NE2-CD2	-6.45	102.55	109.00
2	b	41	ASN	CA-C-O	-6.45	113.91	119.97
8	h	129	HIS	CE1-NE2-CD2	-6.45	102.55	109.00
2	B	21	ILE	N-CA-C	-6.45	104.47	110.53
23	P	339	GLU	CA-C-N	6.45	129.57	120.28
23	P	339	GLU	C-N-CA	6.45	129.57	120.28
24	Q	32	ASP	N-CA-C	6.45	118.31	111.28
18	X	76	VAL	N-CA-CB	6.45	120.24	111.21
25	R	397	ASN	CA-C-N	6.45	128.92	120.28
25	R	397	ASN	C-N-CA	6.45	128.92	120.28
20	Z	305	VAL	N-CA-C	-6.45	98.91	108.45
31	L	161	ARG	CA-C-O	6.45	128.22	120.81
20	Z	27	LYS	O-C-N	6.44	128.71	122.07
32	M	19	ASP	N-CA-C	6.44	118.30	111.28
7	g	142	ASP	CA-C-N	6.44	129.56	120.28
7	g	142	ASP	C-N-CA	6.44	129.56	120.28
13	m	40	ASP	CA-CB-CG	6.44	119.04	112.60
20	Z	516	THR	CA-CB-OG1	6.44	119.26	109.60
10	j	170	ALA	N-CA-C	6.44	118.84	111.11
20	Z	52	LEU	CA-C-N	6.44	129.56	120.42
20	Z	52	LEU	C-N-CA	6.44	129.56	120.42
30	K	168	ASP	N-CA-C	-6.44	98.77	109.46
20	Z	381	LEU	CA-C-N	6.44	129.19	120.44
20	Z	381	LEU	C-N-CA	6.44	129.19	120.44
28	H	344	ASP	CA-C-N	6.44	127.89	119.84
28	H	344	ASP	C-N-CA	6.44	127.89	119.84
30	K	235	ILE	CA-C-O	-6.44	112.73	120.78
31	L	102	GLY	N-CA-C	6.44	119.41	112.33
24	Q	80	HIS	N-CA-CB	6.44	120.56	110.46
30	K	347	ARG	NE-CZ-NH2	-6.44	113.41	119.20
5	e	7	GLU	N-CA-C	-6.43	104.68	113.30
6	f	75	ALA	N-CA-CB	6.43	121.36	110.49
14	n	212	ASN	CA-C-N	6.43	129.43	120.29
14	n	212	ASN	C-N-CA	6.43	129.43	120.29
20	Z	156	HIS	CG-CD2-NE2	6.43	113.64	107.20
8	1	131	LEU	CA-C-N	6.43	128.82	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	131	LEU	C-N-CA	6.43	128.82	121.04
17	T	162	ASP	CA-C-O	6.43	127.37	120.10
27	O	250	TRP	CA-C-N	6.43	128.90	120.28
27	O	250	TRP	C-N-CA	6.43	128.90	120.28
28	H	391	ILE	N-CA-C	6.43	117.22	110.72
1	A	157	THR	CA-CB-CG2	6.43	121.43	110.50
21	N	654	GLN	CA-C-N	6.43	128.80	120.44
21	N	654	GLN	C-N-CA	6.43	128.80	120.44
5	e	83	ALA	CA-C-N	6.43	130.08	120.31
5	e	83	ALA	C-N-CA	6.43	130.08	120.31
3	C	86	ILE	CA-CB-CG1	6.43	121.33	110.40
17	T	103	SER	CA-C-N	6.43	129.42	120.29
17	T	103	SER	C-N-CA	6.43	129.42	120.29
8	1	199	PRO	CA-C-N	6.43	129.42	120.29
8	1	199	PRO	C-N-CA	6.43	129.42	120.29
13	6	168	TYR	CA-C-O	-6.43	114.55	121.36
25	R	49	PHE	N-CA-C	6.43	118.08	111.14
10	j	13	VAL	N-CA-C	-6.42	98.94	108.45
6	F	89	ARG	CA-C-N	6.42	128.89	120.28
6	F	89	ARG	C-N-CA	6.42	128.89	120.28
17	T	102	LYS	CA-C-N	6.42	128.79	120.44
17	T	102	LYS	C-N-CA	6.42	128.79	120.44
21	N	591	LEU	N-CA-C	6.42	118.28	111.28
25	R	72	VAL	CB-CA-C	6.42	121.83	111.29
6	f	190	ILE	CA-C-N	6.42	128.89	120.28
6	f	190	ILE	C-N-CA	6.42	128.89	120.28
20	Z	832	ARG	CA-C-N	6.42	128.88	120.28
20	Z	832	ARG	C-N-CA	6.42	128.88	120.28
1	A	229	THR	N-CA-C	-6.42	100.45	109.69
31	L	233	LYS	CA-C-N	6.42	128.79	120.44
31	L	233	LYS	C-N-CA	6.42	128.79	120.44
11	4	79	ALA	CB-CA-C	-6.42	100.76	110.90
11	4	96	ARG	NE-CZ-NH1	-6.42	115.08	121.50
11	4	165	VAL	N-CA-CB	6.42	119.27	110.54
22	S	369	GLN	CA-C-N	6.42	128.78	120.44
22	S	369	GLN	C-N-CA	6.42	128.78	120.44
30	K	199	GLU	O-C-N	6.42	128.92	122.12
4	D	127	ARG	NE-CZ-NH2	-6.42	113.42	119.20
22	S	120	SER	N-CA-CB	6.42	120.23	110.28
25	R	343	GLU	CA-C-O	6.42	127.22	120.42
29	I	89	GLN	CA-C-N	6.42	128.78	120.44
29	I	89	GLN	C-N-CA	6.42	128.78	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	185	ASN	N-CA-CB	6.42	120.25	110.44
10	3	150	CYS	O-C-N	-6.42	115.32	122.12
20	Z	281	ALA	CA-C-N	6.42	129.53	120.42
20	Z	281	ALA	C-N-CA	6.42	129.53	120.42
24	Q	333	SER	CA-C-O	6.41	127.22	120.42
33	J	357	ASP	CA-CB-CG	-6.41	106.19	112.60
3	c	139	GLY	O-C-N	6.41	129.55	123.65
22	S	61	SER	N-CA-C	6.41	119.09	111.33
30	K	269	ILE	CA-C-O	-6.41	113.47	120.71
2	b	113	GLU	CA-C-N	6.41	129.24	120.46
2	b	113	GLU	C-N-CA	6.41	129.24	120.46
20	Z	809	MET	CB-CA-C	-6.41	100.78	110.90
21	N	141	ILE	N-CA-CB	6.41	118.77	110.57
23	P	344	ARG	N-CA-C	6.41	118.27	111.28
24	Q	247	HIS	ND1-CE1-NE2	6.41	114.81	108.40
28	H	105	ILE	N-CA-C	-6.41	99.24	108.53
30	K	391	GLY	CA-C-N	6.41	129.39	120.29
30	K	391	GLY	C-N-CA	6.41	129.39	120.29
8	1	113	ASP	CA-CB-CG	-6.41	106.19	112.60
28	H	177	ASP	CA-C-O	-6.41	114.69	121.99
22	S	115	PRO	CA-C-N	6.41	133.34	122.26
22	S	115	PRO	C-N-CA	6.41	133.34	122.26
20	Z	878	LEU	CA-C-O	-6.40	112.86	120.10
21	N	262	VAL	CA-C-N	6.40	128.76	120.44
21	N	262	VAL	C-N-CA	6.40	128.76	120.44
21	N	308	ASN	N-CA-C	-6.40	96.82	108.02
21	N	839	ARG	N-CA-C	-6.40	97.16	110.80
32	M	327	THR	N-CA-C	-6.40	99.00	108.79
22	S	488	GLN	CA-C-N	6.40	129.96	120.87
22	S	488	GLN	C-N-CA	6.40	129.96	120.87
27	O	306	ARG	NE-CZ-NH1	-6.40	115.10	121.50
30	K	164	ASN	N-CA-C	-6.40	104.38	111.36
12	5	128	GLN	CA-C-N	6.40	128.76	120.44
12	5	128	GLN	C-N-CA	6.40	128.76	120.44
3	C	227	GLN	OE1-CD-NE2	-6.40	116.20	122.60
29	I	381	VAL	CB-CA-C	-6.40	103.50	112.14
32	M	161	SER	O-C-N	-6.40	115.46	123.01
1	a	74	CYS	N-CA-C	-6.39	98.79	108.96
15	W	21	PHE	CA-C-O	-6.39	113.13	120.03
24	Q	211	PRO	N-CA-C	6.39	125.64	112.47
29	I	303	GLN	CA-C-O	6.39	127.33	120.55
13	m	70	ASP	CA-C-N	6.39	129.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	70	ASP	C-N-CA	6.39	129.13	120.44
9	2	145	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
16	V	23	THR	CB-CA-C	6.39	120.77	110.16
24	Q	331	THR	N-CA-CB	6.39	119.51	110.12
5	e	203	ILE	O-C-N	6.39	128.41	121.83
11	4	45	SER	N-CA-C	-6.39	100.16	110.32
7	G	228	HIS	O-C-N	-6.39	115.75	123.16
15	W	91	LEU	CA-C-N	6.39	130.02	120.31
15	W	91	LEU	C-N-CA	6.39	130.02	120.31
13	m	197	THR	CA-C-N	6.39	128.84	120.28
13	m	197	THR	C-N-CA	6.39	128.84	120.28
20	Z	255	LEU	N-CA-C	-6.39	104.71	114.16
23	P	394	ASN	OD1-CG-ND2	-6.39	116.21	122.60
2	b	99	ARG	N-CA-C	-6.38	104.94	114.64
8	1	99	LYS	N-CA-C	-6.38	104.40	111.36
21	N	472	ASN	OD1-CG-ND2	6.38	128.99	122.60
28	H	148	ASN	CA-C-O	-6.38	113.23	120.32
31	L	327	THR	CA-C-O	-6.38	114.40	121.23
1	a	132	ALA	CA-C-N	6.38	131.37	120.71
1	a	132	ALA	C-N-CA	6.38	131.37	120.71
3	c	70	ASN	N-CA-C	-6.38	98.44	108.14
30	K	255	ARG	CA-C-N	6.38	128.74	120.44
30	K	255	ARG	C-N-CA	6.38	128.74	120.44
3	c	10	THR	CA-CB-OG1	6.38	119.17	109.60
4	d	39	LYS	N-CA-C	-6.38	106.08	114.31
2	b	162	THR	CA-C-O	6.38	128.14	121.38
9	i	34	GLY	N-CA-C	-6.38	100.30	111.46
15	W	126	ILE	CA-C-N	6.38	130.01	120.31
15	W	126	ILE	C-N-CA	6.38	130.01	120.31
29	I	121	THR	N-CA-C	-6.38	98.50	108.90
30	K	114	THR	CA-C-O	6.38	127.32	119.79
1	a	246	VAL	CA-C-N	6.38	128.73	120.44
1	a	246	VAL	C-N-CA	6.38	128.73	120.44
12	l	87	ILE	N-CA-C	-6.38	98.94	108.12
4	D	197	ARG	NH1-CZ-NH2	6.38	127.59	119.30
7	G	182	HIS	CA-C-N	6.38	131.10	122.56
7	G	182	HIS	C-N-CA	6.38	131.10	122.56
24	Q	3	LEU	O-C-N	-6.38	115.34	120.38
26	U	13	LEU	O-C-N	6.38	128.88	122.12
14	n	157	ASP	CA-C-N	6.37	129.87	120.95
14	n	157	ASP	C-N-CA	6.37	129.87	120.95
22	S	19	HIS	CA-C-N	6.37	129.34	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	19	HIS	C-N-CA	6.37	129.34	120.29
9	i	222	PRO	N-CA-C	-6.37	105.68	114.98
15	W	159	ALA	CA-C-N	6.37	129.11	120.44
15	W	159	ALA	C-N-CA	6.37	129.11	120.44
23	P	243	GLU	O-C-N	6.37	128.87	122.12
26	U	259	ASN	N-CA-C	-6.37	104.25	111.07
33	J	292	MET	N-CA-CB	6.37	121.04	110.85
9	i	203	ASP	N-CA-C	-6.37	99.34	109.59
10	j	190	ILE	CA-C-N	6.37	129.10	120.44
10	j	190	ILE	C-N-CA	6.37	129.10	120.44
13	6	111	PHE	CA-CB-CG	-6.37	107.43	113.80
19	Y	59	ILE	N-CA-C	-6.37	106.79	112.90
20	Z	181	GLY	O-C-N	-6.37	115.00	122.45
25	R	397	ASN	CA-C-O	-6.37	113.80	120.55
26	U	282	VAL	CB-CA-C	-6.37	101.94	112.26
30	K	205	PRO	N-CA-CB	6.37	106.76	103.19
3	C	207	THR	N-CA-CB	6.37	120.60	111.05
28	H	121	ASN	O-C-N	6.37	129.94	122.24
25	R	233	ASP	O-C-N	6.37	130.86	122.33
1	a	85	GLY	CA-C-N	6.36	126.12	119.76
1	a	85	GLY	C-N-CA	6.36	126.12	119.76
5	e	123	PHE	N-CA-C	-6.36	105.16	114.39
7	g	118	GLN	N-CA-CB	6.36	120.10	110.30
21	N	682	PHE	N-CA-CB	6.36	119.47	110.12
23	P	189	LEU	CA-C-N	6.36	129.33	120.29
23	P	189	LEU	C-N-CA	6.36	129.33	120.29
26	U	206	ASP	CA-C-N	6.36	129.46	120.42
26	U	206	ASP	C-N-CA	6.36	129.46	120.42
26	U	103	ASP	CA-C-O	-6.36	111.42	119.31
21	N	199	ASN	CA-C-O	6.36	127.55	120.43
22	S	54	TRP	CD2-CE2-CZ2	-6.36	116.04	122.40
23	P	241	LEU	N-CA-C	-6.36	104.22	112.23
33	J	304	LEU	CA-C-N	6.36	129.32	120.29
33	J	304	LEU	C-N-CA	6.36	129.32	120.29
10	j	159	GLU	CA-C-N	6.36	126.28	119.28
10	j	159	GLU	C-N-CA	6.36	126.28	119.28
20	Z	323	TYR	CA-C-N	6.36	129.09	120.44
20	Z	323	TYR	C-N-CA	6.36	129.09	120.44
12	l	241	HIS	CA-CB-CG	6.36	120.16	113.80
30	K	279	THR	CA-CB-OG1	6.36	119.14	109.60
33	J	9	ASN	N-CA-CB	6.36	122.42	112.25
14	n	63	TYR	N-CA-C	-6.36	102.64	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	91	LEU	CA-C-O	-6.36	111.91	119.35
21	N	410	LEU	CA-C-O	-6.35	113.81	120.55
27	O	173	SER	CA-C-N	6.35	128.79	120.28
27	O	173	SER	C-N-CA	6.35	128.79	120.28
31	L	163	THR	CA-C-N	6.35	129.22	120.39
31	L	163	THR	C-N-CA	6.35	129.22	120.39
15	W	27	GLU	O-C-N	-6.35	115.39	122.12
20	Z	610	GLY	CA-C-N	6.35	131.23	121.83
20	Z	610	GLY	C-N-CA	6.35	131.23	121.83
22	S	103	SER	O-C-N	6.35	129.35	122.05
10	3	14	ALA	CA-C-N	6.35	132.52	122.36
10	3	14	ALA	C-N-CA	6.35	132.52	122.36
22	S	457	PRO	N-CA-C	6.35	122.22	113.65
27	O	95	SER	CB-CA-C	-6.35	100.25	110.79
9	i	218	ASN	CA-CB-CG	-6.35	106.25	112.60
33	J	235	VAL	CB-CA-C	-6.35	103.85	111.97
10	j	114	SER	N-CA-C	-6.35	105.57	113.38
13	m	97	ALA	CA-C-N	6.35	128.78	120.28
13	m	97	ALA	C-N-CA	6.35	128.78	120.28
8	h	164	ILE	CA-C-N	6.34	128.69	120.44
8	h	164	ILE	C-N-CA	6.34	128.69	120.44
2	B	139	HIS	CE1-NE2-CD2	-6.34	102.66	109.00
32	M	170	MET	N-CA-CB	6.34	119.99	110.22
33	J	305	LEU	CB-CA-C	-6.34	100.07	110.85
6	F	172	LEU	CA-C-N	6.34	128.69	120.44
6	F	172	LEU	C-N-CA	6.34	128.69	120.44
20	Z	324	GLU	N-CA-C	-6.34	104.29	111.14
21	N	830	LYS	O-C-N	6.34	128.94	122.09
24	Q	398	TYR	CB-CA-C	-6.34	97.26	109.37
2	b	183	LEU	N-CA-C	-6.34	99.69	109.52
12	l	195	THR	CA-C-O	-6.34	113.52	120.81
1	A	196	GLU	N-CA-CB	6.34	119.36	110.04
33	J	323	ALA	CA-C-N	6.34	128.78	120.28
33	J	323	ALA	C-N-CA	6.34	128.78	120.28
21	N	644	LEU	CA-C-N	6.34	128.68	120.44
21	N	644	LEU	C-N-CA	6.34	128.68	120.44
7	g	185	GLU	N-CA-C	-6.34	105.48	113.72
10	j	30	GLY	O-C-N	6.34	128.95	123.37
5	E	222	ILE	N-CA-C	-6.34	97.99	107.37
20	Z	51	LEU	N-CA-CB	6.34	119.54	110.16
10	j	32	GLN	CA-C-N	6.34	128.77	120.28
10	j	32	GLN	C-N-CA	6.34	128.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	103	ASN	OD1-CG-ND2	6.34	128.94	122.60
12	5	250	VAL	N-CA-CB	6.33	118.59	110.99
14	7	220	ARG	N-CA-CB	-6.33	101.78	111.66
22	S	134	ILE	CA-C-N	6.33	129.29	120.29
22	S	134	ILE	C-N-CA	6.33	129.29	120.29
6	F	232	LYS	N-CA-C	-6.33	104.71	112.88
22	S	263	ASP	CA-CB-CG	-6.33	106.27	112.60
29	I	88	LYS	N-CA-CB	6.33	121.19	110.49
14	n	35	GLN	CG-CD-NE2	6.33	125.90	116.40
10	3	172	LEU	CA-C-N	6.33	129.05	120.44
10	3	172	LEU	C-N-CA	6.33	129.05	120.44
11	4	33	ASP	CA-CB-CG	-6.33	106.27	112.60
31	L	138	SER	N-CA-C	-6.33	105.38	113.23
4	d	197	ARG	CA-C-N	6.33	128.67	120.44
4	d	197	ARG	C-N-CA	6.33	128.67	120.44
30	K	402	ILE	O-C-N	-6.33	116.68	123.14
8	h	27	SER	N-CA-C	6.33	121.08	113.23
1	A	146	VAL	N-CA-C	-6.33	98.62	107.80
16	V	109	HIS	CA-CB-CG	6.33	120.13	113.80
19	Y	81	LEU	N-CA-CB	6.33	119.53	110.16
20	Z	801	HIS	CB-CG-CD2	-6.33	122.97	131.20
33	J	342	ASN	CA-C-O	6.33	127.12	119.78
5	e	147	HIS	CE1-NE2-CD2	-6.33	102.67	109.00
2	B	76	SER	N-CA-C	-6.33	98.31	109.06
4	D	232	TYR	CA-C-O	-6.33	114.18	120.82
9	2	84	VAL	CA-CB-CG1	6.33	121.15	110.40
25	R	325	HIS	CB-CG-ND1	6.33	132.19	122.70
3	c	175	LEU	CA-C-N	6.32	129.27	120.29
3	c	175	LEU	C-N-CA	6.32	129.27	120.29
10	j	102	PRO	CB-CA-C	-6.32	101.93	110.85
11	k	111	LYS	N-CA-C	-6.32	104.80	114.16
11	k	127	GLU	N-CA-CB	6.32	120.59	110.16
14	n	210	ILE	CA-C-O	-6.32	114.15	120.85
2	B	5	TYR	CA-C-O	6.32	126.23	119.34
30	K	311	ASN	OD1-CG-ND2	-6.32	116.28	122.60
13	m	212	ILE	N-CA-C	-6.32	98.41	107.77
20	Z	577	GLN	OE1-CD-NE2	6.32	128.92	122.60
21	N	673	PRO	CA-C-N	6.32	129.27	120.29
21	N	673	PRO	C-N-CA	6.32	129.27	120.29
24	Q	423	VAL	O-C-N	6.32	128.94	121.80
30	K	110	VAL	N-CA-C	-6.32	99.57	108.80
3	c	131	PHE	CA-CB-CG	-6.32	107.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	58	ALA	CA-C-O	6.32	127.25	120.55
13	m	203	HIS	CA-C-O	-6.32	114.69	121.45
21	N	167	GLU	CA-C-O	-6.32	114.19	120.70
22	S	331	SER	CA-C-N	6.32	128.65	120.44
22	S	331	SER	C-N-CA	6.32	128.65	120.44
32	M	53	HIS	CG-CD2-NE2	6.32	113.52	107.20
11	4	101	ASN	N-CA-C	-6.32	99.42	109.59
20	Z	151	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
21	N	11	ALA	O-C-N	6.32	128.81	122.12
22	S	268	LEU	N-CA-CB	6.32	119.51	110.16
22	S	333	PHE	CA-C-N	6.32	128.74	120.28
22	S	333	PHE	C-N-CA	6.32	128.74	120.28
8	h	171	ALA	CA-C-N	6.31	130.66	120.30
8	h	171	ALA	C-N-CA	6.31	130.66	120.30
4	D	234	THR	CA-CB-OG1	6.31	119.07	109.60
12	5	89	VAL	N-CA-C	-6.31	99.38	108.53
12	l	106	VAL	N-CA-CB	6.31	121.64	111.23
2	B	168	SER	N-CA-C	6.31	118.68	111.11
4	D	35	GLY	CA-C-O	6.31	125.86	120.94
20	Z	573	LEU	CA-C-N	6.31	131.26	120.72
20	Z	573	LEU	C-N-CA	6.31	131.26	120.72
22	S	232	MET	O-C-N	-6.31	114.96	122.15
22	S	253	PHE	CA-CB-CG	6.31	120.11	113.80
10	3	99	ARG	CA-C-N	6.31	131.88	123.05
10	3	99	ARG	C-N-CA	6.31	131.88	123.05
16	V	120	SER	CA-C-N	6.31	129.38	120.42
16	V	120	SER	C-N-CA	6.31	129.38	120.42
12	5	159	SER	CA-C-O	-6.30	113.74	120.42
15	W	26	PHE	O-C-N	6.30	128.65	122.09
17	T	37	ASN	CA-CB-CG	-6.30	106.30	112.60
4	d	172	ARG	N-CA-CB	6.30	119.15	110.01
23	P	267	PHE	CA-CB-CG	-6.30	107.50	113.80
23	P	374	SER	N-CA-CB	6.30	119.15	110.01
32	M	313	ASP	CA-CB-CG	6.30	118.90	112.60
24	Q	324	GLU	CA-C-N	6.30	128.63	120.44
24	Q	324	GLU	C-N-CA	6.30	128.63	120.44
26	U	103	ASP	N-CA-CB	6.30	120.67	110.40
28	H	357	ARG	O-C-N	-6.30	115.46	121.57
20	Z	621	LEU	CA-C-N	6.30	128.63	120.44
20	Z	621	LEU	C-N-CA	6.30	128.63	120.44
18	X	113	GLU	N-CA-C	-6.30	102.56	111.56
29	I	54	ARG	CA-C-O	6.30	127.21	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	165	ASP	CB-CA-C	-6.30	103.08	110.76
33	J	60	ASP	CA-CB-CG	6.30	118.90	112.60
26	U	57	GLU	N-CA-CB	6.29	123.22	111.52
31	L	317	ASN	CA-C-N	6.29	131.36	121.99
31	L	317	ASN	C-N-CA	6.29	131.36	121.99
2	b	193	LEU	CA-C-O	-6.29	113.88	120.55
9	2	176	THR	CA-C-N	6.29	128.62	120.44
9	2	176	THR	C-N-CA	6.29	128.62	120.44
32	M	191	GLU	O-C-N	6.29	128.55	122.07
9	i	107	SER	CA-C-N	6.29	128.99	120.44
9	i	107	SER	C-N-CA	6.29	128.99	120.44
4	D	213	THR	CA-CB-OG1	-6.29	100.17	109.60
16	V	250	GLN	CA-C-N	6.29	128.71	120.28
16	V	250	GLN	C-N-CA	6.29	128.71	120.28
23	P	18	LYS	CA-C-O	6.29	126.80	119.32
25	R	401	HIS	CA-CB-CG	6.29	120.09	113.80
28	H	276	GLY	N-CA-C	-6.29	105.21	115.46
32	M	383	THR	N-CA-CB	6.29	120.21	110.46
10	3	72	ASN	CB-CG-ND2	-6.29	106.97	116.40
20	Z	214	HIS	CA-CB-CG	6.29	120.09	113.80
18	X	77	PRO	CB-CA-C	-6.29	101.19	111.31
31	L	213	LYS	N-CA-CB	6.29	117.03	109.74
1	A	149	GLU	CA-C-O	-6.28	111.53	120.51
23	P	86	HIS	CE1-NE2-CD2	-6.28	102.72	109.00
29	I	361	ILE	O-C-N	6.28	128.30	121.83
18	X	120	GLU	O-C-N	-6.28	115.46	122.12
20	Z	380	ASN	OD1-CG-ND2	6.28	128.88	122.60
25	R	359	VAL	N-CA-C	-6.28	99.63	108.80
26	U	248	ASP	CB-CA-C	-6.28	100.36	110.79
8	h	156	SER	N-CA-CB	6.28	119.24	110.26
1	A	226	GLY	O-C-N	-6.28	116.58	123.49
32	M	123	SER	N-CA-C	-6.28	104.09	112.94
33	J	209	LYS	CA-C-O	-6.28	114.97	121.87
5	E	83	ALA	CA-C-N	6.28	129.85	120.31
5	E	83	ALA	C-N-CA	6.28	129.85	120.31
10	3	160	PRO	O-C-N	-6.28	114.70	122.23
17	T	256	LYS	CA-C-N	6.28	133.53	121.54
17	T	256	LYS	C-N-CA	6.28	133.53	121.54
27	O	381	GLY	N-CA-C	6.28	120.26	112.73
9	i	143	HIS	CA-C-N	6.27	129.85	120.31
9	i	143	HIS	C-N-CA	6.27	129.85	120.31
14	n	181	ALA	CA-C-O	6.27	127.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	330	LYS	CA-C-O	6.27	128.02	121.31
33	J	331	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
4	D	70	HIS	CG-CD2-NE2	6.27	113.47	107.20
8	1	134	ALA	CA-C-N	6.27	131.71	122.99
8	1	134	ALA	C-N-CA	6.27	131.71	122.99
29	I	194	ILE	O-C-N	6.27	128.42	121.90
7	g	137	ILE	O-C-N	-6.27	115.32	122.72
18	X	32	GLU	CB-CG-CD	-6.27	101.94	112.60
21	N	517	LEU	O-C-N	-6.27	115.00	122.15
23	P	10	ASP	CA-C-N	6.27	128.97	120.38
23	P	10	ASP	C-N-CA	6.27	128.97	120.38
9	2	57	ASP	CA-CB-CG	-6.27	106.33	112.60
10	3	45	HIS	CA-CB-CG	6.27	120.07	113.80
2	b	208	THR	CA-CB-OG1	6.27	119.00	109.60
11	k	154	THR	CA-C-N	6.27	128.96	120.44
11	k	154	THR	C-N-CA	6.27	128.96	120.44
5	E	117	CYS	N-CA-C	-6.27	105.12	112.89
10	3	198	ARG	NE-CZ-NH2	-6.27	113.56	119.20
21	N	846	ILE	CA-C-N	6.27	131.11	122.77
21	N	846	ILE	C-N-CA	6.27	131.11	122.77
20	Z	802	ASP	CA-C-N	6.27	132.32	122.17
20	Z	802	ASP	C-N-CA	6.27	132.32	122.17
4	d	143	ASP	N-CA-C	-6.26	103.78	112.30
22	S	271	ARG	N-CA-C	6.26	118.11	111.28
22	S	408	CYS	CB-CA-C	-6.26	100.20	110.85
23	P	141	LYS	CA-C-N	6.26	129.19	120.29
23	P	141	LYS	C-N-CA	6.26	129.19	120.29
25	R	116	LYS	N-CA-CB	-6.26	100.91	110.12
26	U	68	LEU	N-CA-C	-6.26	98.78	109.24
26	U	290	ASP	CA-C-N	6.26	129.19	120.29
26	U	290	ASP	C-N-CA	6.26	129.19	120.29
27	O	49	PHE	N-CA-CB	6.26	120.61	110.40
29	I	160	LEU	N-CA-C	-6.26	102.91	112.99
32	M	209	ASP	CB-CA-C	-6.26	101.00	110.90
5	e	20	ARG	NE-CZ-NH2	6.26	124.84	119.20
14	n	111	ASN	CA-C-O	-6.26	114.31	120.26
2	B	230	ASP	CA-CB-CG	6.26	118.86	112.60
16	V	247	ILE	N-CA-C	-6.26	105.60	112.80
27	O	283	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
29	I	260	GLY	N-CA-C	6.26	122.73	115.09
1	a	181	ASN	O-C-N	-6.26	115.48	122.12
2	b	162	THR	N-CA-C	-6.26	99.46	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	41	ASN	N-CA-C	-6.26	104.45	113.21
21	N	217	MET	N-CA-C	6.26	117.59	109.64
24	Q	299	MET	CA-CB-CG	6.26	126.62	114.10
27	O	266	PHE	CA-C-N	6.26	128.67	120.28
27	O	266	PHE	C-N-CA	6.26	128.67	120.28
22	S	224	LYS	CA-C-N	6.26	131.28	122.46
22	S	224	LYS	C-N-CA	6.26	131.28	122.46
23	P	367	GLU	N-CA-CB	6.26	119.98	110.28
13	6	199	ALA	N-CA-C	6.26	120.75	113.18
21	N	544	GLU	CA-C-N	6.26	129.29	120.28
21	N	544	GLU	C-N-CA	6.26	129.29	120.28
1	a	120	ARG	CB-CG-CD	6.25	125.69	111.30
4	d	12	SER	N-CA-C	-6.25	102.80	110.31
8	h	127	SER	N-CA-C	-6.25	97.48	110.80
13	m	64	GLY	CA-C-N	6.25	129.75	120.87
13	m	64	GLY	C-N-CA	6.25	129.75	120.87
30	K	423	LYS	N-CA-C	-6.25	104.90	114.16
11	k	23	ARG	NE-CZ-NH2	6.25	124.83	119.20
13	m	145	ARG	NE-CZ-NH2	6.25	124.83	119.20
4	D	217	PRO	O-C-N	6.25	130.61	122.86
31	L	404	ARG	N-CA-CB	-6.25	100.93	110.12
4	d	79	ASN	CA-C-N	6.25	128.66	120.28
4	d	79	ASN	C-N-CA	6.25	128.66	120.28
2	B	239	THR	N-CA-CB	6.25	119.38	110.44
25	R	110	ILE	CA-C-N	6.25	129.28	120.28
25	R	110	ILE	C-N-CA	6.25	129.28	120.28
26	U	252	HIS	ND1-CE1-NE2	6.25	114.65	108.40
33	J	396	THR	N-CA-C	6.25	118.09	111.28
11	k	162	LYS	N-CA-C	-6.25	104.55	111.36
20	Z	887	GLY	N-CA-C	-6.25	98.37	113.18
21	N	60	MET	O-C-N	6.25	129.27	122.15
30	K	62	THR	CA-C-N	6.25	129.16	120.29
30	K	62	THR	C-N-CA	6.25	129.16	120.29
30	K	226	VAL	CA-C-N	6.25	128.65	120.28
30	K	226	VAL	C-N-CA	6.25	128.65	120.28
1	A	148	GLU	N-CA-CB	6.25	119.53	110.47
4	D	20	VAL	CA-C-N	6.25	128.65	120.28
4	D	20	VAL	C-N-CA	6.25	128.65	120.28
24	Q	74	LEU	N-CA-C	6.25	118.17	111.36
24	Q	163	ARG	NE-CZ-NH2	6.25	124.82	119.20
9	i	170	HIS	N-CA-C	-6.25	104.29	112.41
27	O	87	LYS	O-C-N	-6.25	115.34	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	71	ASP	N-CA-CB	6.24	115.88	109.51
10	j	98	ARG	CA-C-O	6.24	127.10	120.36
25	R	311	THR	CB-CA-C	-6.24	101.08	110.88
27	O	188	PHE	CA-C-O	-6.24	114.27	120.82
28	H	362	ASP	CA-C-O	-6.24	114.95	120.19
30	K	361	SER	CA-C-N	6.24	131.75	121.39
30	K	361	SER	C-N-CA	6.24	131.75	121.39
2	b	110	LEU	CA-C-O	-6.24	112.79	119.97
14	n	157	ASP	O-C-N	-6.24	116.66	123.52
17	T	251	HIS	CA-CB-CG	-6.24	107.56	113.80
24	Q	76	GLU	CA-C-N	6.24	128.64	120.28
24	Q	76	GLU	C-N-CA	6.24	128.64	120.28
31	L	196	VAL	CA-C-O	-6.24	114.03	120.71
1	a	180	THR	CA-C-N	6.24	128.64	120.28
1	a	180	THR	C-N-CA	6.24	128.64	120.28
3	c	240	VAL	O-C-N	-6.24	115.40	121.83
21	N	147	ALA	N-CA-C	-6.24	105.63	113.18
25	R	408	ASP	N-CA-C	-6.24	104.56	111.36
27	O	270	ILE	CA-C-N	6.24	128.64	120.28
27	O	270	ILE	C-N-CA	6.24	128.64	120.28
32	M	229	THR	CA-C-N	6.24	129.46	120.79
32	M	229	THR	C-N-CA	6.24	129.46	120.79
17	T	158	GLN	CA-C-N	6.24	129.15	120.29
17	T	158	GLN	C-N-CA	6.24	129.15	120.29
20	Z	351	PRO	CB-CA-C	-6.24	103.01	110.00
12	l	224	SER	N-CA-C	-6.24	101.23	110.46
4	D	36	VAL	CB-CA-C	-6.24	101.06	111.29
20	Z	102	ILE	CA-C-N	6.24	128.88	120.65
20	Z	102	ILE	C-N-CA	6.24	128.88	120.65
27	O	29	PHE	N-CA-CB	6.24	119.11	110.07
2	b	24	ALA	CA-C-O	6.23	127.14	119.97
8	1	28	ARG	CA-C-O	-6.23	114.33	121.19
16	V	177	THR	N-CA-C	-6.23	104.59	111.82
29	I	240	THR	O-C-N	6.23	129.26	122.15
12	5	263	HIS	ND1-CE1-NE2	6.23	114.63	108.40
17	T	43	ASP	CA-CB-CG	-6.23	106.37	112.60
20	Z	868	ASN	CB-CA-C	-6.23	100.26	110.85
21	N	121	GLU	CB-CG-CD	-6.23	102.01	112.60
21	N	896	PHE	O-C-N	-6.23	115.20	122.87
22	S	192	GLU	CA-C-N	6.23	128.92	120.44
22	S	192	GLU	C-N-CA	6.23	128.92	120.44
22	S	480	ARG	NH1-CZ-NH2	-6.23	111.20	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	423	LEU	CA-C-O	6.23	127.14	119.97
1	A	123	ASN	CA-C-O	6.23	127.03	120.42
1	A	211	ILE	O-C-N	6.23	127.91	121.87
9	2	119	TYR	CB-CA-C	-6.23	96.90	109.55
23	P	79	LEU	N-CA-CB	6.23	119.04	110.01
18	X	109	LEU	CA-C-N	6.23	126.20	119.78
18	X	109	LEU	C-N-CA	6.23	126.20	119.78
29	I	365	HIS	CA-C-N	6.23	129.78	120.31
29	I	365	HIS	C-N-CA	6.23	129.78	120.31
10	j	75	LYS	N-CA-C	6.23	118.07	111.28
20	Z	894	MET	CA-C-O	6.23	127.31	120.71
21	N	173	LYS	N-CA-C	-6.23	104.03	111.69
1	a	27	GLN	CA-C-N	6.23	128.53	120.56
1	a	27	GLN	C-N-CA	6.23	128.53	120.56
13	m	11	ASN	CB-CG-ND2	6.22	125.74	116.40
16	V	301	ASN	CB-CA-C	-6.22	100.46	110.79
31	L	164	ASP	CA-C-N	6.22	125.91	119.56
31	L	164	ASP	C-N-CA	6.22	125.91	119.56
12	l	234	ARG	CA-C-N	6.22	129.12	120.29
12	l	234	ARG	C-N-CA	6.22	129.12	120.29
3	C	39	MET	CA-C-N	6.22	132.36	122.59
3	C	39	MET	C-N-CA	6.22	132.36	122.59
4	D	80	ALA	CB-CA-C	-6.22	100.46	110.79
6	F	24	TYR	CB-CG-CD2	-6.22	111.47	120.80
15	W	21	PHE	CA-C-N	6.22	125.98	119.76
15	W	21	PHE	C-N-CA	6.22	125.98	119.76
16	V	200	ASN	CA-C-N	6.22	130.15	122.37
16	V	200	ASN	C-N-CA	6.22	130.15	122.37
4	D	17	ILE	N-CA-CB	6.22	119.74	111.90
17	T	38	ASN	CA-C-O	-6.22	113.07	120.10
25	R	43	ARG	NE-CZ-NH1	6.22	127.72	121.50
23	P	262	SER	CA-C-N	6.22	128.61	120.28
23	P	262	SER	C-N-CA	6.22	128.61	120.28
28	H	431	ILE	CA-C-O	6.22	127.19	120.47
33	J	306	ARG	NE-CZ-NH2	6.22	124.80	119.20
7	g	22	PHE	N-CA-C	-6.22	105.18	112.89
31	L	72	ASP	N-CA-C	6.22	118.06	111.28
2	b	103	GLU	CA-C-N	6.22	130.13	120.68
2	b	103	GLU	C-N-CA	6.22	130.13	120.68
9	i	95	HIS	ND1-CE1-NE2	6.22	114.62	108.40
6	F	197	ILE	CA-C-N	6.22	129.12	120.29
6	F	197	ILE	C-N-CA	6.22	129.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	95	GLU	CA-C-N	6.22	128.61	120.28
7	G	95	GLU	C-N-CA	6.22	128.61	120.28
22	S	51	ARG	CA-C-N	6.22	128.61	120.28
22	S	51	ARG	C-N-CA	6.22	128.61	120.28
27	O	182	LYS	CA-C-O	-6.22	111.60	119.31
29	I	256	TYR	N-CA-CB	6.22	119.57	109.69
29	I	293	ASP	CA-C-N	6.22	132.15	122.26
29	I	293	ASP	C-N-CA	6.22	132.15	122.26
21	N	512	ASN	CA-CB-CG	-6.21	106.39	112.60
1	a	96	ARG	O-C-N	-6.21	115.54	122.12
13	m	98	ALA	CA-C-N	6.21	129.75	120.31
13	m	98	ALA	C-N-CA	6.21	129.75	120.31
3	C	168	ASN	CA-C-N	6.21	128.51	120.44
3	C	168	ASN	C-N-CA	6.21	128.51	120.44
11	4	142	SER	N-CA-C	-6.21	104.62	111.82
20	Z	388	GLY	O-C-N	6.21	128.21	122.19
28	H	429	PHE	CB-CG-CD2	-6.21	110.14	120.70
8	1	129	HIS	CE1-NE2-CD2	-6.21	102.79	109.00
6	F	40	SER	N-CA-CB	6.21	121.68	111.62
6	f	69	HIS	ND1-CE1-NE2	6.21	114.61	108.40
20	Z	361	HIS	CB-CG-CD2	-6.21	123.13	131.20
27	O	366	MET	CA-C-N	6.21	128.51	120.44
27	O	366	MET	C-N-CA	6.21	128.51	120.44
2	B	226	GLY	O-C-N	6.21	129.71	122.45
24	Q	189	ARG	N-CA-CB	6.21	120.98	110.49
26	U	272	GLU	O-C-N	6.21	128.70	122.12
20	Z	761	PHE	N-CA-CB	6.20	119.24	110.12
15	W	178	PRO	N-CA-C	-6.20	100.04	110.21
28	H	112	SER	O-C-N	-6.20	114.34	122.59
33	J	97	ASP	O-C-N	-6.20	115.18	122.81
2	b	168	SER	N-CA-C	6.20	118.55	111.11
3	c	58	GLU	N-CA-C	-6.20	99.10	108.96
15	W	91	LEU	N-CA-CB	6.20	119.23	110.12
20	Z	497	PHE	CA-CB-CG	-6.20	107.60	113.80
25	R	244	THR	CA-C-N	6.20	133.38	121.54
25	R	244	THR	C-N-CA	6.20	133.38	121.54
26	U	109	LEU	CA-C-N	6.20	131.22	120.68
26	U	109	LEU	C-N-CA	6.20	131.22	120.68
27	O	222	LEU	N-CA-CB	-6.20	100.99	110.16
29	I	365	HIS	CA-CB-CG	6.20	120.00	113.80
33	J	327	ILE	CA-C-N	6.20	128.59	120.28
33	J	327	ILE	C-N-CA	6.20	128.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	62	LEU	N-CA-C	-6.20	103.84	111.40
28	H	50	LYS	N-CA-CB	6.20	119.88	110.28
12	l	229	LEU	N-CA-CB	6.19	118.99	110.01
13	6	103	HIS	CB-CG-ND1	6.19	131.99	122.70
20	Z	362	LEU	CA-C-N	6.19	128.58	120.28
20	Z	362	LEU	C-N-CA	6.19	128.58	120.28
20	Z	771	HIS	ND1-CE1-NE2	6.19	114.59	108.40
6	F	92	CYS	CA-C-O	6.19	126.98	120.42
10	j	116	SER	N-CA-CB	6.19	120.95	110.49
2	B	53	SER	CA-C-N	6.19	125.75	119.19
2	B	53	SER	C-N-CA	6.19	125.75	119.19
2	B	87	ASP	N-CA-C	-6.19	104.61	111.36
6	F	167	GLY	N-CA-C	-6.19	106.98	114.66
33	J	234	PHE	CA-C-N	6.19	128.36	120.56
33	J	234	PHE	C-N-CA	6.19	128.36	120.56
33	J	255	SER	CA-C-N	6.19	128.57	120.28
33	J	255	SER	C-N-CA	6.19	128.57	120.28
3	C	170	SER	CA-C-N	6.19	128.48	120.44
3	C	170	SER	C-N-CA	6.19	128.48	120.44
5	E	181	ALA	N-CA-CB	6.19	118.98	110.01
21	N	461	GLU	O-C-N	6.19	128.77	122.09
22	S	343	LEU	CA-C-N	6.19	126.09	119.28
22	S	343	LEU	C-N-CA	6.19	126.09	119.28
33	J	22	TYR	CA-C-N	6.19	128.86	120.44
33	J	22	TYR	C-N-CA	6.19	128.86	120.44
20	Z	528	LEU	CA-C-N	6.19	128.57	120.28
20	Z	528	LEU	C-N-CA	6.19	128.57	120.28
21	N	689	LYS	N-CA-C	-6.19	106.05	113.97
24	Q	335	PHE	N-CA-CB	6.19	120.09	110.44
2	b	76	SER	N-CA-C	-6.18	98.55	109.06
1	A	117	LEU	CA-C-N	6.18	129.18	120.28
1	A	117	LEU	C-N-CA	6.18	129.18	120.28
22	S	444	GLU	CA-C-N	6.18	129.61	120.95
22	S	444	GLU	C-N-CA	6.18	129.61	120.95
27	O	120	LYS	N-CA-CB	6.18	120.94	110.49
16	V	153	ILE	N-CA-C	-6.18	99.30	108.45
20	Z	440	LEU	N-CA-CB	-6.18	100.70	110.22
32	M	286	ILE	N-CA-C	-6.18	106.74	112.43
9	2	32	ILE	N-CA-C	-6.18	100.19	108.35
18	X	102	GLN	CA-C-N	6.18	130.17	121.02
18	X	102	GLN	C-N-CA	6.18	130.17	121.02
21	N	277	LEU	CA-C-N	6.18	129.07	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	277	LEU	C-N-CA	6.18	129.07	120.29
30	K	244	HIS	CA-CB-CG	-6.18	107.62	113.80
13	m	230	ASP	CB-CA-C	-6.18	98.36	110.10
20	Z	570	LEU	N-CA-CB	6.18	118.97	110.01
5	e	157	HIS	CG-CD2-NE2	6.18	113.38	107.20
20	Z	361	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
27	O	291	ILE	CA-C-N	6.18	129.06	120.29
27	O	291	ILE	C-N-CA	6.18	129.06	120.29
11	k	187	ASP	N-CA-CB	6.17	119.93	110.61
23	P	44	LYS	CA-C-N	6.17	131.23	122.09
23	P	44	LYS	C-N-CA	6.17	131.23	122.09
23	P	72	TRP	CA-C-N	6.17	128.47	120.44
23	P	72	TRP	C-N-CA	6.17	128.47	120.44
26	U	227	GLY	CA-C-N	6.17	129.06	120.29
26	U	227	GLY	C-N-CA	6.17	129.06	120.29
30	K	209	VAL	O-C-N	-6.17	116.59	123.26
12	5	247	GLY	CA-C-O	6.17	125.17	120.91
20	Z	423	GLY	N-CA-C	6.17	121.33	113.24
22	S	59	ASP	CA-C-O	6.17	127.09	120.55
27	O	310	PHE	CA-C-N	6.17	128.55	120.28
27	O	310	PHE	C-N-CA	6.17	128.55	120.28
23	P	425	HIS	CA-C-N	6.17	129.18	120.42
23	P	425	HIS	C-N-CA	6.17	129.18	120.42
16	V	294	SER	N-CA-CB	6.17	118.96	110.01
21	N	570	ARG	CA-C-N	6.17	129.05	120.29
21	N	570	ARG	C-N-CA	6.17	129.05	120.29
23	P	269	VAL	CA-CB-CG1	6.17	120.89	110.40
30	K	69	LYS	N-CA-C	-6.17	104.10	111.69
10	j	168	SER	N-CA-CB	6.17	119.02	110.07
15	W	113	PHE	N-CA-CB	6.17	119.38	110.06
17	T	193	THR	O-C-N	6.17	130.88	122.37
21	N	835	LYS	N-CA-CB	6.17	121.61	111.62
33	J	342	ASN	OD1-CG-ND2	-6.17	116.43	122.60
5	E	233	ASN	CA-CB-CG	-6.17	106.43	112.60
20	Z	49	LEU	N-CA-C	6.17	117.67	111.07
20	Z	810	ASN	CA-CB-CG	-6.17	106.44	112.60
29	I	365	HIS	ND1-CE1-NE2	6.17	114.56	108.40
5	e	71	ASP	N-CA-C	-6.16	101.40	108.49
11	k	194	ASP	N-CA-C	-6.16	99.60	108.60
8	1	57	SER	CA-C-N	6.16	129.04	120.29
8	1	57	SER	C-N-CA	6.16	129.04	120.29
27	O	26	PHE	CA-CB-CG	-6.16	107.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	309	ASP	CA-CB-CG	6.16	118.76	112.60
31	L	191	ARG	NE-CZ-NH2	6.16	124.75	119.20
33	J	362	CYS	N-CA-C	6.16	118.00	111.28
6	F	22	VAL	N-CA-CB	6.16	120.85	110.56
20	Z	44	LYS	O-C-N	-6.16	113.96	122.46
13	m	36	ARG	NE-CZ-NH1	-6.16	115.34	121.50
14	n	232	ILE	N-CA-C	-6.16	98.87	107.80
28	H	306	ILE	CA-CB-CG1	6.16	120.87	110.40
31	L	56	ALA	N-CA-C	6.16	119.90	112.38
2	B	181	ASP	N-CA-C	-6.16	104.63	111.71
10	3	170	ALA	N-CA-C	-6.16	104.57	111.28
13	6	164	PHE	CA-CB-CG	-6.16	107.64	113.80
19	Y	43	TRP	CA-C-N	6.16	133.30	121.54
19	Y	43	TRP	C-N-CA	6.16	133.30	121.54
20	Z	950	THR	N-CA-C	6.16	120.41	113.02
27	O	33	TYR	CA-C-N	6.16	128.53	120.28
27	O	33	TYR	C-N-CA	6.16	128.53	120.28
20	Z	859	LYS	CA-C-O	-6.16	114.64	121.23
21	N	747	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
8	h	202	TYR	N-CA-CB	6.16	119.27	110.16
7	G	78	TYR	O-C-N	-6.16	115.67	123.24
23	P	369	LEU	CA-C-O	-6.16	112.15	119.35
3	c	21	GLN	O-C-N	6.15	128.64	122.12
20	Z	65	GLU	CA-C-N	6.15	129.14	120.28
20	Z	65	GLU	C-N-CA	6.15	129.14	120.28
23	P	394	ASN	CA-C-N	6.15	128.51	120.26
23	P	394	ASN	C-N-CA	6.15	128.51	120.26
29	I	187	LEU	N-CA-C	6.15	119.67	111.30
3	C	163	ILE	CA-CB-CG1	6.15	120.86	110.40
11	4	149	ARG	N-CA-C	-6.15	102.39	110.39
9	i	138	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
16	V	125	THR	CA-C-N	6.15	128.52	120.28
16	V	125	THR	C-N-CA	6.15	128.52	120.28
17	T	204	ASN	OD1-CG-ND2	-6.15	116.45	122.60
22	S	93	LEU	CA-C-N	6.15	129.03	120.29
22	S	93	LEU	C-N-CA	6.15	129.03	120.29
26	U	164	GLU	CA-C-O	-6.15	114.46	121.72
29	I	351	GLU	CA-C-N	6.15	129.01	120.65
29	I	351	GLU	C-N-CA	6.15	129.01	120.65
32	M	364	HIS	CA-CB-CG	-6.15	107.65	113.80
25	R	142	ALA	CA-C-N	6.15	128.43	120.44
25	R	142	ALA	C-N-CA	6.15	128.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	70	LYS	CA-C-N	6.15	130.09	121.24
28	H	70	LYS	C-N-CA	6.15	130.09	121.24
28	H	109	ASN	N-CA-CB	6.15	121.53	110.83
10	j	33	SER	N-CA-C	-6.15	104.58	111.28
21	N	250	ASP	CA-C-N	6.15	131.09	120.58
21	N	250	ASP	C-N-CA	6.15	131.09	120.58
5	e	35	SER	CA-C-N	6.15	129.56	120.95
5	e	35	SER	C-N-CA	6.15	129.56	120.95
9	i	64	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
21	N	481	ALA	CA-C-N	6.15	128.52	120.28
21	N	481	ALA	C-N-CA	6.15	128.52	120.28
30	K	427	TYR	N-CA-C	-6.15	103.94	112.30
14	n	36	GLN	CA-C-N	6.14	126.06	119.85
14	n	36	GLN	C-N-CA	6.14	126.06	119.85
3	C	233	GLN	OE1-CD-NE2	6.14	128.75	122.60
25	R	145	GLY	CA-C-N	6.14	133.28	121.54
25	R	145	GLY	C-N-CA	6.14	133.28	121.54
28	H	353	PHE	CB-CG-CD1	-6.14	110.25	120.70
32	M	393	ALA	CA-C-N	6.14	128.30	120.56
32	M	393	ALA	C-N-CA	6.14	128.30	120.56
11	k	142	SER	CA-C-O	-6.14	113.98	120.55
9	2	95	HIS	CE1-NE2-CD2	-6.14	102.86	109.00
21	N	813	ARG	CA-C-N	6.14	129.12	120.28
21	N	813	ARG	C-N-CA	6.14	129.12	120.28
12	l	82	ARG	NH1-CZ-NH2	-6.14	111.32	119.30
13	m	44	ASN	CB-CG-ND2	-6.14	107.19	116.40
13	m	104	LEU	CA-C-O	6.14	127.06	120.55
14	n	155	ASN	N-CA-C	-6.14	105.95	113.50
18	X	31	GLY	CA-C-O	-6.14	114.93	121.38
31	L	73	GLN	CA-CB-CG	-6.14	101.82	114.10
14	n	86	ILE	O-C-N	-6.14	116.71	123.03
12	5	141	HIS	ND1-CE1-NE2	6.14	114.54	108.40
11	k	153	THR	CA-CB-OG1	6.14	118.80	109.60
21	N	349	ILE	CA-C-N	6.14	131.11	120.68
21	N	349	ILE	C-N-CA	6.14	131.11	120.68
24	Q	191	LEU	CA-C-N	6.14	128.50	120.28
24	Q	191	LEU	C-N-CA	6.14	128.50	120.28
27	O	166	ARG	NE-CZ-NH1	6.14	127.64	121.50
10	j	127	ILE	N-CA-C	-6.13	107.15	113.10
11	k	39	SER	CA-C-N	6.13	127.51	119.84
11	k	39	SER	C-N-CA	6.13	127.51	119.84
22	S	90	LYS	CA-C-N	6.13	128.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	90	LYS	C-N-CA	6.13	128.50	120.28
29	I	185	GLY	CA-C-N	6.13	129.46	121.85
29	I	185	GLY	C-N-CA	6.13	129.46	121.85
20	Z	718	ASP	CA-CB-CG	6.13	118.73	112.60
26	U	279	SER	O-C-N	6.13	128.62	122.12
31	L	280	MET	CG-SD-CE	-6.13	87.41	100.90
2	b	136	ILE	O-C-N	6.13	129.56	123.18
20	Z	722	ASP	CA-C-N	6.13	128.78	120.44
20	Z	722	ASP	C-N-CA	6.13	128.78	120.44
5	E	87	SER	CA-C-N	6.13	128.49	120.28
5	E	87	SER	C-N-CA	6.13	128.49	120.28
20	Z	778	LEU	CA-C-N	6.13	128.49	120.28
20	Z	778	LEU	C-N-CA	6.13	128.49	120.28
23	P	440	HIS	ND1-CE1-NE2	6.13	114.53	108.40
28	H	304	CYS	CA-C-O	6.13	128.37	121.51
17	T	239	SER	CA-C-O	-6.13	114.06	120.55
3	c	15	PRO	N-CA-CB	6.12	109.31	103.19
7	g	125	LEU	CA-C-O	-6.12	111.87	119.28
9	2	181	ILE	O-C-N	6.12	128.27	121.90
10	3	60	VAL	CA-C-O	-6.12	114.36	120.85
12	5	185	PRO	N-CA-C	-6.12	101.58	111.19
25	R	60	ALA	CA-C-O	-6.12	112.40	118.34
28	H	262	ALA	N-CA-C	-6.12	104.53	111.14
6	f	142	ALA	CA-C-O	-6.12	114.46	121.19
15	W	180	LEU	N-CA-CB	6.12	120.83	110.49
33	J	154	THR	O-C-N	6.12	129.13	122.15
10	j	63	LEU	O-C-N	6.12	130.63	122.43
26	U	110	PHE	N-CA-CB	6.12	119.72	110.30
33	J	240	HIS	ND1-CE1-NE2	6.12	114.52	108.40
7	G	121	GLN	OE1-CD-NE2	-6.12	116.48	122.60
22	S	90	LYS	O-C-N	-6.12	115.63	122.12
26	U	161	ILE	N-CA-C	-6.12	99.67	108.48
8	h	88	ALA	CA-C-O	-6.12	114.07	120.55
32	M	42	ARG	CA-C-N	6.12	129.11	120.42
32	M	42	ARG	C-N-CA	6.12	129.11	120.42
4	d	212	ILE	N-CA-C	-6.11	99.67	108.48
16	V	240	ALA	CB-CA-C	-6.11	100.64	110.79
8	1	166	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
20	Z	760	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
24	Q	309	ARG	NE-CZ-NH1	6.11	127.61	121.50
27	O	273	GLN	OE1-CD-NE2	6.11	128.71	122.60
1	a	113	PRO	N-CA-CB	6.11	109.80	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	136	PHE	N-CA-C	-6.11	98.36	108.07
24	Q	285	LYS	CB-CA-C	-6.11	98.26	110.42
26	U	261	LEU	CA-C-N	6.11	128.97	120.29
26	U	261	LEU	C-N-CA	6.11	128.97	120.29
29	I	151	HIS	CA-CB-CG	-6.11	107.69	113.80
7	g	92	GLY	CA-C-N	6.11	128.47	120.28
7	g	92	GLY	C-N-CA	6.11	128.47	120.28
3	c	10	THR	N-CA-CB	6.11	119.48	110.56
5	e	217	ALA	N-CA-C	6.11	118.46	109.24
7	g	38	ILE	CA-C-N	6.11	125.80	121.65
7	g	38	ILE	C-N-CA	6.11	125.80	121.65
13	m	65	PHE	CA-CB-CG	6.11	119.91	113.80
20	Z	559	LYS	CA-C-N	6.11	129.08	120.28
20	Z	559	LYS	C-N-CA	6.11	129.08	120.28
30	K	44	ASN	N-CA-CB	6.11	119.10	110.12
9	2	64	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
14	7	36	GLN	O-C-N	6.11	126.54	121.35
27	O	378	GLU	CB-CA-C	-6.11	100.47	110.85
4	D	68	ASP	N-CA-C	-6.10	101.47	108.49
4	D	201	GLU	N-CA-C	6.10	117.93	111.28
14	7	109	TYR	CA-C-N	6.10	133.19	121.54
14	7	109	TYR	C-N-CA	6.10	133.19	121.54
20	Z	727	GLU	CA-C-O	-6.10	114.48	120.89
5	e	156	PHE	CA-CB-CG	-6.10	107.70	113.80
12	5	81	PHE	CA-C-O	6.10	127.82	120.99
13	6	186	GLU	CA-C-O	-6.10	112.95	119.97
19	Y	6	ALA	CA-C-N	6.10	129.58	120.31
19	Y	6	ALA	C-N-CA	6.10	129.58	120.31
20	Z	858	GLY	CA-C-O	6.10	128.26	121.67
21	N	7	ALA	O-C-N	6.10	126.74	120.70
9	i	66	ILE	CA-C-O	6.10	128.27	120.83
6	F	96	SER	CA-C-N	6.10	128.74	120.44
6	F	96	SER	C-N-CA	6.10	128.74	120.44
7	G	66	LYS	N-CA-C	-6.10	103.55	113.19
12	5	80	ALA	N-CA-CB	6.10	122.87	111.52
14	7	242	LYS	O-C-N	-6.10	116.19	123.27
20	Z	427	GLN	CB-CG-CD	-6.10	102.23	112.60
20	Z	959	HIS	CA-C-N	6.10	131.99	121.07
20	Z	959	HIS	C-N-CA	6.10	131.99	121.07
26	U	219	LEU	N-CA-C	-6.10	101.87	110.29
30	K	213	GLY	CA-C-N	6.10	126.66	120.38
30	K	213	GLY	C-N-CA	6.10	126.66	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	234	ASP	CA-C-O	6.10	127.09	120.32
22	S	127	THR	N-CA-C	-6.10	100.33	108.74
1	a	41	ASN	CA-CB-CG	-6.10	106.50	112.60
13	6	155	MET	CA-C-O	-6.10	111.81	120.16
27	O	360	GLY	CA-C-O	-6.10	114.47	120.75
5	E	133	LEU	CB-CA-C	-6.09	100.09	109.29
20	Z	505	VAL	CA-C-O	6.09	127.81	121.05
27	O	371	VAL	CB-CA-C	-6.09	103.81	112.22
32	M	187	ASP	CA-C-N	6.09	128.94	120.29
32	M	187	ASP	C-N-CA	6.09	128.94	120.29
21	N	866	TYR	CA-C-N	6.09	130.53	122.30
21	N	866	TYR	C-N-CA	6.09	130.53	122.30
27	O	48	PHE	CA-C-O	-6.09	114.42	120.82
31	L	150	ILE	N-CA-C	-6.09	103.76	112.35
8	1	84	THR	O-C-N	-6.09	115.66	122.12
9	2	173	GLN	N-CA-CB	6.09	119.38	109.69
20	Z	482	ASP	CA-C-N	6.09	128.94	120.29
20	Z	482	ASP	C-N-CA	6.09	128.94	120.29
26	U	134	THR	O-C-N	-6.09	115.31	123.23
29	I	383	THR	CA-C-N	6.09	131.50	121.39
29	I	383	THR	C-N-CA	6.09	131.50	121.39
11	k	116	LEU	N-CA-CB	6.09	120.13	110.57
7	G	70	VAL	N-CA-C	-6.09	99.35	108.12
20	Z	93	ARG	CA-C-O	-6.09	111.82	120.16
20	Z	574	TYR	N-CA-C	6.09	119.97	112.54
25	R	72	VAL	N-CA-CB	6.09	121.28	111.23
32	M	330	VAL	O-C-N	-6.09	116.23	122.14
4	D	220	ASP	CA-CB-CG	6.09	118.69	112.60
20	Z	480	ASN	CA-C-O	-6.09	113.81	120.69
26	U	113	TYR	CA-C-O	-6.09	114.10	120.55
33	J	13	GLU	CA-C-O	-6.09	113.22	120.10
25	R	100	ASN	CB-CG-ND2	6.09	125.53	116.40
13	6	184	SER	CA-C-N	6.08	128.80	120.46
13	6	184	SER	C-N-CA	6.08	128.80	120.46
4	D	100	LEU	N-CA-C	-6.08	105.52	113.12
13	6	81	LYS	CA-C-O	6.08	127.21	120.82
21	N	777	ALA	CA-C-O	-6.08	114.93	121.38
22	S	179	ILE	CB-CA-C	-6.08	104.07	112.04
24	Q	177	VAL	CA-C-N	6.08	128.93	120.29
24	Q	177	VAL	C-N-CA	6.08	128.93	120.29
26	U	269	THR	N-CA-C	6.08	117.99	111.36
2	b	138	GLY	CA-C-O	-6.08	115.63	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	59	VAL	N-CA-C	-6.08	99.66	108.17
21	N	905	LEU	N-CA-C	-6.08	98.99	108.90
23	P	189	LEU	N-CA-C	-6.08	104.77	111.82
12	l	267	ASP	CA-C-O	-6.08	113.99	120.92
10	3	49	VAL	O-C-N	6.08	129.34	123.14
13	6	97	ALA	N-CA-C	6.08	117.91	111.28
16	V	288	LEU	CA-C-N	6.08	128.92	120.29
16	V	288	LEU	C-N-CA	6.08	128.92	120.29
16	V	237	ASN	N-CA-C	6.08	117.57	111.07
21	N	630	ALA	CB-CA-C	-6.08	101.34	110.88
30	K	134	SER	CA-C-N	6.08	132.19	121.80
30	K	134	SER	C-N-CA	6.08	132.19	121.80
10	3	159	GLU	CA-C-N	6.08	125.80	119.05
10	3	159	GLU	C-N-CA	6.08	125.80	119.05
4	d	84	ILE	CA-C-N	6.08	128.92	120.29
4	d	84	ILE	C-N-CA	6.08	128.92	120.29
4	d	121	THR	CA-C-N	6.08	128.34	120.44
4	d	121	THR	C-N-CA	6.08	128.34	120.44
6	F	145	LEU	N-CA-CB	6.08	121.47	111.08
16	V	32	ILE	N-CA-CB	6.08	117.66	110.55
20	Z	290	GLU	CA-C-N	6.08	128.42	120.28
20	Z	290	GLU	C-N-CA	6.08	128.42	120.28
23	P	36	LEU	CA-C-N	6.08	129.03	120.28
23	P	36	LEU	C-N-CA	6.08	129.03	120.28
24	Q	68	MET	N-CA-CB	6.08	120.83	110.50
2	b	98	LYS	N-CA-C	-6.07	105.80	112.72
20	Z	208	VAL	CA-CB-CG2	-6.07	100.07	110.40
20	Z	338	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
30	K	323	THR	N-CA-C	-6.07	104.25	112.26
12	l	235	SER	N-CA-CB	6.07	119.14	110.16
4	D	231	GLN	N-CA-CB	6.07	119.14	110.16
23	P	210	ASN	N-CA-C	-6.07	101.72	110.40
30	K	410	ALA	N-CA-C	6.07	117.98	111.36
1	a	95	LEU	N-CA-C	6.07	117.56	111.07
5	e	203	ILE	CA-C-O	-6.07	114.42	120.85
20	Z	593	HIS	N-CA-C	-6.07	100.28	108.11
21	N	129	ILE	N-CA-C	-6.07	99.67	108.17
25	R	262	GLU	N-CA-CB	6.07	118.69	110.38
27	O	93	ASP	CA-CB-CG	-6.07	106.53	112.60
31	L	135	VAL	N-CA-C	-6.07	98.97	108.86
33	J	211	ILE	CA-CB-CG1	6.07	120.71	110.40
1	a	13	ASP	N-CA-C	6.07	123.72	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	95	CYS	CA-C-N	6.07	128.90	120.29
8	h	95	CYS	C-N-CA	6.07	128.90	120.29
13	6	203	HIS	CE1-NE2-CD2	-6.06	102.94	109.00
27	O	51	ASP	CA-CB-CG	-6.06	106.54	112.60
30	K	325	ASP	CA-C-O	-6.06	114.83	119.32
31	L	141	LYS	O-C-N	-6.06	116.13	123.10
6	f	99	PHE	CA-CB-CG	-6.06	107.74	113.80
9	i	237	GLY	CA-C-N	6.06	132.75	122.26
9	i	237	GLY	C-N-CA	6.06	132.75	122.26
9	2	110	GLN	N-CA-C	6.06	117.69	111.14
20	Z	48	ASP	O-C-N	6.06	128.54	122.12
22	S	82	TYR	CA-C-O	-6.06	114.55	120.19
23	P	211	PRO	O-C-N	6.06	130.81	122.38
23	P	290	LEU	N-CA-C	-6.06	105.53	113.17
32	M	28	GLN	OE1-CD-NE2	-6.06	116.54	122.60
25	R	251	THR	CA-CB-OG1	6.06	118.69	109.60
16	V	133	ASN	CA-CB-CG	-6.06	106.54	112.60
22	S	360	PHE	CA-C-N	6.06	128.32	120.44
22	S	360	PHE	C-N-CA	6.06	128.32	120.44
33	J	199	ALA	CA-C-O	-6.06	113.25	120.10
24	Q	261	VAL	CA-C-O	-6.06	114.43	120.85
25	R	80	GLU	N-CA-C	-6.06	105.81	112.72
33	J	319	PRO	CA-C-O	-6.06	114.43	121.34
23	P	368	LEU	CA-C-O	-6.05	114.13	120.55
2	b	64	VAL	CA-C-O	6.05	127.14	120.48
3	c	82	ALA	CA-C-N	6.05	128.39	120.28
3	c	82	ALA	C-N-CA	6.05	128.39	120.28
24	Q	300	LYS	CA-C-N	6.05	128.89	120.29
24	Q	300	LYS	C-N-CA	6.05	128.89	120.29
1	A	87	ILE	CB-CA-C	-6.05	107.94	114.35
5	E	226	ASP	N-CA-C	-6.05	105.85	113.72
20	Z	278	LEU	CA-C-N	6.05	128.88	120.29
20	Z	278	LEU	C-N-CA	6.05	128.88	120.29
28	H	243	PRO	CA-C-O	-6.05	114.44	121.34
31	L	100	SER	N-CA-C	-6.05	104.60	111.14
31	L	398	ALA	CA-C-N	6.05	127.90	120.22
31	L	398	ALA	C-N-CA	6.05	127.90	120.22
4	D	100	LEU	N-CA-CB	6.05	119.67	110.42
14	7	166	LEU	N-CA-C	-6.05	105.90	113.28
27	O	15	ARG	O-C-N	6.05	129.05	122.15
28	H	354	ALA	N-CA-CB	6.05	121.27	110.80
30	K	64	GLN	CB-CA-C	-6.05	100.75	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	197	ASP	CA-CB-CG	-6.05	106.55	112.60
21	N	46	ILE	CA-C-N	6.05	128.38	120.28
21	N	46	ILE	C-N-CA	6.05	128.38	120.28
22	S	18	LEU	CA-C-N	6.05	128.30	120.44
22	S	18	LEU	C-N-CA	6.05	128.30	120.44
23	P	275	ASN	N-CA-C	-6.05	105.39	112.89
2	b	122	THR	N-CA-C	-6.05	105.86	113.72
8	1	37	ASN	CA-CB-CG	-6.05	106.55	112.60
20	Z	761	PHE	CA-C-N	6.05	126.69	119.98
20	Z	761	PHE	C-N-CA	6.05	126.69	119.98
22	S	434	ALA	CA-C-O	6.05	127.77	121.36
23	P	305	THR	CA-C-N	6.05	131.00	121.99
23	P	305	THR	C-N-CA	6.05	131.00	121.99
26	U	217	LYS	CA-C-N	6.05	130.94	122.36
26	U	217	LYS	C-N-CA	6.05	130.94	122.36
23	P	145	GLU	N-CA-CB	6.04	119.53	110.22
24	Q	119	GLU	N-CA-CB	6.04	119.01	110.12
5	e	34	GLY	CA-C-N	6.04	131.08	120.87
5	e	34	GLY	C-N-CA	6.04	131.08	120.87
25	R	345	TYR	CB-CA-C	-6.04	99.07	109.65
2	b	139	HIS	ND1-CE1-NE2	6.04	114.44	108.40
16	V	201	ILE	CA-C-N	6.04	133.73	122.74
16	V	201	ILE	C-N-CA	6.04	133.73	122.74
21	N	163	LEU	N-CA-C	-6.04	104.06	112.45
23	P	432	LEU	CA-C-O	6.04	126.34	119.27
6	f	210	ASN	N-CA-C	-6.04	105.87	113.72
20	Z	737	ALA	O-C-N	6.04	128.52	122.12
21	N	223	LEU	N-CA-C	-6.04	104.26	111.69
22	S	302	HIS	CA-CB-CG	-6.04	107.76	113.80
9	i	32	ILE	N-CA-C	-6.04	99.79	108.48
11	4	96	ARG	CA-C-O	-6.04	113.53	119.69
21	N	700	CYS	CA-C-N	6.04	128.99	120.42
21	N	700	CYS	C-N-CA	6.04	128.99	120.42
25	R	311	THR	O-C-N	6.04	128.29	122.07
5	E	86	ARG	N-CA-C	-6.04	104.62	111.14
20	Z	856	HIS	ND1-CE1-NE2	6.04	114.44	108.40
22	S	28	GLU	CA-C-N	6.04	128.86	120.29
22	S	28	GLU	C-N-CA	6.04	128.86	120.29
25	R	21	VAL	CB-CA-C	-6.04	107.95	114.35
25	R	399	GLN	OE1-CD-NE2	-6.04	116.56	122.60
2	B	236	ARG	CD-NE-CZ	-6.03	115.95	124.40
27	O	367	LYS	N-CA-CB	6.03	118.76	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	57	THR	N-CA-C	-6.03	103.63	111.71
5	e	102	TYR	CB-CG-CD2	6.03	129.85	120.80
21	N	179	THR	CA-C-N	6.03	128.85	120.29
21	N	179	THR	C-N-CA	6.03	128.85	120.29
32	M	38	ASP	CA-C-N	6.03	128.85	120.29
32	M	38	ASP	C-N-CA	6.03	128.85	120.29
11	k	133	HIS	CE1-NE2-CD2	-6.03	102.97	109.00
12	l	141	HIS	CE1-NE2-CD2	-6.03	102.97	109.00
22	S	232	MET	CA-C-N	6.03	129.48	120.31
22	S	232	MET	C-N-CA	6.03	129.48	120.31
31	L	360	ILE	CA-C-N	6.03	128.36	120.28
31	L	360	ILE	C-N-CA	6.03	128.36	120.28
11	k	27	VAL	N-CA-CB	6.03	117.70	110.95
26	U	213	LYS	N-CA-C	6.03	120.47	113.18
31	L	134	SER	O-C-N	6.03	130.17	122.39
14	n	69	PHE	N-CA-C	-6.03	98.02	108.69
14	n	240	THR	N-CA-C	-6.03	98.59	108.41
2	B	186	GLU	O-C-N	-6.03	115.73	122.12
7	G	16	SER	CA-C-N	6.03	125.73	119.82
7	G	16	SER	C-N-CA	6.03	125.73	119.82
26	U	88	LYS	CA-C-O	-6.03	114.71	121.40
1	A	85	GLY	CA-C-N	6.03	127.37	119.84
1	A	85	GLY	C-N-CA	6.03	127.37	119.84
5	E	130	GLU	N-CA-C	-6.03	97.97	110.80
14	7	234	ASP	O-C-N	-6.03	115.83	123.24
28	H	139	ASP	N-CA-C	-6.03	99.57	108.79
30	K	252	ARG	CD-NE-CZ	-6.03	115.97	124.40
33	J	209	LYS	O-C-N	6.03	129.80	122.75
33	J	364	GLU	N-CA-C	6.03	117.93	111.36
4	d	133	THR	CA-CB-OG1	6.02	118.64	109.60
24	Q	214	THR	N-CA-C	-6.02	104.71	111.28
9	i	195	ASP	N-CA-CB	6.02	120.10	110.46
5	E	238	GLU	CB-CG-CD	-6.02	102.36	112.60
25	R	362	ALA	CA-C-N	6.02	128.84	120.29
25	R	362	ALA	C-N-CA	6.02	128.84	120.29
12	l	108	LYS	CA-C-O	6.02	127.05	119.95
13	6	130	VAL	N-CA-C	-6.02	100.02	108.27
1	A	106	TYR	N-CA-C	6.02	119.82	112.23
25	R	169	ASP	CA-C-N	6.02	128.71	120.46
25	R	169	ASP	C-N-CA	6.02	128.71	120.46
25	R	391	ASN	N-CA-C	-6.02	101.29	109.54
23	P	174	SER	CA-C-N	6.02	128.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	174	SER	C-N-CA	6.02	128.26	120.44
4	d	241	GLN	OE1-CD-NE2	6.02	128.62	122.60
25	R	206	ARG	CD-NE-CZ	-6.02	115.98	124.40
3	C	121	GLY	CA-C-N	6.01	130.76	120.72
3	C	121	GLY	C-N-CA	6.01	130.76	120.72
4	D	216	LYS	O-C-N	6.01	126.43	121.32
11	4	10	GLN	CA-C-O	-6.01	114.18	120.55
31	L	311	GLN	OE1-CD-NE2	6.01	128.61	122.60
16	V	104	VAL	N-CA-C	6.01	118.29	109.63
20	Z	878	LEU	O-C-N	6.01	129.25	122.22
3	C	219	GLY	N-CA-C	-6.01	106.28	115.66
7	G	178	LYS	CB-CA-C	-6.01	100.81	110.79
11	4	100	VAL	CA-CB-CG2	-6.01	100.18	110.40
20	Z	60	ASP	CA-C-N	6.01	128.82	120.29
20	Z	60	ASP	C-N-CA	6.01	128.82	120.29
20	Z	898	HIS	CG-CD2-NE2	6.01	113.21	107.20
5	E	227	GLY	CA-C-O	-6.01	114.96	122.65
6	F	196	ALA	CA-C-O	6.01	126.92	120.55
14	n	141	ASN	N-CA-C	-6.01	96.54	109.81
14	n	228	PHE	N-CA-CB	6.01	120.87	111.56
3	C	212	GLU	O-C-N	-6.01	115.38	123.19
24	Q	335	PHE	CA-C-N	6.01	128.25	120.44
24	Q	335	PHE	C-N-CA	6.01	128.25	120.44
10	j	146	LEU	CA-C-N	6.00	128.33	120.28
10	j	146	LEU	C-N-CA	6.00	128.33	120.28
17	T	184	ALA	CA-C-N	6.00	128.13	120.56
17	T	184	ALA	C-N-CA	6.00	128.13	120.56
21	N	361	ASN	OD1-CG-ND2	6.00	128.60	122.60
10	j	123	GLY	N-CA-C	-6.00	101.94	111.18
26	U	5	HIS	CA-CB-CG	6.00	119.80	113.80
26	U	287	ALA	CB-CA-C	-6.00	101.42	110.90
28	H	409	ARG	O-C-N	6.00	128.25	122.07
12	5	232	GLY	CA-C-N	6.00	130.84	120.58
12	5	232	GLY	C-N-CA	6.00	130.84	120.58
24	Q	185	TYR	CA-C-N	6.00	128.32	120.28
24	Q	185	TYR	C-N-CA	6.00	128.32	120.28
32	M	304	THR	CA-CB-OG1	6.00	118.60	109.60
14	7	252	TRP	CB-CG-CD1	6.00	135.90	126.90
22	S	300	ALA	O-C-N	-6.00	115.12	121.30
26	U	272	GLU	CA-C-N	6.00	128.32	120.28
26	U	272	GLU	C-N-CA	6.00	128.32	120.28
8	h	185	VAL	N-CA-C	-6.00	98.89	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	75	ALA	CA-C-O	-6.00	114.74	121.40
7	G	102	LEU	O-C-N	6.00	128.99	122.15
11	4	108	ASP	N-CA-CB	6.00	118.95	109.71
23	P	234	TYR	CA-CB-CG	-6.00	103.10	113.90
24	Q	332	ARG	CA-C-N	6.00	128.81	120.29
24	Q	332	ARG	C-N-CA	6.00	128.81	120.29
25	R	282	THR	N-CA-C	-6.00	106.57	114.31
2	b	70	ASP	CA-CB-CG	-6.00	106.60	112.60
12	l	147	GLU	N-CA-C	-6.00	98.50	108.75
14	n	253	ASP	CA-CB-CG	-6.00	106.60	112.60
21	N	338	PHE	N-CA-C	-6.00	104.82	111.36
26	U	281	LEU	N-CA-CB	6.00	118.94	110.12
2	B	99	ARG	N-CA-C	-6.00	104.80	114.09
26	U	84	ASN	CA-CB-CG	6.00	118.59	112.60
8	1	47	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
26	U	116	ASN	CA-CB-CG	5.99	118.59	112.60
30	K	338	ILE	CA-C-N	5.99	130.39	122.30
30	K	338	ILE	C-N-CA	5.99	130.39	122.30
1	a	51	THR	O-C-N	-5.99	115.87	123.24
7	g	58	LEU	N-CA-CB	5.99	119.56	110.28
13	m	54	CYS	N-CA-C	-5.99	106.58	114.31
1	A	193	HIS	CA-C-N	5.99	129.24	120.91
1	A	193	HIS	C-N-CA	5.99	129.24	120.91
4	D	201	GLU	CB-CA-C	-5.99	100.85	110.79
7	G	43	ASN	OD1-CG-ND2	5.99	128.59	122.60
9	2	214	GLU	CA-C-N	5.99	130.92	121.99
9	2	214	GLU	C-N-CA	5.99	130.92	121.99
17	T	229	VAL	CA-C-O	-5.99	114.01	120.36
21	N	850	LYS	CA-C-N	5.99	131.62	123.11
21	N	850	LYS	C-N-CA	5.99	131.62	123.11
31	L	77	ARG	CB-CA-C	-5.99	100.85	110.79
32	M	203	ARG	CA-C-O	5.99	127.88	120.15
32	M	281	ASP	CA-C-N	5.99	130.91	121.56
32	M	281	ASP	C-N-CA	5.99	130.91	121.56
7	G	182	HIS	ND1-CE1-NE2	5.99	114.39	108.40
12	5	129	PHE	N-CA-CB	5.99	118.69	110.01
33	J	62	LEU	CA-C-N	5.99	128.22	120.44
33	J	62	LEU	C-N-CA	5.99	128.22	120.44
10	j	167	ILE	O-C-N	-5.99	115.03	121.80
10	3	61	THR	N-CA-C	-5.99	104.33	111.69
23	P	440	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
29	I	143	PRO	N-CA-CB	5.99	108.56	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	142	ASP	O-C-N	-5.98	116.19	123.19
17	T	142	LEU	CB-CA-C	-5.98	99.24	110.01
31	L	235	VAL	N-CA-C	5.98	116.72	110.62
1	a	193	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
7	g	181	ASP	CB-CA-C	-5.98	100.68	110.85
13	m	205	GLN	OE1-CD-NE2	5.98	128.58	122.60
13	m	229	ARG	N-CA-C	-5.98	104.11	112.25
8	1	74	LEU	N-CA-CB	5.98	118.92	110.12
16	V	52	LEU	CA-C-O	-5.98	114.11	121.11
18	X	97	TYR	N-CA-C	-5.98	99.31	108.76
23	P	100	VAL	N-CA-C	-5.98	104.68	110.72
29	I	270	VAL	CA-C-N	5.98	128.30	120.28
29	I	270	VAL	C-N-CA	5.98	128.30	120.28
31	L	217	GLY	O-C-N	-5.98	114.92	122.70
6	f	185	ASN	N-CA-CB	5.98	120.59	110.43
8	h	136	ALA	N-CA-CB	5.98	120.83	111.56
6	F	69	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
7	G	148	LEU	N-CA-C	-5.98	98.89	109.06
20	Z	300	ALA	N-CA-C	5.98	117.80	111.28
30	K	37	ASN	CA-CB-CG	5.98	118.58	112.60
3	c	10	THR	N-CA-C	-5.98	105.56	112.92
29	I	299	GLU	N-CA-C	-5.98	104.70	112.23
33	J	122	LEU	CA-C-N	5.98	132.96	121.54
33	J	122	LEU	C-N-CA	5.98	132.96	121.54
2	b	80	PRO	O-C-N	5.98	129.70	122.23
7	g	72	ARG	N-CA-C	-5.98	103.31	111.56
9	2	145	HIS	CA-CB-CG	-5.98	107.82	113.80
17	T	191	LYS	CA-C-O	-5.98	114.21	120.55
21	N	7	ALA	CA-C-N	5.98	126.13	119.32
21	N	7	ALA	C-N-CA	5.98	126.13	119.32
23	P	257	TRP	N-CA-CB	5.98	120.14	110.40
4	D	198	SER	CB-CA-C	-5.98	100.87	110.79
20	Z	282	ILE	CA-C-N	5.98	128.29	120.28
20	Z	282	ILE	C-N-CA	5.98	128.29	120.28
7	G	130	ARG	NE-CZ-NH1	-5.97	115.53	121.50
7	G	193	VAL	N-CA-CB	5.97	118.22	110.57
21	N	203	ARG	N-CA-CB	-5.97	101.34	110.12
22	S	395	ILE	CA-C-N	5.97	128.29	120.28
22	S	395	ILE	C-N-CA	5.97	128.29	120.28
23	P	415	TRP	CB-CA-C	-5.97	99.20	110.67
25	R	21	VAL	CA-C-O	-5.97	113.77	118.85
26	U	7	LYS	N-CA-C	-5.97	100.06	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	58	TYR	N-CA-C	-5.97	105.95	113.18
12	5	87	ILE	O-C-N	-5.97	116.73	123.18
21	N	393	SER	N-CA-C	-5.97	103.38	112.99
9	2	251	ASP	O-C-N	-5.97	115.95	123.17
20	Z	751	ASP	CA-C-N	5.97	128.90	120.42
20	Z	751	ASP	C-N-CA	5.97	128.90	120.42
5	E	124	GLY	N-CA-C	-5.97	99.04	113.18
9	2	93	GLU	CA-C-N	5.97	128.20	120.44
9	2	93	GLU	C-N-CA	5.97	128.20	120.44
31	L	351	LEU	CA-C-N	5.97	125.99	119.90
31	L	351	LEU	C-N-CA	5.97	125.99	119.90
3	c	94	HIS	CA-C-N	5.97	128.28	120.28
3	c	94	HIS	C-N-CA	5.97	128.28	120.28
3	c	176	LEU	CB-CA-C	-5.97	100.71	110.85
20	Z	24	THR	CA-C-O	-5.97	111.99	120.16
22	S	160	ARG	CB-CG-CD	5.97	125.02	111.30
23	P	194	SER	O-C-N	5.97	128.44	122.12
29	I	125	MET	CA-C-O	-5.97	112.55	118.34
33	J	322	ALA	N-CA-C	-5.97	104.86	111.36
2	B	114	VAL	CA-C-N	5.96	128.27	120.28
2	B	114	VAL	C-N-CA	5.96	128.27	120.28
15	W	29	GLN	OE1-CD-NE2	5.96	128.56	122.60
21	N	56	SER	N-CA-C	-5.96	105.77	113.16
21	N	600	THR	CA-CB-OG1	5.96	118.55	109.60
3	c	156	ASN	N-CA-C	-5.96	100.08	108.96
11	4	135	TYR	CA-C-N	5.96	129.37	120.31
11	4	135	TYR	C-N-CA	5.96	129.37	120.31
20	Z	338	HIS	CA-C-N	5.96	132.93	121.54
20	Z	338	HIS	C-N-CA	5.96	132.93	121.54
25	R	267	LYS	CA-C-O	5.96	127.08	120.82
29	I	167	MET	CA-C-N	5.96	128.63	120.46
29	I	167	MET	C-N-CA	5.96	128.63	120.46
31	L	401	PHE	CA-C-O	-5.96	114.10	120.42
13	6	96	SER	O-C-N	5.96	128.94	122.15
2	B	66	LEU	N-CA-CB	5.96	119.58	109.87
6	F	122	SER	O-C-N	-5.96	115.32	122.65
8	1	64	ILE	N-CA-C	5.96	116.70	110.62
20	Z	307	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
26	U	94	HIS	N-CA-C	-5.96	99.19	108.90
28	H	194	SER	O-C-N	-5.96	114.67	122.59
31	L	198	GLU	N-CA-C	5.96	117.78	111.28
5	E	177	GLU	CB-CA-C	-5.96	100.72	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	100	ASP	CA-CB-CG	-5.96	106.64	112.60
11	4	104	ILE	N-CA-C	-5.96	97.23	107.24
14	7	99	LEU	N-CA-CB	5.96	118.98	110.16
20	Z	337	GLU	N-CA-C	5.96	117.57	111.14
20	Z	370	SER	N-CA-C	-5.96	105.84	114.12
21	N	175	ASP	N-CA-CB	5.96	120.56	110.49
23	P	128	ASN	N-CA-C	-5.96	100.91	110.14
27	O	161	ASP	CA-CB-CG	-5.96	106.64	112.60
32	M	77	TYR	N-CA-CB	5.96	120.79	111.56
8	1	47	HIS	CA-C-N	5.96	128.75	120.29
8	1	47	HIS	C-N-CA	5.96	128.75	120.29
32	M	253	GLN	CA-C-N	5.96	133.16	122.38
32	M	253	GLN	C-N-CA	5.96	133.16	122.38
1	a	157	THR	N-CA-C	-5.95	99.19	108.90
11	4	13	VAL	CA-CB-CG2	5.95	120.52	110.40
29	I	170	VAL	CA-C-N	5.95	128.18	120.44
29	I	170	VAL	C-N-CA	5.95	128.18	120.44
7	g	183	HIS	CG-CD2-NE2	5.95	113.15	107.20
17	T	126	LEU	CA-C-N	5.95	128.25	120.28
17	T	126	LEU	C-N-CA	5.95	128.25	120.28
20	Z	151	HIS	CG-CD2-NE2	5.95	113.15	107.20
11	k	147	HIS	CA-CB-CG	-5.95	107.85	113.80
12	l	144	ARG	CA-C-O	-5.95	114.11	120.42
14	n	130	ALA	CA-C-N	5.95	128.25	120.28
14	n	130	ALA	C-N-CA	5.95	128.25	120.28
21	N	270	LEU	CA-C-N	5.95	128.25	120.28
21	N	270	LEU	C-N-CA	5.95	128.25	120.28
22	S	185	PHE	CA-C-N	5.95	128.74	120.29
22	S	185	PHE	C-N-CA	5.95	128.74	120.29
28	H	253	GLY	CA-C-N	5.95	128.74	120.29
28	H	253	GLY	C-N-CA	5.95	128.74	120.29
23	P	301	LYS	CA-C-N	5.95	129.35	120.31
23	P	301	LYS	C-N-CA	5.95	129.35	120.31
29	I	399	ALA	O-C-N	5.95	128.43	122.12
2	B	56	ALA	N-CA-CB	5.95	118.73	110.17
24	Q	401	GLU	N-CA-C	-5.95	104.69	113.61
4	d	196	VAL	CA-C-N	5.95	128.25	120.28
4	d	196	VAL	C-N-CA	5.95	128.25	120.28
22	S	241	PHE	CA-CB-CG	5.95	119.75	113.80
25	R	210	TYR	CB-CG-CD2	-5.95	111.88	120.80
32	M	44	PHE	CA-C-N	5.95	128.25	120.28
32	M	44	PHE	C-N-CA	5.95	128.25	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	265	ASP	CB-CA-C	-5.95	101.51	110.90
2	B	133	SER	N-CA-C	-5.94	99.71	109.40
2	b	10	THR	O-C-N	5.94	129.36	122.17
2	B	151	ASP	CA-C-N	5.94	126.05	119.87
2	B	151	ASP	C-N-CA	5.94	126.05	119.87
7	G	57	LYS	N-CA-C	-5.94	105.34	112.59
15	W	188	SER	O-C-N	-5.94	114.99	121.53
2	b	244	ASN	OD1-CG-ND2	-5.94	116.66	122.60
8	h	113	ASP	CA-CB-CG	-5.94	106.66	112.60
11	k	162	LYS	CA-C-N	5.94	128.24	120.28
11	k	162	LYS	C-N-CA	5.94	128.24	120.28
5	E	96	ALA	CA-C-N	5.94	128.60	120.46
5	E	96	ALA	C-N-CA	5.94	128.60	120.46
20	Z	477	TYR	CA-C-O	-5.94	114.25	120.55
23	P	118	VAL	CB-CA-C	-5.94	104.12	112.14
25	R	74	ASN	N-CA-C	-5.94	100.04	109.07
14	n	202	THR	CA-CB-OG1	5.94	118.51	109.60
6	F	118	LYS	N-CA-CB	5.94	118.95	110.16
21	N	499	HIS	CA-C-N	5.94	128.71	120.63
21	N	499	HIS	C-N-CA	5.94	128.71	120.63
3	c	94	HIS	CG-CD2-NE2	5.94	113.14	107.20
28	H	261	ARG	CA-C-N	5.94	128.52	120.44
28	H	261	ARG	C-N-CA	5.94	128.52	120.44
2	b	192	ALA	CA-C-N	5.94	128.23	120.28
2	b	192	ALA	C-N-CA	5.94	128.23	120.28
7	g	238	GLU	CA-C-N	5.93	128.23	120.28
7	g	238	GLU	C-N-CA	5.93	128.23	120.28
22	S	228	GLU	O-C-N	5.93	128.41	122.12
1	a	197	GLU	CB-CA-C	-5.93	97.51	109.55
20	Z	130	GLY	N-CA-C	-5.93	106.91	115.27
20	Z	593	HIS	CG-CD2-NE2	5.93	113.13	107.20
23	P	349	ASN	CA-C-O	-5.93	114.22	120.63
27	O	308	LEU	N-CA-C	-5.93	99.68	108.99
28	H	202	GLU	N-CA-CB	5.93	120.24	110.69
24	Q	104	PHE	CA-C-N	5.93	128.71	120.29
24	Q	104	PHE	C-N-CA	5.93	128.71	120.29
28	H	88	ARG	CB-CA-C	-5.93	101.53	110.90
5	e	71	ASP	O-C-N	-5.93	118.66	123.11
10	j	155	GLU	CA-C-O	-5.93	113.86	119.55
4	D	113	VAL	N-CA-C	5.93	116.71	110.72
6	F	210	ASN	N-CA-C	-5.93	106.38	113.97
22	S	28	GLU	CB-CA-C	-5.93	100.95	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	247	VAL	N-CA-C	5.93	116.10	110.53
23	P	315	GLN	N-CA-C	-5.93	104.73	111.07
25	R	299	SER	CB-CA-C	5.93	119.69	111.63
24	Q	199	THR	N-CA-C	-5.93	104.90	111.36
30	K	190	LEU	CA-C-N	5.93	125.47	119.19
30	K	190	LEU	C-N-CA	5.93	125.47	119.19
32	M	216	LYS	CA-C-O	-5.93	114.60	120.82
23	P	22	PRO	CA-C-N	5.93	128.71	120.29
23	P	22	PRO	C-N-CA	5.93	128.71	120.29
27	O	28	GLN	N-CA-C	5.93	118.53	111.71
29	I	301	GLU	CA-C-N	5.93	128.58	120.46
29	I	301	GLU	C-N-CA	5.93	128.58	120.46
12	5	264	GLY	CA-C-O	-5.92	117.12	122.57
10	j	104	PHE	CA-CB-CG	-5.92	107.88	113.80
6	F	224	ILE	N-CA-C	-5.92	99.88	108.17
17	T	48	ASN	N-CA-C	-5.92	99.95	108.60
24	Q	165	PHE	N-CA-C	-5.92	103.77	111.71
5	E	201	LEU	CA-C-N	5.92	128.70	120.29
5	E	201	LEU	C-N-CA	5.92	128.70	120.29
21	N	294	PRO	CA-C-N	5.92	129.31	120.31
21	N	294	PRO	C-N-CA	5.92	129.31	120.31
23	P	263	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
25	R	50	VAL	CA-C-N	5.92	128.70	120.29
25	R	50	VAL	C-N-CA	5.92	128.70	120.29
26	U	116	ASN	N-CA-C	-5.92	99.73	108.79
28	H	398	VAL	CA-C-N	5.92	129.24	120.95
28	H	398	VAL	C-N-CA	5.92	129.24	120.95
15	W	124	GLU	CA-C-O	-5.92	114.60	120.82
24	Q	336	ASN	CA-C-O	-5.92	114.60	120.82
30	K	68	ILE	CA-CB-CG1	5.92	120.46	110.40
4	d	42	VAL	N-CA-C	-5.92	99.69	108.45
4	d	175	LEU	CA-C-N	5.92	129.02	120.79
4	d	175	LEU	C-N-CA	5.92	129.02	120.79
32	M	235	CYS	CA-C-O	-5.92	114.61	120.82
33	J	49	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	49	ASP	CA-CB-CG	5.92	118.52	112.60
21	N	856	PHE	N-CA-C	-5.92	100.14	108.96
24	Q	118	CYS	CA-C-N	5.92	128.21	120.28
24	Q	118	CYS	C-N-CA	5.92	128.21	120.28
25	R	291	SER	CA-C-N	5.92	128.21	120.28
25	R	291	SER	C-N-CA	5.92	128.21	120.28
25	R	422	ARG	CA-C-N	5.92	128.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	422	ARG	C-N-CA	5.92	128.21	120.28
27	O	106	PHE	CB-CA-C	-5.92	99.31	110.67
28	H	333	MET	N-CA-CB	5.92	118.59	110.01
33	J	258	VAL	N-CA-C	-5.92	104.97	110.53
4	D	212	ILE	O-C-N	-5.91	116.79	123.18
16	V	292	ILE	N-CA-C	-5.91	104.75	110.72
24	Q	416	VAL	CA-C-N	5.91	126.65	120.03
24	Q	416	VAL	C-N-CA	5.91	126.65	120.03
29	I	222	TYR	N-CA-C	5.91	117.84	108.79
5	e	72	ARG	NE-CZ-NH2	5.91	124.52	119.20
20	Z	955	VAL	CB-CA-C	-5.91	101.59	111.29
21	N	677	ASP	CA-CB-CG	-5.91	106.69	112.60
10	j	63	LEU	CA-C-O	-5.91	112.11	119.38
13	6	11	ASN	CA-CB-CG	5.91	118.51	112.60
21	N	180	SER	O-C-N	-5.91	115.41	122.15
23	P	24	ILE	CB-CA-C	5.91	119.54	111.97
30	K	195	ALA	CA-C-N	5.91	128.68	120.29
30	K	195	ALA	C-N-CA	5.91	128.68	120.29
20	Z	49	LEU	CB-CA-C	-5.91	101.60	110.88
20	Z	907	GLY	N-CA-C	-5.91	100.67	111.25
33	J	67	GLU	CA-C-N	5.91	126.24	119.92
33	J	67	GLU	C-N-CA	5.91	126.24	119.92
1	a	209	HIS	CG-CD2-NE2	5.91	113.11	107.20
4	d	140	PRO	N-CA-C	-5.91	106.76	114.03
7	G	61	PRO	CA-C-N	5.91	131.21	122.82
7	G	61	PRO	C-N-CA	5.91	131.21	122.82
1	a	241	ILE	CA-C-O	-5.91	114.59	120.85
2	B	61	LEU	N-CA-CB	5.91	118.75	109.83
2	B	176	GLU	CA-C-O	5.91	127.02	120.82
6	F	219	ASP	N-CA-C	-5.91	103.76	113.50
20	Z	22	LYS	N-CA-C	-5.91	106.11	113.38
21	N	288	ASN	CA-C-O	5.91	126.81	120.55
21	N	584	ARG	NE-CZ-NH1	-5.91	115.59	121.50
25	R	149	ASN	CA-CB-CG	-5.91	106.69	112.60
29	I	86	GLU	N-CA-C	-5.91	105.42	114.16
31	L	251	ILE	N-CA-C	-5.91	107.51	113.47
10	j	102	PRO	CA-C-O	-5.90	114.40	121.48
17	T	177	PHE	N-CA-C	-5.90	106.24	113.50
25	R	191	LEU	CA-C-O	-5.90	112.16	119.18
2	b	94	HIS	CA-C-N	5.90	128.11	120.44
2	b	94	HIS	C-N-CA	5.90	128.11	120.44
4	d	55	GLN	CB-CG-CD	-5.90	102.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	110	PHE	CA-C-N	5.90	127.86	122.37
13	6	110	PHE	C-N-CA	5.90	127.86	122.37
14	7	253	ASP	N-CA-C	-5.90	106.05	113.72
22	S	354	LEU	N-CA-C	-5.90	106.08	113.28
32	M	380	ALA	CA-C-O	-5.90	114.16	120.42
1	A	122	ALA	CA-C-O	-5.90	114.30	120.55
2	B	70	ASP	N-CA-C	-5.90	105.39	113.30
4	D	203	VAL	N-CA-CB	5.90	120.42	110.56
26	U	186	LEU	CA-C-N	5.90	128.67	120.29
26	U	186	LEU	C-N-CA	5.90	128.67	120.29
32	M	15	ASP	CA-CB-CG	-5.90	106.70	112.60
33	J	286	LYS	CD-CE-NZ	5.90	130.78	111.90
3	C	48	ALA	CA-C-N	5.90	131.79	122.94
3	C	48	ALA	C-N-CA	5.90	131.79	122.94
26	U	294	ASN	OD1-CG-ND2	5.90	128.50	122.60
27	O	371	VAL	CA-CB-CG1	5.90	120.43	110.40
13	m	135	PRO	N-CA-C	-5.90	108.55	114.68
2	B	144	GLY	O-C-N	5.90	128.50	122.90
3	C	108	VAL	O-C-N	5.90	127.69	121.91
3	C	225	VAL	CA-C-N	-5.90	114.45	122.77
3	C	225	VAL	C-N-CA	-5.90	114.45	122.77
19	Y	60	TRP	N-CA-C	-5.90	100.81	109.18
27	O	138	LEU	N-CA-C	-5.90	104.85	111.28
29	I	67	ASP	CA-C-N	5.90	128.66	120.29
29	I	67	ASP	C-N-CA	5.90	128.66	120.29
30	K	382	VAL	CA-C-N	5.90	128.80	120.42
30	K	382	VAL	C-N-CA	5.90	128.80	120.42
2	B	8	SER	CA-C-N	5.90	131.80	122.60
2	B	8	SER	C-N-CA	5.90	131.80	122.60
5	E	192	THR	O-C-N	5.89	130.70	123.10
9	2	254	GLU	N-CA-CB	5.89	118.72	109.94
14	7	119	ALA	CA-C-O	5.89	127.80	121.55
22	S	412	ASN	N-CA-CB	5.89	120.45	110.49
28	H	167	ASP	O-C-N	-5.89	114.97	122.34
2	b	231	LYS	N-CA-C	-5.89	98.68	108.34
11	k	177	LYS	N-CA-CB	5.89	121.03	112.13
20	Z	593	HIS	CA-CB-CG	5.89	119.69	113.80
21	N	203	ARG	NE-CZ-NH2	-5.89	113.90	119.20
21	N	322	ASP	CA-CB-CG	-5.89	106.71	112.60
23	P	336	HIS	O-C-N	-5.89	115.27	122.34
25	R	37	LYS	N-CA-C	-5.89	106.43	113.97
30	K	406	ASP	CB-CA-C	-5.89	100.83	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	LYS	N-CA-C	-5.89	104.78	111.14
30	K	86	VAL	CA-C-N	5.89	128.66	120.29
30	K	86	VAL	C-N-CA	5.89	128.66	120.29
4	d	167	ASN	CA-C-N	5.89	128.17	120.28
4	d	167	ASN	C-N-CA	5.89	128.17	120.28
9	i	91	ASN	OD1-CG-ND2	5.89	128.49	122.60
20	Z	551	LEU	CA-C-N	5.89	128.17	120.28
20	Z	551	LEU	C-N-CA	5.89	128.17	120.28
21	N	845	GLY	N-CA-C	-5.89	102.95	112.31
28	H	293	GLU	N-CA-C	5.89	117.37	111.07
28	H	294	LEU	CA-C-O	-5.89	114.18	120.42
32	M	192	GLU	N-CA-CB	5.89	118.87	110.16
33	J	15	HIS	CA-C-N	5.89	128.17	120.28
33	J	15	HIS	C-N-CA	5.89	128.17	120.28
1	a	47	GLY	N-CA-C	-5.89	102.53	112.77
6	f	13	PHE	CA-CB-CG	-5.89	107.91	113.80
17	T	198	ASP	N-CA-C	-5.89	106.64	113.88
25	R	117	ILE	O-C-N	5.89	127.58	121.87
4	D	153	SER	N-CA-C	-5.88	105.93	113.23
20	Z	457	ILE	CA-C-O	-5.88	114.83	120.95
21	N	734	VAL	CA-CB-CG1	5.88	120.40	110.40
23	P	260	VAL	CA-C-N	5.88	128.16	120.28
23	P	260	VAL	C-N-CA	5.88	128.16	120.28
31	L	231	LEU	N-CA-C	-5.88	104.27	112.45
33	J	46	ALA	CA-C-N	5.88	128.65	120.29
33	J	46	ALA	C-N-CA	5.88	128.65	120.29
7	G	94	GLU	CA-C-N	5.88	128.16	120.28
7	G	94	GLU	C-N-CA	5.88	128.16	120.28
33	J	172	GLU	CB-CA-C	5.88	120.56	110.79
9	i	138	HIS	CG-CD2-NE2	5.88	113.08	107.20
2	B	99	ARG	N-CA-CB	5.88	120.19	111.01
27	O	160	LYS	O-C-N	5.88	129.95	123.01
29	I	295	ASN	O-C-N	5.88	130.41	122.59
16	V	36	LYS	N-CA-C	5.88	117.36	111.07
20	Z	841	GLU	CA-C-N	5.88	131.70	122.17
20	Z	841	GLU	C-N-CA	5.88	131.70	122.17
21	N	109	TYR	CA-C-N	5.88	128.09	120.56
21	N	109	TYR	C-N-CA	5.88	128.09	120.56
8	h	23	LEU	N-CA-C	-5.88	100.71	110.17
15	W	98	LEU	CA-C-N	5.88	128.64	120.29
15	W	98	LEU	C-N-CA	5.88	128.64	120.29
20	Z	387	ASN	O-C-N	-5.88	115.89	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	145	PHE	CA-CB-CG	-5.88	107.92	113.80
11	k	172	MET	O-C-N	-5.88	116.36	121.35
16	V	287	THR	CA-C-N	5.88	128.16	120.28
16	V	287	THR	C-N-CA	5.88	128.16	120.28
23	P	242	GLN	N-CA-C	-5.88	105.00	111.82
27	O	83	LEU	CA-C-N	5.88	128.63	120.29
27	O	83	LEU	C-N-CA	5.88	128.63	120.29
20	Z	938	GLN	N-CA-C	-5.88	97.90	108.48
22	S	280	ASN	OD1-CG-ND2	5.88	128.47	122.60
1	a	228	ALA	N-CA-CB	5.87	120.00	110.43
3	c	75	VAL	CA-C-N	5.87	133.26	122.92
3	c	75	VAL	C-N-CA	5.87	133.26	122.92
20	Z	721	ASN	CA-C-N	5.87	128.15	120.28
20	Z	721	ASN	C-N-CA	5.87	128.15	120.28
4	d	105	THR	N-CA-CB	5.87	118.67	109.69
2	B	53	SER	O-C-N	-5.87	114.57	121.32
20	Z	2	VAL	CA-C-N	5.87	130.72	121.56
20	Z	2	VAL	C-N-CA	5.87	130.72	121.56
27	O	373	TRP	CB-CG-CD1	5.87	135.71	126.90
14	n	208	GLU	N-CA-C	-5.87	104.88	111.28
9	2	85	THR	N-CA-CB	5.87	118.85	110.16
17	T	160	ALA	CA-C-O	5.87	126.77	120.55
28	H	363	PRO	N-CA-C	5.87	121.55	113.98
7	G	42	CYS	N-CA-C	-5.87	100.39	109.14
28	H	299	ARG	NE-CZ-NH1	5.87	127.37	121.50
29	I	328	THR	CA-C-N	5.87	128.42	120.44
29	I	328	THR	C-N-CA	5.87	128.42	120.44
32	M	307	GLU	CA-C-N	5.87	128.07	120.44
32	M	307	GLU	C-N-CA	5.87	128.07	120.44
11	k	146	HIS	N-CA-C	-5.87	104.80	111.14
3	C	126	GLY	O-C-N	5.87	129.09	123.05
11	4	92	ILE	N-CA-C	5.87	120.66	112.50
31	L	297	ALA	CA-C-O	5.87	126.60	119.38
1	A	228	ALA	O-C-N	-5.87	116.64	123.27
19	Y	25	ASN	CA-C-N	5.87	128.06	120.44
19	Y	25	ASN	C-N-CA	5.87	128.06	120.44
19	Y	60	TRP	CE2-CD2-CE3	5.87	124.67	118.80
20	Z	747	ALA	CA-C-N	5.87	128.62	120.29
20	Z	747	ALA	C-N-CA	5.87	128.62	120.29
27	O	66	VAL	N-CA-CB	5.87	121.39	110.77
31	L	312	MET	CG-SD-CE	-5.87	87.99	100.90
8	1	94	LEU	N-CA-CB	5.86	118.57	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	116	HIS	ND1-CE1-NE2	5.86	114.26	108.40
23	P	137	ALA	N-CA-C	5.86	117.67	111.28
29	I	121	THR	O-C-N	-5.86	116.32	123.30
6	f	116	ALA	O-C-N	5.86	128.42	122.09
22	S	58	LYS	CB-CG-CD	5.86	124.78	111.30
33	J	322	ALA	CB-CA-C	-5.86	100.88	110.85
8	h	82	PRO	CA-C-N	5.86	133.23	122.92
8	h	82	PRO	C-N-CA	5.86	133.23	122.92
3	C	125	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
17	T	151	TRP	N-CA-CB	5.86	118.74	110.12
20	Z	19	SER	CA-C-N	5.86	126.67	120.11
20	Z	19	SER	C-N-CA	5.86	126.67	120.11
9	i	94	LEU	CB-CA-C	-5.86	100.89	110.85
21	N	544	GLU	N-CA-C	5.86	119.08	109.76
22	S	421	TYR	N-CA-CB	5.86	118.73	110.12
14	n	185	ASN	OD1-CG-ND2	-5.86	116.74	122.60
24	Q	384	LYS	N-CA-CB	5.86	120.39	110.49
25	R	350	LEU	CA-C-N	5.86	128.05	120.44
25	R	350	LEU	C-N-CA	5.86	128.05	120.44
9	i	115	HIS	CA-C-N	5.86	129.97	120.60
9	i	115	HIS	C-N-CA	5.86	129.97	120.60
13	m	186	GLU	N-CA-C	5.86	117.66	111.28
21	N	291	SER	N-CA-C	-5.86	104.49	111.69
3	c	114	ARG	CA-C-N	5.85	128.60	120.29
3	c	114	ARG	C-N-CA	5.85	128.60	120.29
1	a	105	ARG	CA-C-O	-5.85	114.35	120.55
12	l	201	ILE	N-CA-C	-5.85	99.92	108.11
23	P	27	LEU	CA-C-O	-5.85	114.35	120.55
27	O	40	GLN	CA-C-N	5.85	128.60	120.29
27	O	40	GLN	C-N-CA	5.85	128.60	120.29
32	M	233	ARG	CA-C-N	5.85	128.60	120.29
32	M	233	ARG	C-N-CA	5.85	128.60	120.29
4	d	195	THR	CA-C-N	5.85	128.48	120.46
4	d	195	THR	C-N-CA	5.85	128.48	120.46
32	M	343	LEU	N-CA-C	-5.85	99.80	108.99
4	d	58	ARG	CA-C-N	5.85	129.89	120.82
4	d	58	ARG	C-N-CA	5.85	129.89	120.82
20	Z	721	ASN	CA-CB-CG	5.85	118.45	112.60
23	P	332	GLU	CA-C-O	-5.85	114.22	120.42
26	U	21	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
32	M	304	THR	CA-C-N	5.85	128.60	120.29
32	M	304	THR	C-N-CA	5.85	128.60	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	382	PHE	CA-C-N	5.85	128.04	120.44
33	J	382	PHE	C-N-CA	5.85	128.04	120.44
12	l	270	GLU	CA-C-N	5.85	128.11	120.28
12	l	270	GLU	C-N-CA	5.85	128.11	120.28
14	n	86	ILE	CA-C-O	5.85	126.04	120.25
14	n	111	ASN	CA-C-N	5.85	127.15	119.84
14	n	111	ASN	C-N-CA	5.85	127.15	119.84
1	A	235	THR	N-CA-C	-5.85	99.66	109.07
7	G	128	SER	N-CA-C	-5.85	105.73	112.92
18	X	67	ILE	CA-CB-CG1	5.85	120.34	110.40
20	Z	281	ALA	N-CA-CB	5.85	118.49	110.01
20	Z	823	ASN	CA-C-O	5.85	126.72	120.46
21	N	68	VAL	CA-CB-CG2	-5.85	100.46	110.40
24	Q	21	ASN	CA-C-O	-5.85	114.64	120.90
13	m	74	LYS	N-CA-C	5.84	117.73	111.36
15	W	19	GLY	CA-C-N	5.84	131.02	122.08
15	W	19	GLY	C-N-CA	5.84	131.02	122.08
20	Z	400	ILE	CA-CB-CG1	5.84	120.34	110.40
21	N	455	MET	CA-C-O	-5.84	113.98	120.70
3	c	123	THR	N-CA-C	-5.84	104.33	112.45
7	g	115	ARG	O-C-N	-5.84	115.49	122.15
9	i	87	LEU	CA-C-N	5.84	127.92	120.56
9	i	87	LEU	C-N-CA	5.84	127.92	120.56
16	V	268	THR	N-CA-CB	5.84	118.78	110.13
20	Z	757	SER	N-CA-C	5.84	118.60	111.82
21	N	691	GLN	CG-CD-NE2	-5.84	107.64	116.40
22	S	219	LYS	N-CA-CB	-5.84	101.60	110.07
31	L	183	ILE	CB-CA-C	5.84	118.86	110.33
13	6	76	PHE	N-CA-C	5.84	117.64	111.28
27	O	392	TRP	O-C-N	5.84	130.36	122.59
30	K	139	LEU	CA-C-O	-5.84	114.56	121.16
10	j	184	GLY	O-C-N	5.84	129.41	122.64
21	N	653	ARG	CA-C-N	5.84	128.03	120.44
21	N	653	ARG	C-N-CA	5.84	128.03	120.44
22	S	382	ARG	N-CA-C	-5.84	106.12	113.18
3	c	113	ARG	NE-CZ-NH1	-5.84	115.66	121.50
10	j	107	PRO	N-CA-C	5.84	119.68	111.33
13	m	98	ALA	N-CA-CB	5.84	118.70	110.12
24	Q	130	ARG	CA-C-N	5.84	128.46	120.46
24	Q	130	ARG	C-N-CA	5.84	128.46	120.46
24	Q	233	LYS	N-CA-CB	5.84	119.29	110.30
29	I	137	ASP	N-CA-CB	5.84	119.81	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	194	ARG	NE-CZ-NH2	-5.84	113.95	119.20
6	f	63	ILE	N-CA-CB	5.83	119.46	111.41
23	P	186	LEU	CA-C-O	-5.83	113.26	119.97
24	Q	305	ALA	N-CA-CB	5.83	118.70	110.12
2	b	140	ASP	CA-CB-CG	-5.83	106.77	112.60
1	A	211	ILE	CA-C-N	5.83	128.02	120.44
1	A	211	ILE	C-N-CA	5.83	128.02	120.44
23	P	402	PHE	N-CA-CB	5.83	118.70	110.24
24	Q	343	LEU	CA-C-O	5.83	126.95	120.82
25	R	101	GLU	CA-C-N	5.83	128.41	120.54
25	R	101	GLU	C-N-CA	5.83	128.41	120.54
29	I	87	LYS	CA-C-O	-5.83	115.07	121.31
2	b	136	ILE	N-CA-CB	5.83	119.75	111.82
10	j	199	TYR	CB-CG-CD1	-5.83	112.05	120.80
14	n	39	VAL	N-CA-C	-5.83	100.29	108.80
1	A	90	ALA	CA-C-N	5.83	128.09	120.28
1	A	90	ALA	C-N-CA	5.83	128.09	120.28
8	1	107	ILE	O-C-N	-5.83	116.56	123.03
28	H	318	ARG	NE-CZ-NH2	-5.83	113.95	119.20
30	K	220	THR	CA-CB-CG2	5.83	120.42	110.50
32	M	153	TYR	N-CA-C	-5.83	97.72	107.99
9	i	242	LEU	N-CA-CB	-5.83	101.62	110.07
5	E	47	VAL	N-CA-C	-5.83	99.24	107.75
24	Q	10	GLU	CA-C-N	5.83	128.09	120.28
24	Q	10	GLU	C-N-CA	5.83	128.09	120.28
25	R	305	PHE	CA-CB-CG	5.83	119.63	113.80
27	O	70	TYR	CA-C-O	5.83	128.84	120.51
28	H	150	LYS	N-CA-C	-5.83	106.03	113.02
30	K	166	LYS	CA-C-N	5.83	125.52	119.05
30	K	166	LYS	C-N-CA	5.83	125.52	119.05
3	C	94	HIS	ND1-CG-CD2	5.83	111.93	106.10
20	Z	501	LYS	N-CA-C	-5.83	103.31	110.65
32	M	115	LYS	N-CA-C	-5.83	99.23	108.73
8	h	90	VAL	N-CA-CB	5.83	118.46	110.54
17	T	55	LEU	CA-C-N	5.83	128.09	120.28
17	T	55	LEU	C-N-CA	5.83	128.09	120.28
21	N	308	ASN	N-CA-CB	5.83	119.85	110.65
22	S	335	GLN	CA-C-N	5.83	129.14	120.87
22	S	335	GLN	C-N-CA	5.83	129.14	120.87
1	A	233	PHE	CA-CB-CG	-5.82	107.98	113.80
13	6	180	LEU	O-C-N	5.82	130.03	122.87
20	Z	617	ILE	CA-C-N	5.82	128.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	617	ILE	C-N-CA	5.82	128.09	120.28
20	Z	712	ASP	CA-C-N	5.82	128.36	120.44
20	Z	712	ASP	C-N-CA	5.82	128.36	120.44
21	N	578	ASP	N-CA-C	-5.82	99.03	108.52
23	P	422	LEU	O-C-N	5.82	128.79	122.15
12	l	263	HIS	CG-CD2-NE2	5.82	113.02	107.20
4	D	57	THR	CA-CB-OG1	5.82	118.33	109.60
22	S	132	ALA	O-C-N	-5.82	116.07	122.07
6	f	80	ASP	CA-C-N	5.82	128.55	120.29
6	f	80	ASP	C-N-CA	5.82	128.55	120.29
14	7	257	ASP	N-CA-CB	5.82	118.61	109.94
20	Z	550	PHE	CA-CB-CG	-5.82	107.98	113.80
29	I	104	LEU	O-C-N	-5.82	116.37	123.30
1	a	197	GLU	N-CA-C	5.82	120.44	113.23
6	F	27	GLU	CA-C-O	5.82	126.66	119.97
6	F	93	ASN	CA-CB-CG	-5.82	106.78	112.60
20	Z	781	GLY	CA-C-N	5.82	128.43	120.46
20	Z	781	GLY	C-N-CA	5.82	128.43	120.46
12	l	239	ALA	CA-C-O	5.82	126.72	120.55
5	E	133	LEU	N-CA-C	-5.82	105.80	114.64
27	O	207	LEU	CB-CA-C	-5.82	101.14	110.79
30	K	408	GLU	N-CA-C	5.82	118.40	111.71
32	M	275	PRO	N-CD-CG	5.82	110.78	103.80
3	c	82	ALA	CB-CA-C	-5.82	100.96	110.85
4	d	181	ARG	CA-C-N	5.82	128.33	120.65
4	d	181	ARG	C-N-CA	5.82	128.33	120.65
8	1	131	LEU	N-CA-C	-5.82	96.96	109.81
24	Q	236	PHE	CA-CB-CG	5.82	119.61	113.80
3	c	7	ASP	CA-C-N	5.81	128.34	120.44
3	c	7	ASP	C-N-CA	5.81	128.34	120.44
6	f	107	ARG	NE-CZ-NH1	-5.81	115.69	121.50
11	k	72	ASP	N-CA-CB	5.81	120.31	110.49
22	S	50	PRO	CA-C-N	5.81	128.00	120.44
22	S	50	PRO	C-N-CA	5.81	128.00	120.44
9	i	61	ALA	N-CA-C	-5.81	99.81	109.46
14	7	131	THR	CA-C-N	5.81	129.83	120.30
14	7	131	THR	C-N-CA	5.81	129.83	120.30
9	i	191	GLY	CA-C-N	5.81	128.67	120.42
9	i	191	GLY	C-N-CA	5.81	128.67	120.42
9	2	157	GLY	N-CA-C	-5.81	104.27	111.70
20	Z	911	LYS	N-CA-C	-5.81	98.41	108.69
21	N	178	SER	O-C-N	-5.81	116.30	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	348	CYS	CA-C-N	5.81	127.99	120.44
24	Q	348	CYS	C-N-CA	5.81	127.99	120.44
9	i	118	LYS	N-CA-C	5.81	117.61	111.28
9	2	172	LYS	N-CA-C	-5.81	100.24	109.07
21	N	885	ILE	CB-CG1-CD1	5.81	126.00	113.80
27	O	240	GLU	CB-CA-C	-5.81	101.76	110.88
6	f	170	THR	CA-CB-CG2	5.81	120.37	110.50
1	A	79	ILE	N-CA-CB	5.81	119.19	111.64
4	D	106	VAL	N-CA-C	5.81	116.54	110.62
17	T	244	ASP	N-CA-CB	5.81	118.75	110.16
6	f	151	GLY	CA-C-N	5.80	129.00	120.82
6	f	151	GLY	C-N-CA	5.80	129.00	120.82
21	N	196	THR	CA-CB-CG2	5.80	120.37	110.50
23	P	216	LEU	CA-C-N	5.80	128.06	120.28
23	P	216	LEU	C-N-CA	5.80	128.06	120.28
26	U	16	LEU	N-CA-C	5.80	117.69	111.36
10	3	103	TYR	O-C-N	5.80	129.79	122.65
21	N	216	ASN	CA-CB-CG	5.80	118.40	112.60
33	J	244	ILE	N-CA-C	-5.80	100.12	108.48
1	A	185	HIS	ND1-CE1-NE2	5.80	114.20	108.40
9	2	177	LYS	O-C-N	-5.80	116.09	122.07
13	6	155	MET	O-C-N	-5.80	114.65	121.32
20	Z	260	GLU	CA-C-N	5.80	128.53	120.29
20	Z	260	GLU	C-N-CA	5.80	128.53	120.29
28	H	202	GLU	CB-CG-CD	-5.80	102.74	112.60
1	a	179	THR	CA-C-N	5.80	128.53	120.29
1	a	179	THR	C-N-CA	5.80	128.53	120.29
2	b	117	ILE	CA-C-N	5.80	128.53	120.29
2	b	117	ILE	C-N-CA	5.80	128.53	120.29
4	d	92	GLU	CA-C-N	5.80	128.05	120.28
4	d	92	GLU	C-N-CA	5.80	128.05	120.28
8	h	134	ALA	N-CA-C	-5.80	100.53	109.52
1	A	51	THR	N-CA-C	-5.80	100.34	109.50
2	B	19	GLY	CA-C-N	5.80	129.13	120.31
2	B	19	GLY	C-N-CA	5.80	129.13	120.31
6	F	198	SER	CA-C-N	5.80	128.52	120.29
6	F	198	SER	C-N-CA	5.80	128.52	120.29
12	5	76	THR	CA-C-N	5.80	131.02	121.86
12	5	76	THR	C-N-CA	5.80	131.02	121.86
16	V	127	LYS	CA-C-O	5.80	126.70	120.55
26	U	285	ILE	CA-C-N	5.80	128.41	120.46
26	U	285	ILE	C-N-CA	5.80	128.41	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	397	LYS	N-CA-C	-5.80	106.16	113.18
10	j	150	CYS	O-C-N	-5.80	115.54	122.15
3	C	169	THR	CA-C-N	5.80	127.98	120.44
3	C	169	THR	C-N-CA	5.80	127.98	120.44
4	D	210	ILE	N-CA-C	-5.80	99.99	108.11
25	R	172	LEU	CA-C-N	5.80	128.05	120.28
25	R	172	LEU	C-N-CA	5.80	128.05	120.28
30	K	271	ILE	N-CA-C	-5.80	99.99	108.11
10	3	86	THR	N-CA-CB	5.80	118.74	110.16
13	6	203	HIS	CG-CD2-NE2	5.80	113.00	107.20
16	V	204	HIS	CA-CB-CG	5.80	119.60	113.80
26	U	168	GLU	CB-CA-C	-5.80	101.17	110.79
31	L	230	LEU	N-CA-CB	5.80	118.64	110.12
1	A	40	ILE	N-CA-CB	5.79	120.79	111.23
7	G	58	LEU	CA-C-N	5.79	129.50	120.75
7	G	58	LEU	C-N-CA	5.79	129.50	120.75
12	5	96	THR	CA-CB-CG2	-5.79	100.65	110.50
16	V	296	LEU	N-CA-C	5.79	117.27	111.07
8	h	15	VAL	CA-C-O	-5.79	114.42	120.27
9	i	54	ILE	CB-CA-C	-5.79	102.96	110.84
21	N	578	ASP	O-C-N	5.79	130.10	123.27
33	J	50	ALA	CA-C-O	-5.79	114.28	120.42
5	e	10	ARG	NH1-CZ-NH2	5.79	126.83	119.30
14	n	132	VAL	CA-C-N	5.79	128.51	120.29
14	n	132	VAL	C-N-CA	5.79	128.51	120.29
3	C	206	LEU	N-CA-C	-5.79	99.75	108.96
7	G	205	GLU	N-CA-C	-5.79	106.22	113.28
16	V	69	PHE	N-CA-C	-5.79	98.06	108.48
16	V	286	GLU	CA-C-O	-5.79	114.74	120.82
18	X	124	LYS	O-C-N	5.79	128.34	122.09
20	Z	151	HIS	ND1-CE1-NE2	5.79	114.19	108.40
24	Q	161	LEU	CA-C-N	5.79	128.51	120.29
24	Q	161	LEU	C-N-CA	5.79	128.51	120.29
31	L	378	ALA	O-C-N	-5.79	114.70	122.23
25	R	378	ASN	CA-CB-CG	5.79	118.39	112.60
10	j	132	GLU	CA-C-N	5.79	131.76	121.75
10	j	132	GLU	C-N-CA	5.79	131.76	121.75
2	B	165	GLY	N-CA-C	-5.79	104.59	112.52
7	G	35	THR	N-CA-CB	5.79	119.76	110.85
16	V	256	GLU	CB-CA-C	-5.79	101.01	110.85
22	S	239	ARG	CB-CG-CD	5.79	124.61	111.30
1	a	91	ARG	CB-CA-C	-5.79	101.19	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	104	ALA	CA-C-O	-5.79	115.42	121.55
9	i	150	VAL	CA-CB-CG2	-5.79	100.56	110.40
14	n	215	ARG	CA-C-N	5.79	128.63	120.42
14	n	215	ARG	C-N-CA	5.79	128.63	120.42
1	A	193	HIS	CB-CA-C	-5.79	98.01	110.45
12	5	167	GLY	N-CA-C	-5.79	106.17	115.08
16	V	93	ASP	CA-CB-CG	5.79	118.39	112.60
16	V	193	ASN	N-CA-C	5.79	117.67	111.36
19	Y	74	THR	CA-C-N	5.79	127.96	120.44
19	Y	74	THR	C-N-CA	5.79	127.96	120.44
6	f	29	ILE	CA-C-N	5.78	128.30	120.38
6	f	29	ILE	C-N-CA	5.78	128.30	120.38
7	g	238	GLU	CB-CG-CD	-5.78	102.77	112.60
9	2	118	LYS	CA-C-N	5.78	131.84	121.66
9	2	118	LYS	C-N-CA	5.78	131.84	121.66
24	Q	356	CYS	CA-C-O	5.78	128.15	120.98
25	R	293	THR	CA-C-O	-5.78	114.29	120.42
6	f	62	LYS	N-CA-C	-5.78	104.94	113.61
24	Q	181	GLU	CA-C-O	-5.78	114.42	120.55
27	O	353	VAL	N-CA-CB	5.78	121.45	111.39
5	e	106	ASP	O-C-N	-5.78	115.76	122.87
9	i	145	HIS	CE1-NE2-CD2	-5.78	103.22	109.00
11	k	62	ALA	CA-C-N	5.78	128.50	120.29
11	k	62	ALA	C-N-CA	5.78	128.50	120.29
21	N	658	ILE	O-C-N	5.78	127.48	121.87
24	Q	32	ASP	O-C-N	5.78	128.25	122.12
26	U	173	HIS	CE1-NE2-CD2	-5.78	103.22	109.00
27	O	152	ASP	CA-CB-CG	-5.78	106.82	112.60
33	J	211	ILE	CA-C-O	-5.78	113.56	120.78
3	C	37	GLY	CA-C-N	5.78	130.71	123.14
3	C	37	GLY	C-N-CA	5.78	130.71	123.14
1	a	27	GLN	CB-CG-CD	-5.78	102.78	112.60
11	4	54	VAL	O-C-N	-5.78	115.89	121.90
17	T	92	ASN	N-CA-C	-5.78	104.35	111.40
3	c	158	THR	CA-C-N	5.78	127.06	120.53
3	c	158	THR	C-N-CA	5.78	127.06	120.53
11	4	156	GLU	CB-CG-CD	-5.78	102.78	112.60
16	V	166	ASN	CA-C-N	5.78	130.78	122.35
16	V	166	ASN	C-N-CA	5.78	130.78	122.35
17	T	34	LEU	CA-C-N	5.78	128.37	120.46
17	T	34	LEU	C-N-CA	5.78	128.37	120.46
17	T	236	ASN	CA-C-N	5.78	128.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	236	ASN	C-N-CA	5.78	128.29	120.44
21	N	427	ILE	N-CA-CB	5.78	117.96	110.57
5	e	43	LYS	O-C-N	5.77	129.12	122.25
24	Q	190	ASN	OD1-CG-ND2	5.77	128.37	122.60
24	Q	223	GLY	CA-C-N	5.77	128.37	120.46
24	Q	223	GLY	C-N-CA	5.77	128.37	120.46
28	H	184	GLU	N-CA-C	-5.77	102.24	111.02
5	e	29	GLU	CA-C-N	5.77	128.01	120.28
5	e	29	GLU	C-N-CA	5.77	128.01	120.28
3	C	154	SER	N-CA-C	-5.77	106.24	113.28
11	4	149	ARG	CA-C-N	5.77	127.06	119.84
11	4	149	ARG	C-N-CA	5.77	127.06	119.84
16	V	168	LEU	CA-C-N	5.77	127.31	120.09
16	V	168	LEU	C-N-CA	5.77	127.31	120.09
22	S	425	ARG	CA-C-N	5.77	129.84	120.60
22	S	425	ARG	C-N-CA	5.77	129.84	120.60
25	R	253	ALA	N-CA-C	-5.77	105.07	111.36
25	R	419	ALA	CA-C-O	-5.77	114.43	120.55
27	O	61	LEU	CA-C-N	5.77	128.01	120.28
27	O	61	LEU	C-N-CA	5.77	128.01	120.28
27	O	359	SER	CA-C-N	5.77	126.39	119.98
27	O	359	SER	C-N-CA	5.77	126.39	119.98
30	K	380	GLY	N-CA-C	-5.77	107.76	115.32
3	c	72	LYS	O-C-N	5.77	128.05	121.93
4	d	193	LYS	N-CA-CB	5.77	119.11	110.22
10	j	15	MET	CB-CA-C	-5.77	97.99	111.09
25	R	330	VAL	O-C-N	5.77	127.56	121.91
6	f	27	GLU	CA-C-O	5.77	126.67	120.55
10	3	2	SER	CA-C-N	5.77	128.41	120.39
10	3	2	SER	C-N-CA	5.77	128.41	120.39
23	P	102	GLU	N-CA-C	5.77	118.03	111.11
32	M	357	ARG	CA-C-N	5.77	128.01	120.28
32	M	357	ARG	C-N-CA	5.77	128.01	120.28
8	h	192	VAL	CA-C-N	-5.77	114.87	123.00
8	h	192	VAL	C-N-CA	-5.77	114.87	123.00
9	i	117	PHE	N-CA-CB	-5.77	101.62	110.16
2	B	203	GLU	N-CA-C	-5.77	103.98	113.50
12	5	263	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
25	R	405	LYS	CA-C-N	5.77	128.48	120.29
25	R	405	LYS	C-N-CA	5.77	128.48	120.29
28	H	421	SER	O-C-N	-5.77	116.01	122.12
30	K	184	ILE	CA-C-N	5.77	128.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	184	ILE	C-N-CA	5.77	128.59	120.28
4	d	240	LYS	CA-C-N	5.77	127.94	120.44
4	d	240	LYS	C-N-CA	5.77	127.94	120.44
5	e	233	ASN	CA-C-N	5.77	128.01	120.28
5	e	233	ASN	C-N-CA	5.77	128.01	120.28
11	4	25	ILE	N-CA-C	-5.77	107.36	112.90
11	4	124	THR	CA-C-O	5.77	126.45	120.40
13	6	221	ARG	CD-NE-CZ	-5.77	116.33	124.40
21	N	151	LYS	N-CA-CB	5.77	119.18	110.30
23	P	261	LEU	CA-C-O	-5.77	114.44	120.55
4	d	224	LEU	CA-C-O	5.76	126.53	120.36
11	4	80	VAL	N-CA-C	-5.76	104.89	110.42
16	V	227	MET	N-CA-C	-5.76	100.99	109.81
16	V	273	ARG	CD-NE-CZ	-5.76	116.33	124.40
21	N	18	ASP	CA-C-O	-5.76	114.76	120.70
21	N	280	GLN	N-CA-C	-5.76	106.08	113.23
1	A	21	PRO	O-C-N	5.76	128.87	122.24
10	3	110	ALA	N-CA-C	-5.76	99.95	108.99
20	Z	5	SER	N-CA-C	5.76	116.53	108.00
32	M	146	VAL	CA-C-O	5.76	127.12	121.19
19	Y	38	PHE	CA-CB-CG	-5.76	108.04	113.80
20	Z	357	ILE	CA-C-N	5.76	128.57	120.28
20	Z	357	ILE	C-N-CA	5.76	128.57	120.28
22	S	281	ALA	N-CA-C	5.76	117.56	111.28
23	P	93	ILE	CB-CG1-CD1	5.76	125.89	113.80
31	L	431	THR	N-CA-C	-5.76	104.79	113.89
32	M	324	LEU	N-CA-C	-5.76	100.75	109.85
33	J	147	TYR	O-C-N	-5.76	116.01	122.12
4	D	27	VAL	CB-CA-C	-5.76	104.37	112.14
21	N	507	GLU	N-CA-CB	5.76	118.68	110.16
27	O	78	VAL	O-C-N	-5.76	116.28	121.87
1	A	245	LEU	N-CA-C	-5.76	105.09	111.36
14	7	225	SER	N-CA-C	-5.76	99.77	108.46
21	N	78	ALA	N-CA-CB	5.76	118.52	109.94
23	P	93	ILE	CA-C-N	5.76	129.06	120.31
23	P	93	ILE	C-N-CA	5.76	129.06	120.31
33	J	278	GLN	O-C-N	5.75	130.04	122.33
20	Z	61	SER	N-CA-CB	5.75	118.67	110.16
20	Z	627	LYS	N-CA-C	5.75	117.55	111.28
22	S	378	GLN	CB-CA-C	-5.75	101.07	110.85
23	P	369	LEU	CA-C-N	5.75	130.30	122.19
23	P	369	LEU	C-N-CA	5.75	130.30	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	425	GLN	OE1-CD-NE2	5.75	128.35	122.60
27	O	372	GLU	CA-C-N	5.75	127.92	120.44
27	O	372	GLU	C-N-CA	5.75	127.92	120.44
30	K	91	SER	O-C-N	5.75	129.41	122.85
32	M	386	PHE	N-CA-CB	5.75	119.63	110.65
7	g	183	HIS	CA-CB-CG	-5.75	108.05	113.80
8	1	98	ASN	N-CA-C	-5.75	103.52	110.88
22	S	84	ASP	N-CA-CB	5.75	120.21	110.49
30	K	124	SER	N-CA-CB	5.75	118.45	110.17
30	K	203	ILE	N-CA-CB	5.75	120.55	110.49
12	5	253	TYR	N-CA-C	-5.75	99.96	108.99
28	H	227	LEU	CA-C-O	-5.75	112.76	118.34
1	a	12	TYR	CA-C-N	5.75	132.52	121.54
1	a	12	TYR	C-N-CA	5.75	132.52	121.54
6	f	159	THR	O-C-N	-5.75	117.22	123.26
7	g	28	VAL	N-CA-C	-5.75	104.76	110.62
9	i	41	VAL	CA-C-O	-5.75	116.13	120.96
1	A	101	ALA	O-C-N	-5.75	116.15	122.07
3	C	105	ASP	O-C-N	-5.75	116.46	122.96
13	6	136	VAL	CA-C-O	-5.75	112.58	119.36
16	V	67	ASP	N-CA-CB	5.75	120.31	111.46
22	S	39	ASN	CA-CB-CG	-5.75	106.85	112.60
29	I	360	LYS	N-CA-CB	5.75	118.57	110.12
33	J	181	GLN	N-CA-CB	5.75	120.94	111.17
6	f	112	LEU	CA-C-O	-5.75	113.61	120.10
13	m	97	ALA	O-C-N	5.75	128.21	122.12
5	E	127	ALA	N-CA-CB	5.75	120.20	110.49
21	N	253	LEU	CA-C-N	5.75	128.45	120.29
21	N	253	LEU	C-N-CA	5.75	128.45	120.29
22	S	45	THR	N-CA-C	5.75	118.60	110.50
7	g	197	ALA	CA-C-N	5.75	128.55	120.28
7	g	197	ALA	C-N-CA	5.75	128.55	120.28
16	V	212	MET	N-CA-C	5.74	117.22	111.07
20	Z	516	THR	N-CA-C	-5.74	103.87	112.54
20	Z	543	THR	CA-C-O	5.74	126.43	119.31
22	S	215	MET	N-CA-C	-5.74	105.10	111.36
7	g	64	ASN	N-CA-C	-5.74	99.30	109.06
7	G	193	VAL	CA-CB-CG1	5.74	120.16	110.40
20	Z	413	ASP	CA-C-N	5.74	126.35	119.98
20	Z	413	ASP	C-N-CA	5.74	126.35	119.98
27	O	149	LEU	CA-C-O	-5.74	113.37	119.97
30	K	261	ALA	CA-C-O	-5.74	114.46	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	160	LYS	O-C-N	5.74	130.05	122.30
13	m	203	HIS	CE1-NE2-CD2	-5.74	103.26	109.00
16	V	87	PHE	CA-CB-CG	-5.74	108.06	113.80
17	T	58	THR	CA-C-N	5.74	127.90	120.44
17	T	58	THR	C-N-CA	5.74	127.90	120.44
4	d	179	TYR	N-CA-CB	5.74	118.49	109.83
10	j	112	ILE	N-CA-C	-5.74	99.86	108.12
12	l	273	TRP	CD2-CE2-CZ2	-5.74	116.66	122.40
7	G	180	VAL	CA-C-O	-5.74	115.09	121.17
15	W	122	ARG	NE-CZ-NH1	-5.74	115.76	121.50
16	V	151	VAL	O-C-N	5.74	128.93	122.67
20	Z	276	ASN	CA-CB-CG	5.74	118.34	112.60
20	Z	734	ASP	CA-C-N	5.74	128.54	120.28
20	Z	734	ASP	C-N-CA	5.74	128.54	120.28
21	N	383	LYS	CA-C-N	5.74	127.97	120.28
21	N	383	LYS	C-N-CA	5.74	127.97	120.28
19	Y	43	TRP	CG-CD2-CE3	-5.74	128.16	133.90
15	W	76	LEU	CA-C-O	-5.74	114.34	120.42
19	Y	44	ALA	CA-C-N	5.74	129.01	120.87
19	Y	44	ALA	C-N-CA	5.74	129.01	120.87
20	Z	187	SER	CA-C-O	5.74	125.21	118.90
28	H	201	GLU	N-CA-C	-5.74	100.05	109.40
30	K	329	LEU	N-CA-C	-5.74	96.65	108.18
31	L	83	ASP	O-C-N	5.74	127.98	122.07
33	J	21	PRO	CA-C-N	5.74	128.44	120.29
33	J	21	PRO	C-N-CA	5.74	128.44	120.29
23	P	428	THR	CA-CB-OG1	5.73	118.20	109.60
8	h	120	TYR	N-CA-C	-5.73	99.67	109.24
11	k	9	VAL	N-CA-C	-5.73	101.15	109.29
13	m	115	VAL	N-CA-C	-5.73	100.78	108.35
5	E	75	GLY	N-CA-C	-5.73	102.77	111.14
16	V	176	ASN	N-CA-CB	5.73	120.89	111.31
20	Z	265	LEU	N-CA-C	-5.73	105.17	111.82
24	Q	46	VAL	N-CA-C	-5.73	107.70	113.20
31	L	111	GLU	CA-C-O	-5.73	115.47	121.55
9	i	178	GLU	CA-C-O	-5.73	113.88	120.24
2	B	42	GLY	CA-C-N	5.73	131.50	122.33
2	B	42	GLY	C-N-CA	5.73	131.50	122.33
11	4	75	LEU	N-CA-C	-5.73	100.94	110.17
13	6	11	ASN	CB-CA-C	5.73	115.84	110.17
16	V	144	ILE	CA-C-O	5.73	125.28	119.20
20	Z	196	SER	CA-C-N	5.73	127.89	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	196	SER	C-N-CA	5.73	127.89	120.44
22	S	208	ILE	CA-C-O	-5.73	114.78	120.85
30	K	221	MET	N-CA-C	-5.73	106.92	114.31
32	M	394	VAL	CA-C-O	-5.73	115.10	121.17
11	k	166	GLN	O-C-N	-5.73	116.05	122.12
29	I	414	GLU	O-C-N	5.73	127.97	122.07
12	l	154	ALA	N-CA-C	5.73	117.33	111.14
20	Z	168	GLN	CB-CG-CD	-5.73	102.86	112.60
22	S	261	HIS	ND1-CE1-NE2	5.73	114.13	108.40
25	R	325	HIS	CB-CG-CD2	-5.73	123.75	131.20
27	O	63	ASP	CA-CB-CG	-5.73	106.87	112.60
2	b	91	LYS	CA-C-N	5.73	129.69	120.30
2	b	91	LYS	C-N-CA	5.73	129.69	120.30
27	O	7	ILE	CA-C-O	-5.73	112.60	119.36
3	C	114	ARG	CA-C-O	-5.72	114.81	120.82
10	3	87	PHE	CA-CB-CG	-5.72	108.08	113.80
16	V	98	THR	N-CA-C	-5.72	106.34	113.38
16	V	201	ILE	N-CA-CB	5.72	117.53	111.00
20	Z	715	ALA	O-C-N	5.72	128.19	122.12
21	N	664	LEU	N-CA-C	-5.72	104.70	112.26
24	Q	33	LYS	CA-C-N	5.72	127.95	120.28
24	Q	33	LYS	C-N-CA	5.72	127.95	120.28
7	g	43	ASN	N-CA-C	-5.72	106.15	113.02
10	j	111	GLY	N-CA-C	-5.72	101.16	110.55
25	R	162	ILE	N-CA-CB	5.72	120.40	110.96
26	U	159	CYS	O-C-N	5.72	129.12	122.19
6	f	175	THR	CA-C-N	5.72	128.22	120.38
6	f	175	THR	C-N-CA	5.72	128.22	120.38
8	h	47	HIS	CB-CG-CD2	-5.72	123.76	131.20
6	f	110	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
4	D	145	PRO	CA-C-O	-5.72	114.98	122.19
5	E	51	GLU	N-CA-C	-5.72	100.57	109.72
21	N	5	THR	N-CA-CB	5.72	118.70	110.06
24	Q	276	ASP	O-C-N	-5.72	116.06	122.12
32	M	173	ASP	CA-CB-CG	5.72	118.32	112.60
16	V	96	LYS	CA-C-O	5.72	126.61	120.55
21	N	652	VAL	N-CA-C	-5.72	104.94	110.72
13	m	155	MET	N-CA-C	5.72	121.28	113.16
13	6	125	ASP	CA-CB-CG	-5.72	106.88	112.60
16	V	190	HIS	CA-C-N	5.72	127.54	120.34
16	V	190	HIS	C-N-CA	5.72	127.54	120.34
17	T	226	TRP	CB-CA-C	-5.72	104.51	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	918	ASP	CA-CB-CG	-5.72	106.88	112.60
21	N	218	PRO	N-CA-CB	5.72	109.25	103.25
1	a	175	GLN	CA-C-N	5.71	128.21	120.38
1	a	175	GLN	C-N-CA	5.71	128.21	120.38
12	l	141	HIS	CG-CD2-NE2	5.71	112.91	107.20
13	m	59	VAL	N-CA-CB	5.71	119.02	111.25
4	D	126	VAL	N-CA-C	-5.71	100.81	108.35
24	Q	203	THR	CA-C-O	5.71	126.48	120.42
30	K	174	VAL	CA-C-N	5.71	127.48	120.22
30	K	174	VAL	C-N-CA	5.71	127.48	120.22
30	K	299	LEU	CB-CA-C	5.71	119.76	110.96
31	L	58	ASN	CA-C-N	5.71	127.94	120.28
31	L	58	ASN	C-N-CA	5.71	127.94	120.28
33	J	271	THR	CA-C-N	5.71	128.41	120.29
33	J	271	THR	C-N-CA	5.71	128.41	120.29
4	D	108	TYR	CA-C-N	5.71	128.21	120.44
4	D	108	TYR	C-N-CA	5.71	128.21	120.44
22	S	301	PRO	CA-C-O	-5.71	114.25	122.31
6	f	221	PRO	CA-C-O	-5.71	114.81	121.95
8	h	115	ASN	CA-C-N	5.71	132.45	121.54
8	h	115	ASN	C-N-CA	5.71	132.45	121.54
9	i	78	ALA	CA-C-N	5.71	128.40	120.29
9	i	78	ALA	C-N-CA	5.71	128.40	120.29
16	V	285	ASP	O-C-N	5.71	128.66	122.15
21	N	844	LYS	CA-C-N	5.71	129.84	121.96
21	N	844	LYS	C-N-CA	5.71	129.84	121.96
27	O	229	ASN	N-CA-C	-5.71	99.42	108.73
27	O	306	ARG	CA-C-N	5.71	132.07	121.62
27	O	306	ARG	C-N-CA	5.71	132.07	121.62
30	K	226	VAL	CA-C-O	-5.71	114.71	121.05
31	L	68	ARG	NE-CZ-NH1	-5.71	115.79	121.50
33	J	252	SER	CA-C-N	5.71	128.53	120.42
33	J	252	SER	C-N-CA	5.71	128.53	120.42
14	n	129	LEU	CA-C-O	-5.71	114.50	120.55
3	C	156	ASN	CA-CB-CG	5.71	118.31	112.60
6	F	99	PHE	CA-CB-CG	-5.71	108.09	113.80
27	O	161	ASP	N-CA-C	-5.71	104.89	112.94
7	g	231	VAL	N-CA-CB	5.71	117.51	111.00
20	Z	156	HIS	CB-CA-C	-5.71	101.92	110.88
20	Z	816	GLY	CA-C-N	5.71	128.40	120.29
20	Z	816	GLY	C-N-CA	5.71	128.40	120.29
24	Q	95	LYS	CA-C-O	-5.71	114.82	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	185	LEU	CB-CA-C	-5.71	101.46	110.02
28	H	241	ASP	CA-CB-CG	-5.71	106.89	112.60
29	I	233	ALA	CB-CA-C	-5.71	101.14	110.85
14	7	185	ASN	CB-CA-C	-5.71	101.03	111.64
26	U	168	GLU	CA-C-N	5.71	128.28	120.46
26	U	168	GLU	C-N-CA	5.71	128.28	120.46
5	e	163	THR	N-CA-CB	5.71	119.59	110.46
16	V	80	VAL	N-CA-C	-5.71	105.31	113.07
2	b	219	PRO	CA-C-N	5.70	131.12	121.14
2	b	219	PRO	C-N-CA	5.70	131.12	121.14
2	B	68	THR	N-CA-C	-5.70	98.91	109.06
8	1	144	TYR	CB-CG-CD2	5.70	129.35	120.80
12	5	282	PHE	N-CA-C	-5.70	103.41	111.56
18	X	109	LEU	CA-C-O	-5.70	114.24	120.17
20	Z	861	THR	O-C-N	-5.70	115.00	122.59
21	N	284	PRO	N-CA-C	-5.70	106.57	114.27
21	N	697	PHE	N-CA-C	-5.70	104.97	111.07
4	d	19	GLN	CA-C-N	5.70	127.86	120.56
4	d	19	GLN	C-N-CA	5.70	127.86	120.56
12	5	254	HIS	ND1-CE1-NE2	5.70	114.10	108.40
5	E	213	ASP	CA-CB-CG	-5.70	106.90	112.60
20	Z	541	ASP	CA-C-N	5.70	128.84	120.91
20	Z	541	ASP	C-N-CA	5.70	128.84	120.91
21	N	260	ASP	CA-CB-CG	-5.70	106.90	112.60
23	P	344	ARG	NE-CZ-NH2	5.70	124.33	119.20
28	H	358	PRO	N-CA-C	-5.70	108.14	114.92
30	K	395	VAL	CA-C-N	5.70	127.92	120.28
30	K	395	VAL	C-N-CA	5.70	127.92	120.28
5	E	242	GLU	O-C-N	5.70	128.89	122.22
7	G	147	HIS	CG-CD2-NE2	5.70	112.90	107.20
20	Z	112	LYS	CA-C-N	5.70	128.17	120.65
20	Z	112	LYS	C-N-CA	5.70	128.17	120.65
22	S	123	THR	CA-C-N	5.70	127.85	120.44
22	S	123	THR	C-N-CA	5.70	127.85	120.44
33	J	204	HIS	CA-CB-CG	5.70	119.50	113.80
33	J	310	ILE	CA-C-O	-5.70	114.41	120.39
13	6	46	ARG	CA-C-O	5.70	125.96	119.18
22	S	489	GLN	CA-C-O	-5.70	114.78	121.16
31	L	421	LYS	CA-C-O	-5.70	114.38	120.42
32	M	64	ASP	CA-C-N	5.70	127.85	120.44
32	M	64	ASP	C-N-CA	5.70	127.85	120.44
1	A	157	THR	CA-CB-OG1	-5.70	101.06	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	4	ASN	OD1-CG-ND2	5.70	128.30	122.60
21	N	761	ILE	N-CA-C	-5.70	100.28	108.48
3	c	191	GLU	N-CA-C	5.69	117.49	111.28
3	C	178	MET	CG-SD-CE	-5.69	88.37	100.90
5	E	157	HIS	N-CA-C	-5.69	99.13	108.41
20	Z	623	ARG	CA-C-O	5.69	126.80	120.82
24	Q	265	MET	O-C-N	5.69	128.16	122.12
30	K	50	LYS	N-CA-CB	5.69	118.33	110.07
3	c	235	ILE	CA-C-N	5.69	127.91	120.28
3	c	235	ILE	C-N-CA	5.69	127.91	120.28
6	f	27	GLU	N-CA-CB	5.69	118.49	110.12
6	F	225	TYR	N-CA-CB	5.69	119.91	110.52
13	6	90	LYS	O-C-N	-5.69	116.53	123.19
7	g	116	LEU	CB-CA-C	-5.69	101.34	110.79
7	g	182	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
18	X	39	GLU	CA-C-N	5.69	131.81	121.97
18	X	39	GLU	C-N-CA	5.69	131.81	121.97
20	Z	916	LEU	N-CA-C	-5.69	106.88	113.88
21	N	436	ASP	CA-C-N	5.69	128.37	120.29
21	N	436	ASP	C-N-CA	5.69	128.37	120.29
12	5	227	ASP	N-CA-C	-5.69	105.84	112.89
28	H	146	VAL	O-C-N	5.69	129.08	122.99
7	g	94	GLU	CA-C-O	5.69	126.45	120.42
4	D	108	TYR	N-CA-C	-5.69	105.16	111.36
15	W	77	HIS	CA-C-O	5.69	126.45	120.42
16	V	196	TYR	CB-CG-CD2	5.69	129.33	120.80
29	I	346	ARG	CB-CG-CD	5.69	124.38	111.30
12	l	204	VAL	CB-CA-C	-5.69	100.53	110.71
9	2	176	THR	N-CA-C	-5.69	101.78	110.14
20	Z	925	VAL	CB-CA-C	-5.69	104.59	112.04
2	b	82	TYR	CA-C-O	-5.68	114.52	120.55
2	b	94	HIS	CB-CG-CD2	-5.68	123.81	131.20
9	i	252	ILE	CB-CA-C	5.68	120.61	111.29
17	T	104	LYS	CB-CG-CD	5.68	124.37	111.30
21	N	223	LEU	N-CA-CB	5.68	118.67	110.20
21	N	862	SER	N-CA-CB	5.68	120.10	110.49
25	R	394	ASP	CA-C-O	5.68	124.77	118.52
27	O	144	VAL	N-CA-C	5.68	116.46	110.72
31	L	420	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	a	41	ASN	N-CA-C	-5.68	100.52	109.50
5	e	176	SER	CA-C-N	5.68	127.89	120.28
5	e	176	SER	C-N-CA	5.68	127.89	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	52	LYS	N-CA-CB	5.68	119.63	110.65
16	V	271	VAL	O-C-N	5.68	129.67	122.57
22	S	39	ASN	CA-C-O	-5.68	114.40	120.42
24	Q	12	ARG	CA-C-N	5.68	127.89	120.28
24	Q	12	ARG	C-N-CA	5.68	127.89	120.28
5	e	63	SER	O-C-N	-5.68	115.52	122.34
20	Z	800	SER	N-CA-C	-5.68	105.61	112.54
22	S	55	ARG	NE-CZ-NH1	-5.68	115.82	121.50
22	S	471	LEU	CA-C-O	-5.68	114.40	120.42
25	R	345	TYR	N-CA-CB	5.68	120.36	110.81
15	W	87	MET	N-CA-C	5.68	117.15	111.07
20	Z	743	ILE	N-CA-C	-5.68	104.98	110.72
27	O	186	ASN	N-CA-CB	5.68	118.57	110.16
32	M	357	ARG	CA-C-O	-5.68	114.86	120.82
33	J	6	THR	CA-CB-CG2	5.68	120.16	110.50
9	i	178	GLU	O-C-N	5.68	129.61	122.23
8	1	48	ASP	N-CA-C	-5.68	105.17	111.36
29	I	150	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
14	n	207	GLU	CB-CG-CD	-5.68	102.95	112.60
21	N	83	LEU	CA-C-N	5.68	133.73	121.64
21	N	83	LEU	C-N-CA	5.68	133.73	121.64
29	I	56	LYS	N-CA-C	-5.68	105.23	111.82
7	g	211	ASP	CA-C-N	5.67	131.44	122.36
7	g	211	ASP	C-N-CA	5.67	131.44	122.36
10	j	73	LEU	N-CA-CB	5.67	119.08	110.28
7	G	20	ARG	O-C-N	-5.67	116.28	122.92
11	4	143	LEU	CA-C-N	5.67	128.35	120.29
11	4	143	LEU	C-N-CA	5.67	128.35	120.29
14	7	252	TRP	CB-CG-CD2	-5.67	118.86	126.80
17	T	250	MET	CG-SD-CE	-5.67	88.42	100.90
20	Z	19	SER	N-CA-C	-5.67	97.27	109.81
20	Z	33	GLU	CB-CG-CD	-5.67	102.95	112.60
23	P	36	LEU	CA-C-O	-5.67	114.41	120.42
9	i	230	LYS	CA-C-O	-5.67	115.20	121.33
1	A	43	LEU	N-CA-C	-5.67	98.27	108.48
20	Z	921	GLU	CA-C-N	5.67	126.93	119.84
20	Z	921	GLU	C-N-CA	5.67	126.93	119.84
22	S	49	ASP	CA-C-N	5.67	125.52	119.28
22	S	49	ASP	C-N-CA	5.67	125.52	119.28
26	U	41	ALA	O-C-N	5.67	128.96	123.29
28	H	292	ARG	N-CA-C	5.67	117.46	111.28
2	b	164	ILE	N-CA-C	-5.67	99.65	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	109	HIS	CB-CG-ND1	5.67	131.21	122.70
18	X	36	LYS	CA-C-O	-5.67	113.53	120.05
3	c	89	ASN	CA-C-N	5.67	128.34	120.29
3	c	89	ASN	C-N-CA	5.67	128.34	120.29
5	E	188	HIS	N-CA-C	-5.67	100.87	108.86
20	Z	80	SER	N-CA-CB	5.67	120.07	110.49
21	N	186	ILE	CA-C-N	5.67	128.93	120.31
21	N	186	ILE	C-N-CA	5.67	128.93	120.31
31	L	289	ARG	CA-C-N	5.67	132.37	121.54
31	L	289	ARG	C-N-CA	5.67	132.37	121.54
9	i	144	ALA	N-CA-C	5.67	118.39	111.82
9	2	88	ILE	CA-C-O	-5.67	114.65	120.71
16	V	121	VAL	CA-C-N	5.67	128.92	120.31
16	V	121	VAL	C-N-CA	5.67	128.92	120.31
16	V	150	LYS	N-CA-C	-5.67	106.91	113.88
25	R	276	LEU	CB-CA-C	-5.67	101.95	110.90
30	K	197	LEU	N-CA-C	5.67	117.13	111.07
3	c	174	THR	N-CA-C	-5.67	105.11	111.28
1	A	71	TYR	N-CA-C	-5.67	98.73	110.80
30	K	273	GLU	N-CA-C	-5.67	100.46	109.07
33	J	217	GLU	N-CA-CB	5.67	119.44	110.55
14	n	235	LYS	CA-C-N	5.66	128.87	119.35
14	n	235	LYS	C-N-CA	5.66	128.87	119.35
8	1	16	THR	CA-C-O	5.66	128.49	121.81
23	P	194	SER	CA-C-N	5.66	127.87	120.28
23	P	194	SER	C-N-CA	5.66	127.87	120.28
26	U	115	GLN	OE1-CD-NE2	5.66	128.26	122.60
16	V	259	LYS	N-CA-C	-5.66	105.58	112.88
24	Q	72	ASP	CA-C-N	5.66	127.80	120.44
24	Q	72	ASP	C-N-CA	5.66	127.80	120.44
25	R	49	PHE	O-C-N	5.66	128.20	122.09
27	O	164	PRO	N-CA-C	5.66	119.90	111.41
10	j	157	ASN	N-CA-CB	5.66	120.05	110.49
4	D	205	THR	CA-C-O	-5.66	114.49	121.11
7	G	119	TYR	CA-C-N	5.66	128.45	120.42
7	G	119	TYR	C-N-CA	5.66	128.45	120.42
20	Z	146	PHE	N-CA-CB	5.66	120.05	110.49
24	Q	231	ASP	N-CA-CB	5.66	119.59	110.65
32	M	15	ASP	N-CA-C	-5.66	101.65	110.42
9	2	238	THR	N-CA-C	-5.66	105.88	112.89
2	b	150	VAL	O-C-N	5.66	128.52	123.03
2	b	153	SER	N-CA-C	-5.66	104.59	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	111	ARG	CA-C-N	5.66	128.32	120.29
4	d	111	ARG	C-N-CA	5.66	128.32	120.29
11	k	33	ASP	N-CA-C	-5.66	100.02	109.24
3	C	203	SER	N-CA-CB	5.66	119.09	109.87
24	Q	15	VAL	N-CA-CB	5.66	117.17	110.55
25	R	159	SER	O-C-N	5.66	128.60	122.15
29	I	199	GLU	CB-CA-C	-5.66	101.24	110.85
7	g	47	VAL	N-CA-C	-5.65	100.03	108.46
19	Y	11	GLN	CA-C-N	5.65	127.86	120.28
19	Y	11	GLN	C-N-CA	5.65	127.86	120.28
24	Q	160	ASP	CA-CB-CG	5.65	118.25	112.60
2	b	135	LEU	N-CA-C	-5.65	100.19	109.40
3	c	129	ARG	CA-C-N	5.65	126.13	120.14
3	c	129	ARG	C-N-CA	5.65	126.13	120.14
5	e	109	VAL	N-CA-C	5.65	116.39	110.62
9	i	52	GLY	CA-C-N	5.65	126.72	120.45
9	i	52	GLY	C-N-CA	5.65	126.72	120.45
14	n	77	PRO	N-CA-CB	5.65	108.27	103.35
12	5	159	SER	N-CA-C	-5.65	105.20	111.36
21	N	522	ALA	CA-C-N	5.65	127.86	120.28
21	N	522	ALA	C-N-CA	5.65	127.86	120.28
21	N	677	ASP	CA-C-N	5.65	128.45	120.42
21	N	677	ASP	C-N-CA	5.65	128.45	120.42
5	e	157	HIS	ND1-CE1-NE2	5.65	114.05	108.40
6	f	126	ARG	CB-CA-C	5.65	118.29	109.42
11	k	162	LYS	N-CA-CB	-5.65	101.80	110.16
5	E	231	TYR	CB-CG-CD1	-5.65	112.32	120.80
6	F	119	ASN	OD1-CG-ND2	-5.65	116.95	122.60
15	W	107	HIS	CE1-NE2-CD2	-5.65	103.35	109.00
21	N	922	GLN	CA-C-N	5.65	128.31	120.29
21	N	922	GLN	C-N-CA	5.65	128.31	120.29
22	S	186	TYR	N-CA-C	5.65	117.52	111.36
32	M	142	PRO	CA-C-N	5.65	132.63	123.93
32	M	142	PRO	C-N-CA	5.65	132.63	123.93
9	i	200	SER	N-CA-CB	5.65	120.04	110.49
7	G	28	VAL	N-CA-CB	5.65	118.22	110.54
3	c	115	LEU	CB-CA-C	5.65	120.45	110.85
8	h	95	CYS	N-CA-CB	5.65	118.52	110.16
7	G	16	SER	N-CA-C	-5.65	103.53	110.31
23	P	402	PHE	CB-CA-C	-5.65	101.51	111.05
28	H	196	THR	CA-C-N	5.65	127.85	120.28
28	H	196	THR	C-N-CA	5.65	127.85	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	329	VAL	N-CA-C	-5.65	104.65	112.50
29	I	376	ASN	CA-C-N	5.65	127.78	120.44
29	I	376	ASN	C-N-CA	5.65	127.78	120.44
31	L	225	GLY	N-CA-C	-5.65	106.38	115.08
11	4	143	LEU	N-CA-C	5.65	117.51	111.36
17	T	107	SER	CA-C-N	5.65	128.41	120.28
17	T	107	SER	C-N-CA	5.65	128.41	120.28
23	P	260	VAL	O-C-N	-5.65	116.38	121.91
9	i	59	ASN	CA-CB-CG	-5.64	106.96	112.60
13	m	160	ASN	O-C-N	5.64	128.10	122.12
13	m	173	ASN	CA-CB-CG	-5.64	106.95	112.60
2	B	53	SER	N-CA-C	-5.64	97.33	109.81
9	2	181	ILE	CA-C-N	5.64	127.84	120.28
9	2	181	ILE	C-N-CA	5.64	127.84	120.28
16	V	119	SER	O-C-N	-5.64	115.76	122.65
23	P	407	ASN	CA-CB-CG	5.64	118.25	112.60
5	e	73	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
1	A	228	ALA	CA-C-O	5.64	126.58	120.43
2	B	233	PRO	O-C-N	5.64	129.50	123.01
3	C	179	ASP	O-C-N	-5.64	115.41	122.35
21	N	211	PHE	O-C-N	5.64	128.10	122.12
26	U	189	ARG	NE-CZ-NH2	5.64	124.28	119.20
26	U	197	LEU	CA-C-O	5.64	126.40	120.42
29	I	98	GLU	CA-C-N	5.64	127.67	120.56
29	I	98	GLU	C-N-CA	5.64	127.67	120.56
29	I	255	LYS	CA-C-N	5.64	128.86	120.90
29	I	255	LYS	C-N-CA	5.64	128.86	120.90
32	M	110	ASN	N-CA-C	5.64	117.51	111.36
32	M	207	PHE	N-CA-C	5.64	117.11	111.07
13	6	68	ASP	N-CA-C	-5.64	105.28	111.82
2	b	90	ARG	CA-C-O	-5.64	114.90	120.82
12	l	113	ASN	N-CA-CB	5.64	117.10	111.29
22	S	362	SER	CA-C-N	5.64	128.15	120.54
22	S	362	SER	C-N-CA	5.64	128.15	120.54
26	U	11	ALA	CA-C-N	5.64	125.26	119.56
26	U	11	ALA	C-N-CA	5.64	125.26	119.56
5	e	43	LYS	N-CA-C	-5.64	105.61	112.88
5	e	225	GLN	N-CA-C	-5.64	104.51	111.33
6	F	177	ASP	CA-CB-CG	5.64	118.24	112.60
16	V	237	ASN	CA-C-N	5.64	127.83	120.28
16	V	237	ASN	C-N-CA	5.64	127.83	120.28
28	H	405	GLU	N-CA-CB	5.64	118.50	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	60	GLU	CB-CA-C	-5.64	101.43	110.79
5	E	146	GLY	O-C-N	5.64	131.36	123.64
21	N	457	SER	O-C-N	5.64	128.57	121.64
31	L	137	ARG	CA-C-N	5.64	131.58	121.66
31	L	137	ARG	C-N-CA	5.64	131.58	121.66
9	i	125	ALA	N-CA-CB	5.63	120.01	110.49
13	6	190	LYS	CA-C-N	5.63	127.83	120.28
13	6	190	LYS	C-N-CA	5.63	127.83	120.28
20	Z	85	VAL	CA-C-N	5.63	126.88	119.84
20	Z	85	VAL	C-N-CA	5.63	126.88	119.84
20	Z	735	GLU	N-CA-CB	5.63	118.90	110.22
1	A	36	ASN	CB-CG-OD1	-5.63	109.53	120.80
20	Z	570	LEU	O-C-N	-5.63	116.27	122.07
26	U	94	HIS	CB-CG-CD2	-5.63	123.88	131.20
7	G	74	ILE	N-CA-C	-5.63	99.53	107.75
8	1	151	PHE	N-CA-CB	5.63	118.68	109.95
12	5	179	TYR	N-CA-C	-5.63	96.57	107.44
21	N	553	PHE	N-CA-C	-5.63	106.41	113.28
32	M	210	MET	CA-C-O	-5.63	114.58	120.55
32	M	389	ALA	O-C-N	5.63	128.17	122.09
5	E	212	LEU	CB-CA-C	-5.63	101.06	110.29
21	N	841	THR	N-CA-C	-5.63	98.81	110.80
26	U	231	ASP	N-CA-C	5.63	117.42	111.28
27	O	82	LEU	CA-C-N	5.63	128.28	120.29
27	O	82	LEU	C-N-CA	5.63	128.28	120.29
6	f	131	GLY	CA-C-O	-5.63	115.80	120.92
6	f	143	HIS	ND1-CE1-NE2	5.63	114.03	108.40
33	J	33	LYS	CA-C-N	5.63	128.41	120.42
33	J	33	LYS	C-N-CA	5.63	128.41	120.42
16	V	21	ASP	CA-C-N	5.63	130.81	122.82
16	V	21	ASP	C-N-CA	5.63	130.81	122.82
27	O	341	ILE	O-C-N	-5.63	117.18	123.26
28	H	208	TYR	N-CA-C	-5.63	105.07	112.72
21	N	832	HIS	ND1-CE1-NE2	5.62	114.03	108.40
29	I	141	LEU	CA-C-O	5.62	127.47	121.11
11	k	25	ILE	CB-CA-C	5.62	118.99	111.85
21	N	14	ARG	CA-C-O	-5.62	113.50	119.97
21	N	404	SER	CA-C-O	5.62	126.42	119.79
25	R	388	VAL	CG1-CB-CG2	-5.62	98.43	110.80
6	f	231	ALA	N-CA-C	-5.62	106.01	112.92
12	l	196	ARG	N-CA-C	-5.62	99.12	108.34
20	Z	787	ASP	CA-CB-CG	-5.62	106.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	73	TYR	N-CA-C	-5.62	98.83	110.80
8	1	160	THR	N-CA-C	-5.62	105.07	111.14
9	2	242	LEU	N-CA-C	-5.62	105.53	112.72
25	R	53	LYS	CA-C-N	5.62	128.16	120.46
25	R	53	LYS	C-N-CA	5.62	128.16	120.46
28	H	115	THR	CA-C-N	5.62	128.07	120.65
28	H	115	THR	C-N-CA	5.62	128.07	120.65
12	l	157	ILE	CA-CB-CG2	5.62	120.05	110.50
4	D	88	LYS	CA-C-N	5.62	128.27	120.29
4	D	88	LYS	C-N-CA	5.62	128.27	120.29
21	N	889	ARG	N-CA-C	5.62	117.85	111.11
23	P	346	ILE	O-C-N	-5.62	114.79	122.26
27	O	141	ASN	N-CA-CB	5.62	119.98	110.49
31	L	69	ARG	NE-CZ-NH1	-5.62	115.88	121.50
31	L	333	LEU	O-C-N	-5.62	116.84	123.25
32	M	378	GLU	CA-CB-CG	-5.62	102.86	114.10
13	6	78	ASN	CA-CB-CG	5.62	118.22	112.60
20	Z	312	TYR	CA-CB-CG	-5.62	103.79	113.90
33	J	299	ILE	N-CA-C	-5.62	105.38	113.07
20	Z	541	ASP	N-CA-CB	5.62	120.61	111.74
21	N	639	ASP	N-CA-CB	5.62	118.38	110.12
24	Q	404	ASN	CA-C-O	5.62	125.46	119.34
25	R	71	LEU	CA-C-N	5.62	132.08	121.97
25	R	71	LEU	C-N-CA	5.62	132.08	121.97
25	R	114	ASN	CA-C-O	-5.62	114.60	120.55
28	H	161	GLU	N-CA-C	-5.62	106.47	113.38
30	K	84	GLU	CA-C-N	5.62	127.80	120.28
30	K	84	GLU	C-N-CA	5.62	127.80	120.28
31	L	302	GLN	N-CA-C	5.62	117.40	111.28
10	j	116	SER	CB-CA-C	-5.61	99.25	110.42
12	l	215	LEU	CA-C-N	5.61	127.80	120.28
12	l	215	LEU	C-N-CA	5.61	127.80	120.28
12	l	225	VAL	N-CA-CB	5.61	119.00	110.58
17	T	246	GLU	N-CA-C	5.61	117.40	111.28
27	O	277	ILE	CA-CB-CG1	5.61	119.94	110.40
10	j	37	SER	N-CA-C	-5.61	100.18	108.99
17	T	259	ILE	CA-C-N	5.61	128.15	120.46
17	T	259	ILE	C-N-CA	5.61	128.15	120.46
21	N	389	TYR	N-CA-C	-5.61	106.48	113.38
13	m	140	GLU	CA-C-O	5.61	127.39	121.33
24	Q	304	GLU	CA-C-N	5.61	127.80	120.28
24	Q	304	GLU	C-N-CA	5.61	127.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	346	VAL	CA-C-O	5.61	127.12	121.17
26	U	26	GLN	N-CA-CB	5.61	120.00	111.70
26	U	292	ILE	CA-C-O	5.61	127.12	121.17
13	m	26	GLU	N-CA-C	-5.61	106.43	113.72
7	G	241	ASP	N-CA-C	5.61	117.47	111.36
9	2	88	ILE	N-CA-C	-5.61	104.89	111.00
23	P	287	ASP	O-C-N	-5.61	116.62	122.96
28	H	110	GLY	N-CA-C	-5.61	107.58	115.32
29	I	106	ILE	CA-C-O	-5.61	115.81	121.59
33	J	43	ARG	NE-CZ-NH2	-5.61	114.15	119.20
7	g	169	ARG	CA-C-N	5.61	128.25	120.29
7	g	169	ARG	C-N-CA	5.61	128.25	120.29
9	i	143	HIS	N-CA-C	-5.61	101.88	109.95
11	k	60	ILE	N-CA-C	5.61	116.38	110.72
1	A	188	LYS	CB-CA-C	-5.61	101.32	110.85
3	C	188	ASP	CA-C-N	5.61	127.73	120.44
3	C	188	ASP	C-N-CA	5.61	127.73	120.44
4	D	152	PRO	N-CA-CB	5.61	108.80	103.19
11	4	43	LEU	N-CA-C	-5.61	99.29	108.76
13	6	51	VAL	N-CA-C	-5.61	99.67	107.80
18	X	48	PHE	CA-CB-CG	-5.61	108.19	113.80
18	X	94	ASN	CA-CB-CG	-5.61	106.99	112.60
20	Z	570	LEU	CA-C-N	5.61	127.15	120.14
20	Z	570	LEU	C-N-CA	5.61	127.15	120.14
21	N	433	THR	N-CA-C	-5.61	104.69	112.03
21	N	888	ASP	CA-CB-CG	-5.61	107.00	112.60
24	Q	102	GLU	CB-CA-C	-5.61	101.48	110.79
30	K	65	GLU	CB-CG-CD	-5.61	103.07	112.60
15	W	49	VAL	CA-CB-CG2	-5.60	100.87	110.40
20	Z	760	HIS	ND1-CE1-NE2	5.60	114.00	108.40
22	S	136	CYS	CA-C-O	5.60	126.47	120.70
24	Q	2	SER	CA-C-N	5.60	126.73	119.78
24	Q	2	SER	C-N-CA	5.60	126.73	119.78
7	g	46	VAL	N-CA-C	-5.60	100.41	108.42
9	i	151	GLY	CA-C-O	-5.60	113.32	122.56
8	1	203	GLU	N-CA-C	-5.60	105.25	111.36
22	S	417	GLN	CA-C-N	5.60	127.72	120.44
22	S	417	GLN	C-N-CA	5.60	127.72	120.44
25	R	170	VAL	CB-CA-C	5.60	119.70	112.14
27	O	30	GLU	N-CA-C	5.60	117.39	111.28
29	I	194	ILE	CA-C-N	5.60	127.79	120.28
29	I	194	ILE	C-N-CA	5.60	127.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	280	PHE	CA-C-O	5.60	126.28	120.40
33	J	116	ARG	N-CA-C	-5.60	98.87	110.80
20	Z	370	SER	CA-C-N	5.60	129.21	120.75
20	Z	370	SER	C-N-CA	5.60	129.21	120.75
23	P	291	LYS	N-CA-C	-5.60	105.76	112.59
25	R	85	SER	O-C-N	5.60	129.15	122.26
31	L	387	ASN	OD1-CG-ND2	5.60	128.20	122.60
5	e	51	GLU	N-CA-C	-5.60	100.27	109.40
11	k	64	ILE	N-CA-CB	5.60	118.98	110.58
7	G	20	ARG	CA-C-O	5.60	127.30	121.36
9	2	30	THR	O-C-N	-5.60	114.04	123.00
20	Z	633	GLU	CA-C-O	-5.60	114.61	120.55
23	P	384	VAL	CA-C-N	5.60	128.24	120.29
23	P	384	VAL	C-N-CA	5.60	128.24	120.29
25	R	177	LEU	N-CA-C	5.60	118.15	111.71
28	H	425	GLU	CA-C-N	5.60	128.82	120.31
28	H	425	GLU	C-N-CA	5.60	128.82	120.31
3	c	36	ILE	CA-C-O	-5.60	114.33	120.43
4	d	239	GLU	CA-C-O	-5.60	113.53	119.97
5	E	70	ILE	N-CA-CB	-5.60	106.05	112.21
10	3	101	GLY	CA-C-N	5.60	126.84	119.84
10	3	101	GLY	C-N-CA	5.60	126.84	119.84
25	R	395	ASN	O-C-N	-5.60	117.14	123.13
9	i	177	LYS	CA-C-O	-5.60	114.94	120.82
20	Z	277	GLU	CA-C-N	5.60	130.93	121.14
20	Z	277	GLU	C-N-CA	5.60	130.93	121.14
24	Q	247	HIS	CE1-NE2-CD2	-5.60	103.40	109.00
4	d	54	LEU	N-CA-CB	5.59	118.28	109.94
12	l	108	LYS	O-C-N	-5.59	115.38	122.26
1	A	130	GLN	OE1-CD-NE2	5.59	128.19	122.60
11	4	180	ILE	N-CA-CB	5.59	117.22	110.95
17	T	20	TYR	N-CA-C	-5.59	106.50	113.38
20	Z	109	PRO	N-CD-CG	5.59	111.59	103.20
21	N	607	GLN	CA-C-O	5.59	126.48	120.55
21	N	806	THR	N-CA-CB	5.59	118.84	110.22
32	M	354	GLU	CA-C-N	5.59	130.19	120.68
32	M	354	GLU	C-N-CA	5.59	130.19	120.68
9	2	122	HIS	CA-CB-CG	5.59	119.39	113.80
20	Z	146	PHE	CA-C-N	5.59	128.05	120.44
20	Z	146	PHE	C-N-CA	5.59	128.05	120.44
24	Q	217	GLU	CA-C-N	5.59	127.71	120.44
24	Q	217	GLU	C-N-CA	5.59	127.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	91	TRP	CA-CB-CG	5.59	124.23	113.60
27	O	267	ASP	CA-C-N	5.59	127.71	120.44
27	O	267	ASP	C-N-CA	5.59	127.71	120.44
31	L	96	LYS	N-CA-CB	5.59	118.34	110.12
5	E	214	GLU	N-CA-C	-5.59	106.42	113.18
7	G	82	ILE	CA-C-O	-5.59	114.46	118.71
20	Z	447	VAL	N-CA-CB	5.59	120.89	110.77
20	Z	566	LEU	CA-C-N	5.59	128.23	120.29
20	Z	566	LEU	C-N-CA	5.59	128.23	120.29
23	P	295	SER	N-CA-CB	5.59	118.53	110.20
25	R	24	TYR	CA-C-N	5.59	127.71	120.44
25	R	24	TYR	C-N-CA	5.59	127.71	120.44
25	R	110	ILE	N-CA-C	-5.59	105.05	110.42
27	O	235	HIS	N-CA-C	-5.59	104.69	112.30
28	H	216	ASP	CA-C-O	-5.59	114.62	120.55
29	I	292	TYR	N-CA-C	-5.59	104.82	111.03
29	I	372	SER	N-CA-CB	5.59	119.94	110.49
8	h	34	TYR	N-CA-C	-5.59	101.17	110.17
8	1	38	ARG	CA-C-O	5.59	126.24	119.31
10	3	54	THR	N-CA-C	-5.59	102.19	110.46
10	3	154	TYR	CA-C-O	5.59	127.24	120.81
12	5	168	ALA	N-CA-C	-5.59	106.13	113.17
13	6	84	HIS	CA-C-O	-5.59	114.95	120.82
20	Z	564	ARG	CD-NE-CZ	5.59	132.23	124.40
20	Z	967	THR	CA-C-N	5.59	130.88	123.00
20	Z	967	THR	C-N-CA	5.59	130.88	123.00
21	N	553	PHE	N-CA-CB	5.59	119.23	110.46
25	R	241	ILE	CB-CG1-CD1	5.59	125.54	113.80
22	S	294	ILE	N-CA-C	-5.59	105.08	110.72
30	K	140	HIS	CB-CG-CD2	-5.59	123.94	131.20
31	L	175	GLN	CB-CG-CD	-5.59	103.10	112.60
31	L	369	LYS	CA-C-O	5.59	127.00	120.80
14	n	208	GLU	CA-C-O	-5.59	114.63	120.55
14	n	263	THR	N-CA-CB	5.59	119.36	110.65
8	1	122	ILE	N-CA-C	-5.59	101.62	107.60
10	3	145	GLN	N-CA-C	5.59	117.05	111.07
21	N	47	GLU	CA-C-O	-5.59	114.63	120.55
22	S	20	HIS	O-C-N	5.59	128.52	122.15
23	P	425	HIS	CA-CB-CG	-5.59	108.21	113.80
30	K	303	MET	O-C-N	-5.59	115.64	122.34
31	L	113	SER	N-CA-C	-5.59	100.44	108.60
32	M	170	MET	CB-CA-C	-5.59	100.30	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	SER	CA-C-O	-5.58	115.25	121.51
28	H	107	LYS	N-CA-C	-5.58	99.80	108.90
28	H	420	ARG	NE-CZ-NH2	5.58	124.23	119.20
3	c	170	SER	CA-C-N	5.58	127.70	120.44
3	c	170	SER	C-N-CA	5.58	127.70	120.44
8	h	174	TRP	N-CA-C	-5.58	105.07	112.94
5	E	237	ALA	CA-C-N	5.58	127.76	120.28
5	E	237	ALA	C-N-CA	5.58	127.76	120.28
12	5	152	ALA	CA-C-N	5.58	128.03	120.44
12	5	152	ALA	C-N-CA	5.58	128.03	120.44
22	S	458	GLN	O-C-N	5.58	128.04	122.12
30	K	205	PRO	CA-C-N	5.58	126.05	120.52
30	K	205	PRO	C-N-CA	5.58	126.05	120.52
32	M	315	PHE	N-CA-CB	5.58	119.72	111.01
2	b	243	ILE	N-CA-CB	5.58	118.13	110.54
10	3	183	TRP	CE2-CD2-CE3	5.58	124.38	118.80
13	6	40	ASP	CA-CB-CG	-5.58	107.02	112.60
15	W	86	HIS	CA-C-N	5.58	127.70	120.44
15	W	86	HIS	C-N-CA	5.58	127.70	120.44
20	Z	620	LEU	N-CA-C	-5.58	98.91	110.80
21	N	667	GLN	N-CA-C	-5.58	98.91	110.80
22	S	345	TYR	CB-CG-CD2	5.58	129.17	120.80
24	Q	346	ASN	CA-C-N	5.58	128.22	120.29
24	Q	346	ASN	C-N-CA	5.58	128.22	120.29
8	h	180	GLY	N-CA-C	-5.58	99.95	113.18
20	Z	358	TYR	N-CA-C	-5.58	105.29	111.71
4	d	133	THR	CA-C-N	5.58	130.70	123.00
4	d	133	THR	C-N-CA	5.58	130.70	123.00
13	m	45	SER	CA-C-N	5.58	130.99	122.29
13	m	45	SER	C-N-CA	5.58	130.99	122.29
2	B	127	VAL	CA-CB-CG2	-5.58	100.92	110.40
3	C	31	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
7	G	240	ILE	CA-C-O	-5.58	115.26	121.17
9	2	178	GLU	CA-C-O	5.58	126.68	120.82
12	5	241	HIS	ND1-CE1-NE2	5.58	113.98	108.40
2	b	219	PRO	N-CA-C	-5.58	105.27	114.75
13	m	155	MET	CA-C-N	5.58	125.42	119.28
13	m	155	MET	C-N-CA	5.58	125.42	119.28
11	k	153	THR	CA-C-N	5.58	127.75	120.28
11	k	153	THR	C-N-CA	5.58	127.75	120.28
12	l	241	HIS	CG-CD2-NE2	5.58	112.78	107.20
13	m	133	PHE	CA-CB-CG	-5.58	108.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	163	VAL	CA-CB-CG2	5.58	119.88	110.40
10	3	113	ASN	CA-CB-CG	-5.58	107.03	112.60
13	6	57	ASN	N-CA-CB	5.58	119.91	110.49
14	7	135	GLN	OE1-CD-NE2	5.58	128.18	122.60
16	V	151	VAL	N-CA-CB	5.58	117.17	110.31
20	Z	390	LEU	N-CA-CB	-5.58	101.74	110.44
26	U	117	ASN	CA-CB-CG	-5.58	107.02	112.60
26	U	171	VAL	N-CA-C	5.58	115.77	110.53
31	L	157	ARG	CA-C-N	5.58	128.89	120.75
31	L	157	ARG	C-N-CA	5.58	128.89	120.75
32	M	351	LEU	CA-C-N	5.58	126.81	119.84
32	M	351	LEU	C-N-CA	5.58	126.81	119.84
2	b	10	THR	CA-CB-CG2	5.57	119.98	110.50
11	k	106	GLY	O-C-N	5.57	128.45	123.60
4	D	213	THR	N-CA-C	-5.57	100.59	109.23
9	2	224	VAL	CA-C-N	5.57	128.78	120.87
9	2	224	VAL	C-N-CA	5.57	128.78	120.87
11	4	113	LYS	CA-C-N	5.57	125.48	119.85
11	4	113	LYS	C-N-CA	5.57	125.48	119.85
12	5	215	LEU	CA-C-O	-5.57	114.96	120.70
23	P	303	PHE	CA-CB-CG	-5.57	108.23	113.80
23	P	376	THR	O-C-N	5.57	128.03	122.12
33	J	52	ASN	N-CA-C	5.57	117.80	111.11
2	B	157	PHE	CA-C-N	5.57	126.05	120.14
2	B	157	PHE	C-N-CA	5.57	126.05	120.14
10	3	176	ASP	CA-CB-CG	-5.57	107.03	112.60
12	5	275	VAL	CA-C-O	5.57	126.27	120.25
21	N	66	SER	N-CA-C	5.57	117.35	111.28
26	U	21	HIS	ND1-CE1-NE2	5.57	113.97	108.40
32	M	195	GLU	CA-C-O	-5.57	114.64	120.55
9	i	33	VAL	O-C-N	-5.57	117.14	123.10
2	B	149	GLN	N-CA-C	-5.57	99.82	108.90
5	E	43	LYS	N-CA-C	-5.57	106.25	113.16
10	3	37	SER	N-CA-C	-5.57	99.59	109.06
13	6	116	HIS	CA-C-N	-5.57	114.35	122.65
13	6	116	HIS	C-N-CA	-5.57	114.35	122.65
25	R	22	PRO	CB-CA-C	-5.57	101.75	110.49
12	5	147	GLU	CA-C-N	5.57	128.75	120.95
12	5	147	GLU	C-N-CA	5.57	128.75	120.95
9	i	82	GLU	CA-C-N	5.57	127.68	120.44
9	i	82	GLU	C-N-CA	5.57	127.68	120.44
14	7	148	ILE	CA-C-O	5.57	125.89	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	366	THR	CA-CB-OG1	5.57	117.95	109.60
31	L	263	ILE	CA-C-N	5.57	127.68	120.44
31	L	263	ILE	C-N-CA	5.57	127.68	120.44
1	A	68	THR	CA-CB-OG1	5.57	117.95	109.60
4	D	10	ILE	O-C-N	-5.57	117.19	123.20
4	D	29	ARG	NE-CZ-NH2	5.57	124.21	119.20
6	F	76	GLY	N-CA-C	-5.57	99.99	113.18
12	5	113	ASN	OD1-CG-ND2	-5.57	117.03	122.60
13	6	87	HIS	ND1-CE1-NE2	5.57	113.97	108.40
21	N	793	GLY	CA-C-N	5.57	128.19	120.29
21	N	793	GLY	C-N-CA	5.57	128.19	120.29
7	G	144	ASN	N-CA-C	-5.56	106.38	112.72
20	Z	324	GLU	CA-C-O	-5.56	114.97	120.70
10	j	49	VAL	N-CA-CB	5.56	116.78	110.72
8	1	91	PHE	N-CA-CB	5.56	118.08	110.01
8	1	129	HIS	CB-CG-CD2	-5.56	123.97	131.20
15	W	75	GLY	CA-C-O	-5.56	114.14	120.09
20	Z	716	THR	CA-C-N	5.56	127.73	120.28
20	Z	716	THR	C-N-CA	5.56	127.73	120.28
29	I	271	ALA	CB-CA-C	-5.56	101.56	110.79
14	n	75	LEU	O-C-N	5.56	129.56	123.22
4	D	14	ASP	N-CA-C	-5.56	106.49	113.72
18	X	89	LEU	N-CA-C	-5.56	98.12	108.02
7	G	188	SER	N-CA-CB	5.56	118.31	110.36
15	W	170	HIS	CA-CB-CG	5.56	119.36	113.80
20	Z	289	GLY	CA-C-N	5.56	130.33	121.66
20	Z	289	GLY	C-N-CA	5.56	130.33	121.66
20	Z	608	TYR	N-CA-CB	5.56	118.95	110.44
24	Q	9	GLU	O-C-N	5.56	127.80	122.07
26	U	243	ASP	CA-CB-CG	-5.56	107.04	112.60
1	a	70	SER	O-C-N	-5.56	116.91	123.25
2	b	170	ALA	CA-C-N	5.56	127.73	120.28
2	b	170	ALA	C-N-CA	5.56	127.73	120.28
1	A	131	ARG	CB-CA-C	-5.56	100.84	110.45
14	7	177	THR	O-C-N	5.56	130.38	123.15
20	Z	214	HIS	CG-CD2-NE2	5.56	112.76	107.20
24	Q	212	THR	N-CA-C	5.56	117.34	111.28
24	Q	334	HIS	CG-CD2-NE2	5.56	112.76	107.20
25	R	254	SER	O-C-N	5.56	127.79	122.07
26	U	228	LYS	N-CA-CB	5.56	118.38	110.16
12	l	239	ALA	CA-C-N	5.56	127.72	120.28
12	l	239	ALA	C-N-CA	5.56	127.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	72	LEU	N-CA-CB	5.56	120.34	111.56
22	S	116	ALA	N-CA-C	-5.56	106.55	113.38
33	J	179	ILE	N-CA-C	-5.56	99.83	108.44
4	d	139	ASP	CA-C-N	5.55	125.65	119.87
4	d	139	ASP	C-N-CA	5.55	125.65	119.87
14	7	39	VAL	CA-C-N	5.55	131.45	122.29
14	7	39	VAL	C-N-CA	5.55	131.45	122.29
15	W	65	PHE	N-CA-CB	5.55	118.19	109.69
26	U	232	VAL	N-CA-C	5.55	116.19	110.36
32	M	164	ASP	CA-C-N	5.55	130.00	120.72
32	M	164	ASP	C-N-CA	5.55	130.00	120.72
26	U	283	ARG	NE-CZ-NH1	5.55	127.05	121.50
7	g	102	LEU	CB-CA-C	-5.55	101.41	110.85
5	E	19	GLY	N-CA-C	-5.55	107.54	115.64
20	Z	460	SER	N-CA-C	-5.55	106.35	113.01
20	Z	532	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
33	J	231	ARG	CD-NE-CZ	-5.55	116.63	124.40
2	b	143	ASN	CA-CB-CG	-5.55	107.05	112.60
6	f	87	TYR	N-CA-C	-5.55	105.13	111.07
9	2	114	GLN	CG-CD-OE1	5.55	131.90	120.80
11	4	86	GLN	CA-C-N	5.55	128.75	120.31
11	4	86	GLN	C-N-CA	5.55	128.75	120.31
16	V	263	GLU	N-CA-C	5.55	117.33	111.28
20	Z	122	LEU	N-CA-C	-5.55	106.01	112.89
21	N	341	ALA	CB-CA-C	-5.55	101.94	110.26
27	O	392	TRP	CA-C-O	-5.55	112.57	120.51
28	H	84	ILE	CA-C-N	5.55	131.73	121.52
28	H	84	ILE	C-N-CA	5.55	131.73	121.52
1	a	72	ILE	N-CA-CB	5.55	117.33	111.00
4	d	87	GLU	N-CA-CB	5.55	118.37	110.16
12	l	137	GLN	OE1-CD-NE2	5.55	128.15	122.60
5	E	165	TYR	O-C-N	-5.55	116.70	123.30
10	3	73	LEU	N-CA-C	5.55	117.33	111.28
27	O	78	VAL	CA-C-N	5.55	129.40	120.30
27	O	78	VAL	C-N-CA	5.55	129.40	120.30
27	O	187	SER	O-C-N	5.55	128.47	122.15
29	I	404	LEU	CA-C-N	5.55	127.71	120.28
29	I	404	LEU	C-N-CA	5.55	127.71	120.28
30	K	418	ASP	N-CA-CB	5.55	121.17	112.46
31	L	132	ARG	NE-CZ-NH1	-5.55	115.95	121.50
9	2	43	ILE	O-C-N	-5.54	117.08	123.07
29	I	278	ILE	N-CA-C	-5.54	100.14	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	19	THR	CA-CB-OG1	-5.54	101.28	109.60
1	A	112	MET	CA-C-N	5.54	125.52	120.03
1	A	112	MET	C-N-CA	5.54	125.52	120.03
3	C	217	ARG	NE-CZ-NH1	-5.54	115.96	121.50
4	D	183	GLU	CB-CA-C	-5.54	104.44	110.98
11	4	9	VAL	CA-C-N	5.54	127.71	120.28
11	4	9	VAL	C-N-CA	5.54	127.71	120.28
13	6	166	ASN	N-CA-CB	5.54	121.17	112.46
14	7	105	THR	CA-C-N	5.54	127.98	120.44
14	7	105	THR	C-N-CA	5.54	127.98	120.44
17	T	230	ASN	CA-CB-CG	5.54	118.14	112.60
20	Z	507	GLY	CA-C-O	5.54	125.99	119.45
21	N	94	LYS	N-CA-C	-5.54	106.10	112.92
23	P	413	ASN	CA-C-N	5.54	127.71	120.28
23	P	413	ASN	C-N-CA	5.54	127.71	120.28
26	U	65	VAL	CB-CA-C	-5.54	102.58	110.12
33	J	193	THR	CA-C-O	5.54	125.78	119.18
9	i	170	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
13	m	189	ILE	CA-C-N	5.54	127.70	120.28
13	m	189	ILE	C-N-CA	5.54	127.70	120.28
9	2	35	VAL	O-C-N	-5.54	117.33	123.20
10	3	156	PRO	N-CA-C	5.54	120.29	111.26
11	4	104	ILE	CA-C-O	5.54	125.74	120.31
20	Z	319	THR	CA-C-N	5.54	127.71	120.28
20	Z	319	THR	C-N-CA	5.54	127.71	120.28
21	N	736	PHE	CA-C-O	-5.54	114.55	120.42
28	H	346	ARG	NE-CZ-NH2	-5.54	114.21	119.20
30	K	179	MET	O-C-N	5.54	128.00	122.12
6	f	208	VAL	O-C-N	5.54	127.34	121.91
4	D	160	SER	N-CA-CB	5.54	118.04	110.01
12	5	153	ALA	CA-C-O	-5.54	114.99	120.70
17	T	268	ILE	CA-C-N	5.54	128.26	120.28
17	T	268	ILE	C-N-CA	5.54	128.26	120.28
23	P	236	GLU	O-C-N	5.54	128.47	122.15
32	M	39	ASN	CA-C-O	-5.54	114.55	120.42
1	a	209	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
11	k	145	ASP	CA-CB-CG	-5.54	107.06	112.60
11	4	145	ASP	CA-CB-CG	-5.54	107.06	112.60
17	T	118	ASN	CA-C-N	5.54	128.73	120.31
17	T	118	ASN	C-N-CA	5.54	128.73	120.31
23	P	360	ILE	N-CA-C	-5.54	100.50	108.42
28	H	321	ASP	CA-C-O	5.54	126.42	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	157	VAL	N-CA-C	-5.54	107.58	112.90
31	L	256	ILE	O-C-N	-5.54	116.18	122.72
20	Z	809	MET	O-C-N	-5.54	116.11	122.09
24	Q	300	LYS	CA-C-O	5.54	126.18	119.31
4	d	36	VAL	CB-CA-C	-5.54	102.21	111.29
4	D	10	ILE	CA-C-O	5.54	126.23	120.36
7	G	71	ASP	CA-CB-CG	-5.54	107.06	112.60
13	6	131	TYR	N-CA-C	5.54	117.98	109.07
20	Z	752	ILE	N-CA-C	-5.54	105.13	110.72
24	Q	340	ASP	CA-C-N	5.54	128.15	120.29
24	Q	340	ASP	C-N-CA	5.54	128.15	120.29
26	U	101	ALA	N-CA-C	-5.54	106.57	113.38
27	O	320	PRO	CA-C-N	5.54	129.96	120.72
27	O	320	PRO	C-N-CA	5.54	129.96	120.72
10	j	126	LEU	N-CA-C	5.53	117.75	111.11
14	n	259	LYS	CB-CA-C	5.53	119.72	109.70
5	E	138	PHE	CA-CB-CG	-5.53	108.27	113.80
5	E	165	TYR	CB-CG-CD1	-5.53	112.50	120.80
12	5	151	VAL	CA-C-N	5.53	127.69	120.28
12	5	151	VAL	C-N-CA	5.53	127.69	120.28
12	5	231	LEU	N-CA-C	-5.53	105.33	111.36
19	Y	40	ILE	CB-CA-C	-5.53	104.77	112.02
20	Z	191	SER	CA-C-N	5.53	126.09	120.00
20	Z	191	SER	C-N-CA	5.53	126.09	120.00
25	R	208	ASN	O-C-N	5.53	127.99	122.12
29	I	213	ILE	N-CA-C	-5.53	100.65	109.17
33	J	251	ASP	CA-CB-CG	5.53	118.13	112.60
33	J	315	GLU	O-C-N	-5.53	116.74	123.27
5	e	7	GLU	CB-CA-C	-5.53	100.82	110.17
5	e	99	HIS	ND1-CE1-NE2	5.53	113.93	108.40
21	N	630	ALA	N-CA-C	5.53	116.99	111.07
24	Q	225	LEU	N-CA-CB	-5.53	101.99	110.12
31	L	340	PRO	N-CA-C	5.53	123.86	112.47
20	Z	856	HIS	O-C-N	5.53	128.98	122.34
23	P	5	ALA	O-C-N	-5.53	114.96	121.32
29	I	102	ASN	CA-C-O	-5.53	114.24	119.55
33	J	271	THR	CA-CB-CG2	5.53	119.90	110.50
5	e	63	SER	CA-C-O	5.53	126.03	119.56
20	Z	766	HIS	CA-CB-CG	-5.53	108.27	113.80
23	P	262	SER	CB-CA-C	-5.53	101.61	110.79
24	Q	231	ASP	N-CA-C	-5.53	98.34	108.02
2	b	102	GLY	CA-C-O	5.53	125.87	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	241	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
29	I	341	PRO	CB-CA-C	-5.53	102.44	111.56
10	3	189	ILE	N-CA-C	-5.53	99.79	107.80
22	S	125	LYS	CA-C-N	5.53	132.09	121.54
22	S	125	LYS	C-N-CA	5.53	132.09	121.54
27	O	121	ASP	N-CA-CB	5.53	119.30	110.46
30	K	211	LEU	N-CA-C	-5.53	99.40	108.41
4	d	12	SER	CA-C-O	-5.52	115.53	121.27
17	T	236	ASN	CB-CA-C	-5.52	101.62	110.79
20	Z	851	ALA	CA-C-N	5.52	127.62	120.44
20	Z	851	ALA	C-N-CA	5.52	127.62	120.44
24	Q	201	ALA	CB-CA-C	-5.52	101.46	110.85
26	U	76	MET	CA-C-N	5.52	128.13	120.29
26	U	76	MET	C-N-CA	5.52	128.13	120.29
30	K	406	ASP	CA-CB-CG	-5.52	107.08	112.60
5	e	108	ASN	N-CA-CB	5.52	118.84	110.45
6	f	136	GLY	CA-C-O	5.52	128.14	121.68
7	G	81	LEU	CA-C-O	5.52	126.62	120.43
8	1	66	ASP	CA-C-N	5.52	128.03	120.46
8	1	66	ASP	C-N-CA	5.52	128.03	120.46
13	6	185	VAL	N-CA-CB	5.52	118.05	110.54
32	M	31	GLN	CA-C-O	-5.52	114.57	120.42
2	b	48	GLU	CA-C-N	-5.52	114.98	122.77
2	b	48	GLU	C-N-CA	-5.52	114.98	122.77
14	n	34	THR	CA-CB-CG2	-5.52	101.11	110.50
1	A	243	GLU	CB-CG-CD	-5.52	103.22	112.60
9	2	106	VAL	CA-C-N	5.52	127.68	120.28
9	2	106	VAL	C-N-CA	5.52	127.68	120.28
21	N	900	ASN	N-CA-C	5.52	117.66	110.43
29	I	156	ILE	N-CA-CB	5.52	117.13	110.95
26	U	268	LYS	CA-C-N	5.52	128.13	120.29
26	U	268	LYS	C-N-CA	5.52	128.13	120.29
27	O	26	PHE	CB-CG-CD1	-5.52	111.32	120.70
30	K	168	ASP	N-CA-CB	5.52	119.27	110.16
30	K	275	ASP	CA-C-O	5.52	125.75	119.18
6	f	86	ASN	CA-C-N	5.52	127.61	120.44
6	f	86	ASN	C-N-CA	5.52	127.61	120.44
14	n	150	ALA	N-CA-C	-5.52	100.41	109.40
7	G	213	GLU	N-CA-C	-5.52	98.92	108.69
16	V	60	ASP	N-CA-C	-5.52	104.40	113.50
21	N	28	ILE	CA-C-N	5.52	128.23	120.28
21	N	28	ILE	C-N-CA	5.52	128.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	150	GLN	N-CA-C	-5.52	99.29	108.34
25	R	361	VAL	CA-C-N	5.52	127.94	120.44
25	R	361	VAL	C-N-CA	5.52	127.94	120.44
13	m	87	HIS	ND1-CE1-NE2	5.52	113.92	108.40
5	E	207	VAL	CA-C-O	5.52	126.16	119.54
10	3	81	ALA	N-CA-CB	5.52	118.11	110.17
26	U	237	PRO	N-CA-CB	5.52	108.22	103.31
30	K	42	ASN	N-CA-C	-5.52	105.35	111.36
13	m	105	LEU	CA-C-N	5.51	128.69	120.31
13	m	105	LEU	C-N-CA	5.51	128.69	120.31
14	7	81	ASN	OD1-CG-ND2	5.51	128.11	122.60
25	R	409	GLY	O-C-N	-5.51	116.27	122.28
30	K	98	GLN	CA-C-N	5.51	128.59	120.82
30	K	98	GLN	C-N-CA	5.51	128.59	120.82
30	K	369	ASP	CA-CB-CG	5.51	118.11	112.60
14	n	109	TYR	N-CA-CB	5.51	118.15	109.83
23	P	116	ILE	CA-C-N	5.51	127.67	120.28
23	P	116	ILE	C-N-CA	5.51	127.67	120.28
24	Q	359	ILE	N-CA-C	-5.51	105.00	110.62
27	O	53	LYS	N-CA-CB	5.51	118.74	110.53
8	h	138	SER	CA-C-O	5.51	125.88	119.32
7	G	100	LYS	N-CA-CB	5.51	118.31	110.16
20	Z	511	PRO	CA-C-N	5.51	128.17	122.27
20	Z	511	PRO	C-N-CA	5.51	128.17	122.27
20	Z	553	ARG	NH1-CZ-NH2	5.51	126.46	119.30
27	O	335	GLY	N-CA-C	-5.51	107.60	115.64
31	L	53	HIS	CG-CD2-NE2	5.51	112.71	107.20
2	b	224	TYR	N-CA-CB	5.51	120.10	111.56
14	n	87	SER	N-CA-C	-5.51	101.38	109.81
20	Z	861	THR	CA-C-O	5.51	128.39	120.51
24	Q	432	VAL	CB-CA-C	-5.51	100.97	110.94
33	J	235	VAL	N-CA-C	-5.51	105.13	110.42
1	a	207	ILE	CA-C-O	-5.51	115.33	121.17
13	m	227	LEU	CA-C-O	5.51	128.18	121.68
1	A	243	GLU	CB-CA-C	-5.51	101.65	110.79
8	1	195	LEU	N-CA-C	-5.51	100.70	109.23
22	S	321	GLN	CB-CG-CD	-5.51	103.24	112.60
30	K	213	GLY	O-C-N	-5.51	116.26	121.77
33	J	363	THR	N-CA-CB	5.51	118.22	110.12
8	h	125	GLY	N-CA-C	-5.50	105.60	113.86
8	h	158	GLU	N-CA-CB	5.50	118.31	110.16
10	j	151	GLU	CA-C-N	5.50	127.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	151	GLU	C-N-CA	5.50	127.66	120.28
14	7	95	HIS	CA-C-O	5.50	126.25	120.42
20	Z	9	GLN	N-CA-C	5.50	118.21	111.82
29	I	275	ALA	N-CA-CB	5.50	117.84	109.75
9	i	50	THR	N-CA-C	-5.50	99.44	108.41
9	2	181	ILE	CA-C-O	-5.50	114.94	121.05
17	T	238	GLN	N-CA-CB	5.50	118.31	110.16
21	N	454	ALA	N-CA-C	-5.50	106.15	112.92
25	R	153	THR	N-CA-CB	5.50	118.78	110.30
30	K	219	LYS	N-CA-C	5.50	118.04	111.71
32	M	41	ILE	CA-C-N	5.50	127.92	120.44
32	M	41	ILE	C-N-CA	5.50	127.92	120.44
33	J	170	HIS	CG-CD2-NE2	5.50	112.70	107.20
9	i	233	LYS	N-CA-C	-5.50	101.20	109.95
16	V	239	ALA	CB-CA-C	-5.50	102.24	110.88
25	R	394	ASP	N-CA-C	-5.50	106.02	114.16
27	O	80	LYS	CA-C-N	5.50	128.10	120.29
27	O	80	LYS	C-N-CA	5.50	128.10	120.29
27	O	213	LEU	CA-C-O	-5.50	114.59	120.42
5	E	136	ARG	NE-CZ-NH2	5.50	124.15	119.20
21	N	506	GLN	N-CA-C	-5.50	104.92	111.69
11	4	133	HIS	CA-C-O	5.50	127.67	121.51
14	7	76	ILE	O-C-N	5.50	125.98	120.59
20	Z	766	HIS	CB-CG-CD2	-5.50	124.05	131.20
21	N	623	PHE	CA-CB-CG	-5.50	108.30	113.80
24	Q	161	LEU	O-C-N	-5.50	115.88	122.15
31	L	223	PRO	CA-C-O	-5.50	112.59	120.56
11	4	10	GLN	N-CA-CB	5.50	118.20	110.12
14	7	146	ALA	N-CA-C	-5.50	99.94	108.90
17	T	170	ASN	CA-C-O	5.50	124.85	119.08
11	4	117	TYR	CA-CB-CG	-5.50	104.01	113.90
12	5	186	THR	CA-CB-CG2	5.50	119.84	110.50
25	R	257	GLY	O-C-N	5.50	127.57	122.13
6	f	3	ARG	NE-CZ-NH2	-5.49	114.26	119.20
13	m	69	GLY	O-C-N	5.49	128.66	122.34
14	n	41	GLY	N-CA-C	-5.49	100.94	112.04
11	4	180	ILE	N-CA-C	-5.49	100.41	108.54
20	Z	611	THR	N-CA-C	-5.49	101.31	109.83
20	Z	736	LEU	CB-CA-C	-5.49	101.67	110.79
30	K	191	PRO	N-CD-CG	5.49	111.44	103.20
2	b	68	THR	CA-C-N	5.49	126.70	119.84
2	b	68	THR	C-N-CA	5.49	126.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	406	TRP	CA-C-N	5.49	127.48	120.56
20	Z	406	TRP	C-N-CA	5.49	127.48	120.56
27	O	84	ALA	O-C-N	5.49	128.41	122.15
29	I	414	GLU	CA-C-N	5.49	127.64	120.28
29	I	414	GLU	C-N-CA	5.49	127.64	120.28
1	a	18	ILE	N-CA-C	-5.49	99.73	107.75
1	a	111	ASP	CA-C-N	5.49	135.20	121.80
1	a	111	ASP	C-N-CA	5.49	135.20	121.80
6	f	168	ALA	CA-C-N	5.49	128.19	120.28
6	f	168	ALA	C-N-CA	5.49	128.19	120.28
9	i	126	TYR	N-CA-C	-5.49	99.33	108.34
9	i	209	ILE	CA-C-O	-5.49	113.92	120.78
13	m	66	ALA	N-CA-C	-5.49	104.94	111.69
16	V	246	LYS	N-CA-C	5.49	117.34	111.36
21	N	758	VAL	N-CA-CB	-5.49	104.79	111.21
24	Q	114	GLN	CB-CA-C	-5.49	101.68	110.79
28	H	399	GLU	N-CA-CB	5.49	118.03	109.85
32	M	277	ILE	N-CA-C	-5.49	99.64	107.77
11	k	4	ILE	N-CA-C	-5.49	100.33	108.45
7	G	201	TYR	N-CA-CB	5.49	118.19	110.12
11	4	166	GLN	CA-C-N	5.49	127.63	120.28
11	4	166	GLN	C-N-CA	5.49	127.63	120.28
12	5	176	ILE	CB-CA-C	5.49	118.99	111.31
15	W	132	LEU	CA-C-O	-5.49	114.73	120.55
20	Z	338	HIS	ND1-CE1-NE2	5.49	113.89	108.40
21	N	776	TYR	CB-CA-C	-5.49	101.11	109.89
27	O	158	ASP	CA-C-N	5.49	127.64	120.28
27	O	158	ASP	C-N-CA	5.49	127.64	120.28
8	1	170	GLN	OE1-CD-NE2	5.49	128.09	122.60
13	6	132	SER	N-CA-CB	5.49	120.38	110.83
16	V	304	ALA	N-CA-CB	5.49	118.03	110.07
21	N	771	PHE	N-CA-CB	5.49	121.06	111.13
13	m	65	PHE	O-C-N	-5.49	116.20	122.89
7	G	115	ARG	NE-CZ-NH1	-5.49	116.01	121.50
22	S	26	ALA	N-CA-CB	5.49	118.18	110.12
5	e	205	LYS	N-CA-C	5.48	118.02	111.71
10	j	51	LEU	N-CA-C	-5.48	99.96	108.90
2	B	139	HIS	CG-CD2-NE2	5.48	112.68	107.20
21	N	811	LYS	N-CA-C	5.48	118.77	111.75
22	S	458	GLN	CA-C-N	5.48	127.63	120.28
22	S	458	GLN	C-N-CA	5.48	127.63	120.28
32	M	96	ASN	N-CA-CB	5.48	119.76	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	39	MET	CG-SD-CE	-5.48	88.84	100.90
6	f	28	ALA	CA-C-O	5.48	126.28	119.97
4	D	81	ASP	CB-CA-C	-5.48	101.53	110.85
14	7	126	PHE	CA-CB-CG	5.48	119.28	113.80
21	N	52	ASP	N-CA-CB	5.48	118.20	110.36
22	S	264	VAL	CB-CA-C	-5.48	103.67	111.40
27	O	215	TYR	CA-CB-CG	-5.48	104.03	113.90
29	I	188	GLU	CA-C-N	5.48	127.90	120.44
29	I	188	GLU	C-N-CA	5.48	127.90	120.44
2	b	205	ASN	N-CA-CB	5.48	119.90	111.46
9	i	143	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
13	6	218	ASP	CB-CA-C	-5.48	101.46	110.72
22	S	80	VAL	N-CA-CB	5.48	118.32	112.07
24	Q	206	ASN	N-CA-C	-5.48	106.26	113.17
20	Z	478	VAL	CA-C-N	5.48	127.62	120.28
20	Z	478	VAL	C-N-CA	5.48	127.62	120.28
20	Z	621	LEU	N-CA-CB	5.48	118.17	110.12
26	U	280	ASN	O-C-N	-5.48	116.31	122.12
7	g	135	SER	N-CA-CB	5.48	119.56	110.63
10	j	190	ILE	N-CA-C	-5.48	99.19	107.73
2	B	234	ARG	CA-C-N	5.48	128.49	120.71
2	B	234	ARG	C-N-CA	5.48	128.49	120.71
3	C	177	GLN	CG-CD-NE2	-5.48	108.18	116.40
16	V	203	TYR	O-C-N	-5.48	116.68	123.36
26	U	169	ILE	CB-CA-C	-5.48	104.75	112.14
4	D	231	GLN	OE1-CD-NE2	-5.48	117.12	122.60
6	F	42	THR	N-CA-C	5.48	120.64	113.30
13	6	164	PHE	N-CA-CB	5.48	120.40	112.13
17	T	230	ASN	N-CA-CB	5.48	120.00	111.84
21	N	243	LYS	CA-C-N	5.48	128.16	120.28
21	N	243	LYS	C-N-CA	5.48	128.16	120.28
21	N	475	ALA	CB-CA-C	-5.48	102.28	110.88
23	P	154	ASP	O-C-N	5.48	128.00	122.09
28	H	335	GLU	CA-C-O	-5.48	114.75	120.55
3	c	130	PRO	N-CA-C	-5.47	102.54	111.68
10	j	49	VAL	N-CA-C	-5.47	100.70	108.58
8	1	58	ALA	CA-C-N	5.47	128.06	120.29
8	1	58	ALA	C-N-CA	5.47	128.06	120.29
16	V	36	LYS	CA-C-N	5.47	127.62	120.28
16	V	36	LYS	C-N-CA	5.47	127.62	120.28
21	N	848	GLU	N-CA-C	-5.47	100.85	109.50
33	J	4	ALA	N-CA-C	-5.47	106.56	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	108	ASN	CA-C-O	-5.47	115.35	121.81
20	Z	535	VAL	CB-CA-C	-5.47	102.94	111.26
22	S	91	ASN	CB-CA-C	-5.47	101.70	110.79
22	S	187	ILE	O-C-N	5.47	127.25	121.89
26	U	275	VAL	O-C-N	-5.47	115.62	121.80
29	I	150	HIS	CG-CD2-NE2	5.47	112.67	107.20
33	J	21	PRO	N-CA-C	5.47	120.95	113.84
2	B	7	PHE	CA-CB-CG	-5.47	108.33	113.80
12	5	103	SER	O-C-N	5.47	129.51	123.33
20	Z	620	LEU	N-CA-CB	5.47	119.74	110.49
3	c	118	ILE	N-CA-C	-5.47	105.39	110.53
4	D	148	TYR	N-CA-C	-5.47	101.10	109.41
12	5	115	PHE	CB-CA-C	-5.47	100.93	110.17
17	T	150	ARG	O-C-N	5.47	127.92	122.12
20	Z	942	PRO	CA-C-O	-5.47	115.30	122.19
22	S	376	THR	CA-C-N	5.47	128.16	120.28
22	S	376	THR	C-N-CA	5.47	128.16	120.28
26	U	125	VAL	CA-C-N	5.47	130.82	122.23
26	U	125	VAL	C-N-CA	5.47	130.82	122.23
29	I	362	LEU	O-C-N	-5.47	115.91	122.15
33	J	81	ASP	CA-C-N	5.47	130.33	122.35
33	J	81	ASP	C-N-CA	5.47	130.33	122.35
11	4	73	TYR	N-CA-C	-5.47	99.15	110.80
18	X	130	ASN	N-CA-C	5.47	118.42	111.69
5	e	197	GLU	N-CA-CB	-5.47	102.08	110.01
12	l	265	ASN	CA-CB-CG	-5.47	107.13	112.60
1	A	17	THR	N-CA-C	-5.47	105.83	112.88
14	7	127	GLU	O-C-N	5.47	128.38	122.15
21	N	390	LEU	N-CA-C	5.47	117.35	109.48
29	I	312	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	a	247	ALA	CA-C-N	5.46	127.55	120.56
1	a	247	ALA	C-N-CA	5.46	127.55	120.56
32	M	129	LEU	N-CA-C	-5.46	101.89	110.14
6	f	207	THR	CA-CB-OG1	5.46	117.79	109.60
12	l	107	LYS	N-CA-C	-5.46	101.08	109.76
25	R	151	GLU	CA-C-N	5.46	127.54	120.44
25	R	151	GLU	C-N-CA	5.46	127.54	120.44
10	j	67	PHE	CB-CA-C	-5.46	98.47	109.55
7	G	42	CYS	CA-C-O	5.46	127.63	121.51
22	S	399	TYR	CB-CG-CD1	5.46	128.99	120.80
3	c	173	GLN	OE1-CD-NE2	5.46	128.06	122.60
14	n	98	ARG	N-CA-CB	5.46	118.24	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	396	VAL	CA-C-N	5.46	127.60	120.28
32	M	396	VAL	C-N-CA	5.46	127.60	120.28
33	J	235	VAL	CA-C-N	5.46	127.60	120.28
33	J	235	VAL	C-N-CA	5.46	127.60	120.28
2	b	188	ALA	CA-C-O	-5.46	113.69	119.97
5	e	157	HIS	CA-CB-CG	5.46	119.26	113.80
9	i	188	ILE	O-C-N	-5.46	116.21	121.83
11	k	109	LYS	O-C-N	5.46	129.57	122.42
9	2	67	SER	CA-C-N	5.46	125.07	119.56
9	2	67	SER	C-N-CA	5.46	125.07	119.56
9	2	193	TRP	CD2-CE2-CZ2	-5.46	116.94	122.40
10	3	94	SER	CB-CA-C	-5.46	102.31	110.88
15	W	107	HIS	ND1-CE1-NE2	5.46	113.86	108.40
20	Z	236	PHE	CB-CG-CD2	-5.46	111.42	120.70
21	N	588	VAL	CA-C-N	5.46	127.94	120.46
21	N	588	VAL	C-N-CA	5.46	127.94	120.46
23	P	110	LEU	CA-C-N	5.46	127.53	120.44
23	P	110	LEU	C-N-CA	5.46	127.53	120.44
25	R	388	VAL	CA-C-O	5.46	126.37	120.53
32	M	432	PHE	N-CA-C	-5.46	105.57	113.21
4	D	193	LYS	CA-C-N	5.46	128.04	120.29
4	D	193	LYS	C-N-CA	5.46	128.04	120.29
9	2	89	GLY	CA-C-N	5.46	128.14	120.28
9	2	89	GLY	C-N-CA	5.46	128.14	120.28
11	4	168	LEU	CA-C-N	5.46	128.14	120.28
11	4	168	LEU	C-N-CA	5.46	128.14	120.28
13	6	213	LEU	N-CA-CB	5.46	119.85	110.68
16	V	20	ARG	N-CA-C	-5.46	101.00	109.24
28	H	260	ALA	N-CA-C	5.46	118.15	111.82
31	L	63	LYS	CA-C-N	5.46	128.04	120.29
31	L	63	LYS	C-N-CA	5.46	128.04	120.29
32	M	381	ARG	CA-C-N	5.46	127.59	120.28
32	M	381	ARG	C-N-CA	5.46	127.59	120.28
5	e	209	GLU	CB-CA-C	-5.46	102.24	111.02
21	N	494	LYS	CA-C-N	5.46	124.97	119.19
21	N	494	LYS	C-N-CA	5.46	124.97	119.19
24	Q	62	GLY	CA-C-N	5.46	128.60	120.31
24	Q	62	GLY	C-N-CA	5.46	128.60	120.31
1	a	157	THR	O-C-N	5.45	129.79	123.30
3	c	96	GLN	N-CA-C	-5.45	106.63	113.28
10	3	149	MET	O-C-N	5.45	128.37	122.15
17	T	122	PHE	CA-CB-CG	5.45	119.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	240	PHE	CA-C-N	5.45	127.59	120.28
24	Q	240	PHE	C-N-CA	5.45	127.59	120.28
1	a	91	ARG	N-CA-CB	5.45	118.14	110.12
14	7	68	ARG	CA-C-O	5.45	126.29	120.24
33	J	41	VAL	CA-CB-CG2	-5.45	101.13	110.40
22	S	207	ASN	CA-C-O	5.45	126.20	120.42
28	H	167	ASP	CA-C-O	5.45	125.73	119.35
10	3	188	TYR	CB-CA-C	-5.45	101.11	110.16
15	W	13	SER	CA-C-N	5.45	131.54	122.66
15	W	13	SER	C-N-CA	5.45	131.54	122.66
20	Z	260	GLU	N-CA-CB	5.45	118.32	110.20
27	O	249	ASP	CA-C-N	5.45	128.03	120.29
27	O	249	ASP	C-N-CA	5.45	128.03	120.29
33	J	398	ILE	CA-C-N	5.45	131.22	122.83
33	J	398	ILE	C-N-CA	5.45	131.22	122.83
8	h	124	LEU	CB-CA-C	5.45	119.43	110.88
25	R	252	TYR	CA-C-N	5.45	128.03	120.29
25	R	252	TYR	C-N-CA	5.45	128.03	120.29
2	b	39	ALA	N-CA-C	-5.45	101.45	109.18
6	f	120	THR	N-CA-C	-5.45	104.76	111.40
5	E	55	THR	CA-C-O	5.45	125.87	119.06
13	6	90	LYS	N-CA-C	-5.45	100.83	109.76
19	Y	23	GLU	CA-C-N	5.45	128.15	120.42
19	Y	23	GLU	C-N-CA	5.45	128.15	120.42
21	N	564	ASN	N-CA-C	-5.45	101.40	110.17
21	N	713	VAL	CB-CA-C	-5.45	104.29	111.70
30	K	50	LYS	CB-CA-C	-5.45	102.30	110.90
1	a	237	SER	CA-C-N	5.44	127.57	120.28
1	a	237	SER	C-N-CA	5.44	127.57	120.28
5	e	210	GLU	N-CA-C	-5.44	101.02	109.24
13	m	84	HIS	CA-CB-CG	-5.44	108.36	113.80
1	A	181	ASN	CA-C-O	5.44	126.31	120.70
25	R	144	ILE	CA-CB-CG2	-5.44	101.25	110.50
28	H	271	PHE	CA-CB-CG	5.44	119.24	113.80
1	a	87	ILE	N-CA-CB	5.44	113.93	110.50
6	f	78	ALA	CA-C-N	5.44	124.90	119.24
6	f	78	ALA	C-N-CA	5.44	124.90	119.24
9	i	72	CYS	N-CA-C	-5.44	100.85	108.96
20	Z	952	SER	CA-C-O	-5.44	114.89	120.99
23	P	410	GLN	O-C-N	-5.44	116.35	122.12
24	Q	65	TYR	CA-C-O	5.44	126.53	120.82
24	Q	183	LYS	CA-C-N	5.44	127.53	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	183	LYS	C-N-CA	5.44	127.53	120.56
28	H	63	ILE	CA-C-N	5.44	128.58	120.31
28	H	63	ILE	C-N-CA	5.44	128.58	120.31
13	m	109	ARG	CA-C-O	5.44	126.28	119.59
8	1	25	ALA	N-CA-C	5.44	116.54	108.60
10	3	70	LYS	CA-C-O	-5.44	114.65	120.42
10	3	189	ILE	CA-C-N	-5.44	116.01	123.14
10	3	189	ILE	C-N-CA	-5.44	116.01	123.14
20	Z	396	ASN	CB-CA-C	-5.44	99.59	109.38
30	K	413	THR	N-CA-C	-5.44	100.80	109.23
32	M	25	LEU	CA-C-N	5.44	130.06	120.87
32	M	25	LEU	C-N-CA	5.44	130.06	120.87
7	g	173	LYS	CA-C-N	5.44	128.01	120.29
7	g	173	LYS	C-N-CA	5.44	128.01	120.29
12	l	253	TYR	N-CA-C	-5.44	99.81	109.06
22	S	44	THR	N-CA-CB	5.44	119.68	110.49
24	Q	110	SER	CA-C-O	5.44	127.17	121.19
30	K	366	ALA	N-CA-C	-5.44	100.84	109.76
12	l	100	TRP	CE2-CD2-CE3	5.44	124.24	118.80
20	Z	49	LEU	CA-C-N	5.44	128.01	120.29
20	Z	49	LEU	C-N-CA	5.44	128.01	120.29
20	Z	61	SER	CA-C-O	-5.44	114.66	120.42
20	Z	376	SER	N-CA-CB	5.44	119.68	110.49
21	N	305	ASN	N-CA-C	-5.44	105.00	111.69
23	P	38	GLN	OE1-CD-NE2	5.44	128.04	122.60
24	Q	386	PHE	CA-C-N	5.44	131.93	121.54
24	Q	386	PHE	C-N-CA	5.44	131.93	121.54
28	H	341	ASP	CA-CB-CG	-5.44	107.16	112.60
30	K	47	ILE	N-CA-C	5.44	115.64	110.42
2	b	116	LYS	O-C-N	5.44	127.88	122.12
3	c	111	LEU	CA-C-N	5.44	128.14	120.42
3	c	111	LEU	C-N-CA	5.44	128.14	120.42
3	c	175	LEU	CA-C-O	-5.44	114.79	120.55
9	i	127	LEU	O-C-N	-5.43	116.75	123.33
2	B	179	TRP	CE2-CD2-CE3	5.43	124.23	118.80
3	C	135	PHE	CA-CB-CG	-5.43	108.37	113.80
9	2	190	ALA	CA-C-O	5.43	126.18	120.42
24	Q	373	VAL	CA-CB-CG2	-5.43	101.16	110.40
25	R	388	VAL	N-CA-CB	5.43	118.31	111.46
28	H	353	PHE	CB-CG-CD2	5.43	129.94	120.70
31	L	240	GLY	CA-C-N	5.43	128.43	120.71
31	L	240	GLY	C-N-CA	5.43	128.43	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	379	LEU	CA-C-N	5.43	128.01	120.29
32	M	379	LEU	C-N-CA	5.43	128.01	120.29
4	d	169	LYS	N-CA-C	5.43	117.63	111.11
1	A	123	ASN	CB-CG-ND2	5.43	124.55	116.40
2	B	187	ASP	O-C-N	-5.43	116.47	122.07
8	1	92	LYS	CA-C-O	-5.43	114.79	120.55
13	6	202	ARG	CD-NE-CZ	-5.43	116.80	124.40
20	Z	15	GLN	CB-CG-CD	5.43	121.84	112.60
22	S	454	SER	N-CA-CB	5.43	117.88	110.38
22	S	491	GLU	O-C-N	-5.43	117.39	123.48
25	R	156	LYS	CG-CD-CE	5.43	123.79	111.30
27	O	244	ASN	CA-CB-CG	-5.43	107.17	112.60
28	H	242	PRO	N-CA-C	5.43	117.33	110.70
29	I	329	ASN	N-CA-C	-5.43	105.27	111.14
31	L	369	LYS	O-C-N	-5.43	116.83	123.19
23	P	102	GLU	CA-C-N	5.43	127.50	120.44
23	P	102	GLU	C-N-CA	5.43	127.50	120.44
31	L	317	ASN	CA-CB-CG	-5.43	107.17	112.60
21	N	808	ALA	CA-C-N	5.43	127.56	120.28
21	N	808	ALA	C-N-CA	5.43	127.56	120.28
20	Z	133	ASP	CA-C-O	-5.43	114.80	120.55
23	P	183	GLN	O-C-N	-5.43	115.87	122.22
23	P	439	MET	CB-CA-C	-5.43	101.62	110.85
24	Q	54	GLN	N-CA-C	5.43	117.20	111.28
1	a	117	LEU	N-CA-CB	5.43	118.28	110.20
10	j	168	SER	CB-CA-C	-5.43	102.33	110.90
1	A	251	GLN	OE1-CD-NE2	5.43	128.03	122.60
5	E	131	GLU	CA-C-N	5.43	129.84	122.19
5	E	131	GLU	C-N-CA	5.43	129.84	122.19
17	T	7	LEU	CA-C-N	5.43	131.50	122.54
17	T	7	LEU	C-N-CA	5.43	131.50	122.54
22	S	400	LYS	CA-C-O	-5.43	113.38	120.00
24	Q	340	ASP	N-CA-CB	5.43	118.10	110.12
27	O	106	PHE	CB-CG-CD1	5.43	129.92	120.70
1	a	146	VAL	N-CA-C	-5.42	99.93	107.80
8	h	24	GLY	N-CA-C	-5.42	100.32	113.18
14	n	143	LEU	CA-C-O	-5.42	114.36	120.43
1	A	36	ASN	OD1-CG-ND2	5.42	128.03	122.60
13	6	197	THR	CB-CA-C	-5.42	101.79	110.79
24	Q	188	LEU	N-CA-C	-5.42	106.62	113.18
7	g	87	HIS	ND1-CE1-NE2	5.42	113.82	108.40
12	l	159	SER	N-CA-C	5.42	117.27	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	38	LEU	N-CA-CB	5.42	120.68	111.57
10	3	145	GLN	O-C-N	5.42	127.66	122.07
25	R	246	TYR	CA-C-N	5.42	127.99	120.29
25	R	246	TYR	C-N-CA	5.42	127.99	120.29
25	R	250	ALA	CA-C-N	5.42	127.55	120.28
25	R	250	ALA	C-N-CA	5.42	127.55	120.28
3	c	218	LYS	N-CA-C	-5.42	106.58	114.12
8	h	126	GLY	O-C-N	5.42	128.29	122.60
12	l	147	GLU	CA-C-N	5.42	128.46	120.82
12	l	147	GLU	C-N-CA	5.42	128.46	120.82
14	n	233	ILE	N-CA-C	-5.42	99.94	107.80
6	F	14	SER	CA-C-N	5.42	125.76	119.47
6	F	14	SER	C-N-CA	5.42	125.76	119.47
6	F	107	ARG	CA-C-N	5.42	127.54	120.28
6	F	107	ARG	C-N-CA	5.42	127.54	120.28
20	Z	926	ASN	CB-CA-C	-5.42	109.34	115.79
16	V	266	LEU	N-CA-CB	5.42	118.09	110.12
20	Z	553	ARG	CB-CA-C	-5.42	100.26	110.67
21	N	815	LYS	CA-CB-CG	5.42	124.94	114.10
4	d	75	PHE	N-CA-C	5.42	117.03	108.96
8	h	80	GLY	CA-C-O	-5.42	115.72	122.65
3	C	164	SER	N-CA-C	-5.42	100.19	109.24
13	6	177	LYS	N-CA-C	5.42	117.68	110.53
16	V	299	GLY	N-CA-C	-5.42	105.73	113.86
21	N	11	ALA	CA-C-O	-5.42	114.81	120.55
21	N	715	ILE	N-CA-C	-5.42	100.08	107.99
28	H	242	PRO	CA-C-N	5.42	125.34	119.76
28	H	242	PRO	C-N-CA	5.42	125.34	119.76
1	a	204	GLU	CA-C-O	-5.42	114.81	120.55
2	b	148	TYR	CB-CA-C	-5.42	98.80	110.45
4	d	204	GLN	N-CA-CB	5.42	119.64	110.49
9	i	85	THR	CA-C-O	-5.42	113.98	120.10
13	m	118	ILE	N-CA-C	-5.42	100.32	108.12
20	Z	538	CYS	N-CA-CB	5.42	117.98	109.69
25	R	399	GLN	O-C-N	5.42	127.65	122.07
25	R	417	TYR	CA-C-N	5.42	125.95	119.94
25	R	417	TYR	C-N-CA	5.42	125.95	119.94
31	L	431	THR	CB-CA-C	5.42	119.06	109.75
5	e	86	ARG	CA-C-N	5.42	127.54	120.28
5	e	86	ARG	C-N-CA	5.42	127.54	120.28
8	h	133	TYR	O-C-N	-5.42	117.42	123.48
14	n	114	ALA	N-CA-C	-5.42	104.94	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ASP	N-CA-C	-5.42	100.87	109.59
3	C	232	PRO	O-C-N	5.42	129.21	122.22
27	O	106	PHE	CA-CB-CG	-5.42	108.39	113.80
11	k	107	TYR	N-CA-C	-5.41	99.70	108.52
13	m	204	ILE	CA-CB-CG2	-5.41	101.30	110.50
3	C	175	LEU	N-CA-C	5.41	117.18	111.28
10	3	105	VAL	CA-C-N	5.41	130.37	121.87
10	3	105	VAL	C-N-CA	5.41	130.37	121.87
11	4	61	GLN	CA-C-N	5.41	127.48	120.44
11	4	61	GLN	C-N-CA	5.41	127.48	120.44
21	N	393	SER	CA-C-O	5.41	124.76	119.08
21	N	602	VAL	CA-C-N	5.41	125.49	119.32
21	N	602	VAL	C-N-CA	5.41	125.49	119.32
24	Q	416	VAL	CA-CB-CG2	-5.41	101.20	110.40
28	H	101	ARG	O-C-N	-5.41	117.08	123.41
28	H	292	ARG	O-C-N	5.41	127.86	122.12
30	K	163	GLU	CB-CA-C	5.41	119.42	109.46
25	R	362	ALA	N-CA-C	-5.41	105.30	111.14
4	d	234	THR	O-C-N	5.41	127.86	122.12
12	l	124	ALA	CB-CA-C	-5.41	102.35	110.90
2	B	85	LEU	CA-C-N	5.41	127.87	120.46
2	B	85	LEU	C-N-CA	5.41	127.87	120.46
2	B	126	GLY	CA-C-O	-5.41	113.20	119.10
20	Z	336	SER	N-CA-CB	5.41	118.17	110.16
21	N	394	ARG	NE-CZ-NH1	-5.41	116.09	121.50
22	S	364	ILE	N-CA-C	-5.41	105.66	113.07
27	O	278	PRO	CA-C-N	5.41	128.10	120.42
27	O	278	PRO	C-N-CA	5.41	128.10	120.42
32	M	195	GLU	O-C-N	5.41	127.86	122.12
10	3	84	PRO	CA-C-N	5.41	127.97	120.29
10	3	84	PRO	C-N-CA	5.41	127.97	120.29
11	4	8	ARG	CD-NE-CZ	-5.41	116.83	124.40
20	Z	562	TRP	CE2-CD2-CE3	5.41	124.21	118.80
23	P	208	PHE	N-CA-C	-5.41	106.36	113.17
25	R	43	ARG	NE-CZ-NH2	-5.41	114.33	119.20
28	H	62	ARG	NE-CZ-NH1	5.41	126.91	121.50
30	K	141	ARG	CA-C-O	-5.41	115.13	120.70
31	L	177	GLU	N-CA-CB	5.41	119.63	110.49
32	M	378	GLU	N-CA-CB	5.41	118.67	110.28
16	V	126	GLN	N-CA-CB	5.41	118.07	110.12
25	R	389	GLU	N-CA-C	-5.41	102.46	110.46
32	M	222	GLY	CA-C-N	5.41	123.61	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	222	GLY	C-N-CA	5.41	123.61	119.66
13	m	110	PHE	N-CA-C	-5.41	104.65	113.19
22	S	366	LYS	CB-CA-C	-5.41	101.66	110.85
1	A	34	ALA	N-CA-C	-5.40	106.36	113.17
4	d	108	TYR	CA-C-O	-5.40	114.69	120.42
9	i	99	THR	N-CA-C	-5.40	106.19	112.89
10	j	152	SER	CB-CA-C	-5.40	101.82	110.79
11	k	100	VAL	N-CA-C	-5.40	99.73	107.78
7	G	9	ASP	N-CA-CB	5.40	119.62	110.49
7	G	200	ILE	CA-C-N	5.40	127.52	120.28
7	G	200	ILE	C-N-CA	5.40	127.52	120.28
15	W	17	ARG	CA-C-N	5.40	129.15	121.42
15	W	17	ARG	C-N-CA	5.40	129.15	121.42
28	H	182	ASN	CA-CB-CG	-5.40	107.20	112.60
28	H	285	GLY	O-C-N	5.40	128.73	122.30
30	K	267	SER	N-CA-C	-5.40	100.10	108.42
4	d	233	VAL	O-C-N	5.40	127.11	121.87
7	g	127	ASN	N-CA-C	-5.40	106.65	113.18
11	k	8	ARG	N-CA-C	-5.40	99.72	108.52
12	5	139	ARG	CA-C-O	-5.40	114.83	120.55
12	5	262	TYR	CA-C-N	5.40	130.97	122.49
12	5	262	TYR	C-N-CA	5.40	130.97	122.49
28	H	120	ASN	CA-C-N	5.40	130.86	122.49
28	H	120	ASN	C-N-CA	5.40	130.86	122.49
29	I	386	ASP	O-C-N	-5.40	116.25	122.95
30	K	366	ALA	CB-CA-C	-5.40	100.41	109.48
10	j	41	GLU	N-CA-CB	5.40	117.91	109.97
19	Y	87	GLU	N-CA-CB	5.40	118.53	110.22
21	N	96	GLN	N-CA-C	-5.40	105.47	111.36
14	7	200	LYS	CA-C-O	5.40	126.02	119.11
23	P	210	ASN	CA-CB-CG	-5.40	107.20	112.60
25	R	109	LYS	CB-CA-C	-5.40	102.37	110.90
26	U	75	ASN	CB-CG-ND2	5.40	124.50	116.40
31	L	206	ILE	O-C-N	-5.40	115.70	121.80
33	J	221	LYS	CG-CD-CE	5.40	123.71	111.30
20	Z	357	ILE	N-CA-C	5.40	117.83	111.09
6	f	178	THR	N-CA-C	-5.39	105.30	111.07
13	m	205	GLN	N-CA-C	-5.39	106.62	114.12
17	T	123	HIS	ND1-CE1-NE2	5.39	113.80	108.40
18	X	75	TRP	CH2-CZ2-CE2	5.39	124.51	117.50
23	P	143	LEU	N-CA-C	-5.39	106.54	113.23
23	P	364	ARG	CA-C-N	5.39	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	364	ARG	C-N-CA	5.39	127.51	120.28
29	I	233	ALA	N-CA-C	-5.39	105.48	111.36
29	I	303	GLN	O-C-N	-5.39	116.40	122.12
30	K	107	THR	N-CA-C	-5.39	99.89	109.06
21	N	329	HIS	CA-C-N	5.39	127.50	120.28
21	N	329	HIS	C-N-CA	5.39	127.50	120.28
25	R	305	PHE	CA-C-O	-5.39	112.77	120.16
29	I	60	LEU	CA-C-N	5.39	127.77	120.44
29	I	60	LEU	C-N-CA	5.39	127.77	120.44
30	K	296	LEU	N-CA-C	5.39	117.58	111.11
32	M	47	GLU	O-C-N	5.39	127.92	122.09
33	J	215	GLY	CA-C-N	5.39	128.89	120.75
33	J	215	GLY	C-N-CA	5.39	128.89	120.75
3	C	76	ALA	N-CA-C	-5.39	101.38	109.95
26	U	27	THR	CA-CB-OG1	5.39	117.69	109.60
26	U	128	GLN	OE1-CD-NE2	5.39	127.99	122.60
9	i	145	HIS	CG-CD2-NE2	5.39	112.59	107.20
13	m	46	ARG	NE-CZ-NH2	-5.39	114.35	119.20
6	F	91	GLN	CB-CG-CD	5.39	121.76	112.60
9	2	249	ILE	N-CA-C	-5.39	107.47	112.43
11	4	155	GLU	CA-C-N	5.39	127.50	120.28
11	4	155	GLU	C-N-CA	5.39	127.50	120.28
14	7	91	SER	CB-CA-C	-5.39	101.84	110.79
20	Z	775	MET	CA-C-O	5.39	127.05	120.31
24	Q	102	GLU	N-CA-CB	5.39	118.04	110.12
26	U	289	ASP	CB-CA-C	-5.39	101.84	110.79
30	K	169	VAL	CA-C-N	5.39	127.77	120.44
30	K	169	VAL	C-N-CA	5.39	127.77	120.44
30	K	400	TYR	CB-CG-CD2	5.39	128.88	120.80
7	G	228	HIS	ND1-CE1-NE2	5.39	113.79	108.40
20	Z	881	ILE	O-C-N	5.39	127.19	121.91
2	B	190	HIS	CA-CB-CG	5.39	119.19	113.80
2	B	237	LYS	CB-CA-C	5.39	118.64	109.75
8	1	187	LEU	N-CA-C	5.39	117.45	108.02
15	W	37	PHE	CB-CA-C	-5.39	102.42	110.88
16	V	195	HIS	N-CA-CB	5.39	119.59	110.49
20	Z	284	LEU	CA-C-N	5.39	128.04	120.28
20	Z	284	LEU	C-N-CA	5.39	128.04	120.28
21	N	70	TYR	N-CA-CB	5.39	118.13	110.16
28	H	439	THR	N-CA-C	-5.39	103.58	110.53
3	c	224	GLU	N-CA-C	-5.38	100.34	108.52
10	j	165	GLU	CB-CG-CD	-5.38	103.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	VAL	CB-CA-C	-5.38	104.87	112.14
1	A	212	ASP	N-CA-CB	5.38	117.82	110.01
17	T	58	THR	O-C-N	-5.38	115.23	122.23
24	Q	209	TYR	CA-C-O	5.38	126.30	119.95
28	H	437	VAL	CA-CB-CG2	5.38	119.56	110.40
32	M	290	ARG	NE-CZ-NH2	5.38	124.05	119.20
32	M	418	GLY	O-C-N	5.38	127.36	122.19
23	P	259	PRO	N-CA-C	-5.38	106.70	114.18
12	5	191	ASP	CA-CB-CG	5.38	117.98	112.60
20	Z	537	THR	N-CA-C	-5.38	100.94	108.96
31	L	187	THR	CA-C-O	-5.38	115.17	120.82
11	4	109	LYS	N-CA-C	-5.38	106.88	113.50
15	W	127	ARG	N-CA-C	-5.38	105.58	111.82
20	Z	47	THR	CA-CB-CG2	-5.38	101.35	110.50
5	e	45	GLY	N-CA-C	-5.38	103.04	111.00
13	m	99	ARG	CA-C-N	5.38	127.43	120.44
13	m	99	ARG	C-N-CA	5.38	127.43	120.44
5	E	30	ALA	CA-C-N	5.38	128.06	120.42
5	E	30	ALA	C-N-CA	5.38	128.06	120.42
10	3	168	SER	CA-C-N	5.38	127.93	120.29
10	3	168	SER	C-N-CA	5.38	127.93	120.29
18	X	74	MET	CG-SD-CE	-5.38	89.07	100.90
20	Z	433	LEU	CA-C-N	5.38	127.93	120.29
20	Z	433	LEU	C-N-CA	5.38	127.93	120.29
21	N	616	HIS	ND1-CE1-NE2	5.38	113.78	108.40
28	H	327	ASN	CA-C-N	5.38	129.82	120.68
28	H	327	ASN	C-N-CA	5.38	129.82	120.68
1	a	15	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
4	d	8	LEU	N-CA-C	-5.38	106.49	113.16
1	A	211	ILE	CA-C-O	-5.38	115.36	120.95
16	V	119	SER	N-CA-CB	5.38	117.75	110.38
20	Z	596	THR	CA-C-O	5.38	126.15	119.97
24	Q	226	HIS	CA-C-N	5.38	127.49	120.28
24	Q	226	HIS	C-N-CA	5.38	127.49	120.28
26	U	202	SER	N-CA-CB	5.38	118.12	110.16
29	I	64	ARG	CB-CA-C	-5.38	102.44	110.88
31	L	179	THR	CA-CB-OG1	5.38	117.66	109.60
32	M	289	LYS	N-CA-C	-5.38	104.84	111.40
15	W	63	SER	O-C-N	-5.38	117.12	123.25
5	E	136	ARG	CA-C-N	5.37	126.56	119.84
5	E	136	ARG	C-N-CA	5.37	126.56	119.84
10	3	18	LYS	CA-C-N	5.37	130.48	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	18	LYS	C-N-CA	5.37	130.48	122.74
14	7	77	PRO	O-C-N	5.37	129.55	123.10
15	W	113	PHE	O-C-N	5.37	129.35	123.01
15	W	122	ARG	CB-CA-C	-5.37	102.44	110.88
20	Z	733	VAL	CA-C-N	5.37	127.92	120.29
20	Z	733	VAL	C-N-CA	5.37	127.92	120.29
30	K	338	ILE	O-C-N	-5.37	117.59	123.18
7	g	61	PRO	O-C-N	5.37	129.83	123.06
13	m	80	VAL	N-CA-CB	5.37	117.84	110.54
15	W	6	THR	CA-C-O	-5.37	114.56	120.36
16	V	93	ASP	N-CA-C	5.37	117.14	111.28
20	Z	214	HIS	CA-C-O	5.37	126.11	120.42
21	N	621	THR	N-CA-C	-5.37	105.34	111.14
23	P	407	ASN	OD1-CG-ND2	-5.37	117.23	122.60
25	R	264	THR	O-C-N	-5.37	116.54	122.07
32	M	58	MET	CG-SD-CE	-5.37	89.08	100.90
5	E	121	LEU	CA-C-N	5.37	129.80	121.26
5	E	121	LEU	C-N-CA	5.37	129.80	121.26
20	Z	631	GLY	CA-C-O	5.37	126.58	121.05
21	N	293	LEU	CA-C-N	5.37	124.88	119.19
21	N	293	LEU	C-N-CA	5.37	124.88	119.19
21	N	696	LYS	CA-C-N	5.37	127.42	120.44
21	N	696	LYS	C-N-CA	5.37	127.42	120.44
23	P	41	VAL	CA-C-N	5.37	128.47	120.31
23	P	41	VAL	C-N-CA	5.37	128.47	120.31
24	Q	229	ASP	N-CA-C	-5.37	106.23	112.89
25	R	197	MET	O-C-N	5.37	128.96	122.35
26	U	10	ILE	CA-C-O	-5.37	114.85	120.27
13	m	150	ALA	N-CA-C	-5.37	106.50	112.57
22	S	306	SER	N-CA-CB	5.37	119.05	110.73
31	L	50	GLN	CG-CD-NE2	-5.37	108.35	116.40
33	J	218	LEU	CA-C-N	5.37	128.04	120.42
33	J	218	LEU	C-N-CA	5.37	128.04	120.42
8	h	148	ASP	O-C-N	5.37	127.81	122.12
2	B	29	LYS	CG-CD-CE	5.37	123.64	111.30
8	1	119	VAL	N-CA-CB	5.37	120.27	111.58
11	4	94	SER	CA-C-N	5.37	127.78	120.54
11	4	94	SER	C-N-CA	5.37	127.78	120.54
12	5	89	VAL	CA-C-O	5.37	126.84	120.72
18	X	45	PHE	CA-CB-CG	-5.37	108.43	113.80
9	i	149	ASP	CA-C-N	-5.37	115.81	123.11
9	i	149	ASP	C-N-CA	-5.37	115.81	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	30	THR	CA-CB-OG1	5.37	117.65	109.60
15	W	38	GLN	CA-C-N	5.37	127.74	120.44
15	W	38	GLN	C-N-CA	5.37	127.74	120.44
21	N	45	ASP	CA-CB-CG	5.37	117.97	112.60
21	N	411	ILE	O-C-N	-5.37	116.32	121.90
22	S	391	GLY	CA-C-O	-5.37	114.40	120.30
32	M	291	PHE	CA-CB-CG	-5.37	108.43	113.80
4	d	210	ILE	N-CA-C	-5.36	100.66	108.17
8	h	155	MET	CA-C-N	5.36	129.93	120.87
8	h	155	MET	C-N-CA	5.36	129.93	120.87
13	m	188	VAL	CA-C-N	5.36	127.41	120.70
13	m	188	VAL	C-N-CA	5.36	127.41	120.70
6	F	223	THR	N-CA-C	-5.36	99.94	109.06
32	M	390	GLN	OE1-CD-NE2	5.36	127.96	122.60
13	m	43	ILE	CB-CA-C	5.36	118.38	110.77
17	T	19	ASP	CA-C-O	5.36	126.20	120.46
31	L	69	ARG	CB-CA-C	-5.36	102.43	110.90
12	l	130	TRP	CE2-CD2-CE3	5.36	124.16	118.80
13	m	189	ILE	N-CA-C	-5.36	105.10	110.30
8	1	98	ASN	CA-C-N	5.36	127.90	120.29
8	1	98	ASN	C-N-CA	5.36	127.90	120.29
21	N	626	GLY	CA-C-O	-5.36	115.53	121.05
21	N	843	LYS	CA-C-N	5.36	127.73	120.44
21	N	843	LYS	C-N-CA	5.36	127.73	120.44
21	N	879	SER	CB-CA-C	-5.36	100.38	110.67
27	O	19	ASP	O-C-N	5.36	127.28	121.60
33	J	124	LYS	CA-C-O	-5.36	115.72	121.45
8	h	67	ILE	N-CA-C	-5.36	105.49	110.53
11	k	13	VAL	N-CA-C	-5.36	100.61	108.11
20	Z	806	GLU	O-C-N	-5.36	115.46	122.59
5	e	164	PHE	N-CA-C	5.36	118.21	110.28
9	i	67	SER	N-CA-CB	5.36	118.16	111.35
20	Z	208	VAL	CA-C-O	-5.36	115.10	118.69
26	U	91	GLY	N-CA-C	-5.36	103.43	110.29
28	H	164	SER	N-CA-C	-5.36	100.19	108.55
20	Z	64	TYR	N-CA-C	-5.36	106.68	113.43
21	N	610	SER	O-C-N	5.36	128.25	122.15
24	Q	111	LEU	O-C-N	5.36	127.66	122.09
27	O	111	SER	N-CA-CB	5.36	118.06	110.13
4	d	24	LEU	CA-C-N	5.35	127.99	120.28
4	d	24	LEU	C-N-CA	5.35	127.99	120.28
13	m	125	ASP	CA-CB-CG	-5.35	107.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	172	SER	N-CA-C	-5.35	101.20	108.11
27	O	240	GLU	N-CA-C	5.35	116.80	111.07
5	E	243	LEU	CA-C-N	5.35	127.45	120.28
5	E	243	LEU	C-N-CA	5.35	127.45	120.28
23	P	166	GLU	CB-CG-CD	-5.35	103.50	112.60
23	P	347	GLU	CA-C-N	5.35	127.72	120.44
23	P	347	GLU	C-N-CA	5.35	127.72	120.44
27	O	144	VAL	O-C-N	5.35	127.34	121.83
27	O	319	LEU	CA-C-N	5.35	126.11	120.11
27	O	319	LEU	C-N-CA	5.35	126.11	120.11
33	J	265	ASP	CA-C-N	5.35	127.99	120.28
33	J	265	ASP	C-N-CA	5.35	127.99	120.28
13	m	87	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
16	V	119	SER	CA-C-O	5.35	128.09	121.99
21	N	572	LEU	CA-C-N	5.35	127.72	120.44
21	N	572	LEU	C-N-CA	5.35	127.72	120.44
23	P	204	LEU	CA-C-N	5.35	127.89	120.29
23	P	204	LEU	C-N-CA	5.35	127.89	120.29
25	R	33	LEU	CA-C-N	5.35	127.76	120.54
25	R	33	LEU	C-N-CA	5.35	127.76	120.54
26	U	5	HIS	ND1-CE1-NE2	5.35	113.75	108.40
28	H	244	LYS	CA-C-N	5.35	127.55	122.36
28	H	244	LYS	C-N-CA	5.35	127.55	122.36
5	e	73	HIS	CB-CG-ND1	5.35	130.72	122.70
6	f	43	HIS	CG-CD2-NE2	5.35	112.55	107.20
9	i	57	ASP	CA-CB-CG	-5.35	107.25	112.60
11	k	141	PHE	CA-C-N	5.35	129.65	120.71
11	k	141	PHE	C-N-CA	5.35	129.65	120.71
12	l	134	LEU	CA-C-O	5.35	126.22	120.55
12	5	254	HIS	CB-CG-CD2	-5.35	124.25	131.20
20	Z	197	LYS	O-C-N	5.35	127.58	122.07
23	P	303	PHE	CB-CG-CD2	-5.35	111.61	120.70
12	l	244	ALA	N-CA-C	-5.35	106.13	113.30
17	T	87	PRO	N-CA-C	-5.35	106.75	114.18
21	N	18	ASP	CA-C-N	5.35	127.45	120.28
21	N	18	ASP	C-N-CA	5.35	127.45	120.28
26	U	173	HIS	N-CA-CB	5.35	118.08	110.16
4	d	170	THR	CA-C-N	5.35	129.07	120.30
4	d	170	THR	C-N-CA	5.35	129.07	120.30
11	k	118	GLN	N-CA-C	-5.35	99.70	108.41
11	4	76	SER	CA-C-O	-5.35	115.13	120.96
20	Z	145	ASP	N-CA-C	-5.35	98.55	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	26	ALA	O-C-N	5.35	127.79	122.12
31	L	393	ASN	CA-C-O	5.35	126.22	120.55
5	E	12	VAL	CA-C-N	5.34	129.94	121.18
5	E	12	VAL	C-N-CA	5.34	129.94	121.18
12	5	228	ALA	CA-C-O	-5.34	114.75	120.42
14	7	259	LYS	O-C-N	5.34	129.02	122.34
18	X	79	LYS	N-CA-CB	5.34	119.56	111.06
20	Z	781	GLY	CA-C-O	5.34	126.26	120.75
28	H	454	TYR	O-C-N	5.34	128.24	122.15
2	B	141	GLU	CB-CG-CD	-5.34	103.52	112.60
5	E	234	GLU	CA-C-N	5.34	127.39	120.44
5	E	234	GLU	C-N-CA	5.34	127.39	120.44
17	T	38	ASN	O-C-N	5.34	128.47	122.22
17	T	158	GLN	CA-C-O	5.34	126.62	120.90
22	S	61	SER	CB-CA-C	-5.34	101.60	110.68
25	R	246	TYR	CG-CD1-CE1	-5.34	113.19	121.20
3	c	129	ARG	N-CA-C	5.34	121.61	109.81
7	g	173	LYS	N-CA-C	-5.34	105.54	111.36
8	h	109	ALA	N-CA-CB	5.34	120.12	110.83
14	7	172	SER	O-C-N	-5.34	117.66	121.83
17	T	90	PHE	N-CA-CB	5.34	118.36	110.56
22	S	65	ASN	CA-C-N	5.34	127.88	120.29
22	S	65	ASN	C-N-CA	5.34	127.88	120.29
23	P	48	GLN	CA-C-N	5.34	127.44	120.28
23	P	48	GLN	C-N-CA	5.34	127.44	120.28
29	I	434	GLY	CA-C-N	5.34	127.70	120.44
29	I	434	GLY	C-N-CA	5.34	127.70	120.44
33	J	144	ASP	O-C-N	5.34	129.88	122.78
8	h	202	TYR	N-CA-C	5.34	117.18	111.36
5	E	13	SER	N-CA-C	-5.34	104.75	113.19
11	4	52	ASP	O-C-N	5.34	128.24	122.15
13	6	43	ILE	CA-C-N	5.34	127.70	120.44
13	6	43	ILE	C-N-CA	5.34	127.70	120.44
20	Z	338	HIS	CG-CD2-NE2	5.34	112.54	107.20
23	P	137	ALA	CA-C-N	5.34	129.71	120.58
23	P	137	ALA	C-N-CA	5.34	129.71	120.58
23	P	384	VAL	CB-CA-C	-5.34	105.21	111.94
24	Q	379	GLN	O-C-N	5.34	127.78	122.12
27	O	236	HIS	ND1-CE1-NE2	5.34	113.74	108.40
27	O	347	LEU	N-CA-CB	5.34	119.85	111.20
30	K	211	LEU	CA-C-O	-5.34	114.59	120.30
6	f	68	GLU	CB-CA-C	-5.34	102.13	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ALA	CB-CA-C	-5.34	101.78	110.85
2	B	60	THR	CA-C-N	5.34	128.29	120.71
2	B	60	THR	C-N-CA	5.34	128.29	120.71
21	N	920	VAL	CA-C-O	5.34	126.04	119.58
25	R	157	SER	CA-C-N	5.34	127.87	120.29
25	R	157	SER	C-N-CA	5.34	127.87	120.29
26	U	30	ASN	N-CA-CB	5.34	119.51	110.49
27	O	93	ASP	N-CA-C	-5.34	105.54	111.36
33	J	11	VAL	N-CA-C	5.34	120.44	109.34
1	A	73	PHE	CA-CB-CG	-5.34	108.46	113.80
8	1	170	GLN	N-CA-CB	5.34	117.96	110.12
13	6	84	HIS	O-C-N	5.34	127.57	122.07
15	W	77	HIS	ND1-CE1-NE2	5.34	113.74	108.40
19	Y	23	GLU	CB-CG-CD	-5.34	103.53	112.60
20	Z	56	LEU	N-CA-C	-5.34	101.53	109.11
21	N	768	ILE	CA-C-O	-5.34	112.80	119.95
27	O	392	TRP	N-CA-CB	5.34	119.51	110.49
29	I	209	GLU	CA-C-O	-5.34	114.76	120.42
5	e	55	THR	N-CA-C	-5.33	106.53	114.64
9	2	247	VAL	CB-CA-C	5.33	118.53	110.63
32	M	145	LEU	N-CA-CB	5.33	118.87	110.23
13	m	140	GLU	CA-C-N	5.33	129.45	121.72
13	m	140	GLU	C-N-CA	5.33	129.45	121.72
7	G	147	HIS	N-CA-C	-5.33	99.63	108.75
12	5	256	THR	CA-CB-OG1	5.33	117.60	109.60
16	V	128	SER	CA-C-N	5.33	128.42	120.31
16	V	128	SER	C-N-CA	5.33	128.42	120.31
21	N	616	HIS	CA-CB-CG	-5.33	108.47	113.80
21	N	924	LYS	N-CA-C	5.33	119.94	113.38
24	Q	114	GLN	N-CA-CB	5.33	117.96	110.12
24	Q	267	LEU	CA-C-O	-5.33	115.20	121.07
27	O	174	THR	N-CA-C	-5.33	105.47	111.28
28	H	112	SER	CB-CA-C	5.33	121.03	110.42
10	j	194	GLU	N-CA-CB	5.33	118.11	110.06
17	T	258	ASN	CA-CB-CG	5.33	117.93	112.60
20	Z	165	TYR	CB-CG-CD1	-5.33	112.80	120.80
20	Z	442	VAL	CA-C-N	5.33	131.72	121.54
20	Z	442	VAL	C-N-CA	5.33	131.72	121.54
21	N	210	SER	CB-CA-C	-5.33	101.94	110.79
22	S	349	THR	CA-C-O	-5.33	115.22	120.82
28	H	395	SER	O-C-N	-5.33	115.71	122.27
30	K	408	GLU	CB-CG-CD	-5.33	103.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	61	LYS	CA-C-N	5.33	127.42	120.28
31	L	61	LYS	C-N-CA	5.33	127.42	120.28
31	L	62	ARG	N-CA-CB	5.33	117.96	110.12
21	N	743	PHE	CA-C-O	-5.33	112.86	120.16
10	j	126	LEU	O-C-N	5.33	127.63	122.09
14	7	34	THR	CA-C-N	5.33	128.33	120.82
14	7	34	THR	C-N-CA	5.33	128.33	120.82
14	7	128	TYR	CB-CG-CD2	-5.33	112.81	120.80
22	S	20	HIS	N-CA-C	-5.33	105.55	111.36
27	O	267	ASP	CA-C-O	-5.33	114.90	120.55
20	Z	453	LEU	CA-C-O	-5.33	114.90	120.55
23	P	58	VAL	CA-C-N	5.33	127.95	120.28
23	P	58	VAL	C-N-CA	5.33	127.95	120.28
3	c	194	LEU	CA-C-N	5.33	127.42	120.28
3	c	194	LEU	C-N-CA	5.33	127.42	120.28
9	2	51	GLN	N-CA-C	-5.33	98.54	108.02
9	2	197	GLY	N-CA-C	-5.33	108.34	115.32
17	T	101	LYS	CA-C-N	5.33	127.68	120.38
17	T	101	LYS	C-N-CA	5.33	127.68	120.38
20	Z	259	PRO	O-C-N	5.33	129.09	122.22
20	Z	494	GLY	CA-C-N	5.33	127.38	120.56
20	Z	494	GLY	C-N-CA	5.33	127.38	120.56
20	Z	593	HIS	N-CA-CB	5.33	118.17	110.77
21	N	326	SER	CA-C-N	5.33	127.68	120.44
21	N	326	SER	C-N-CA	5.33	127.68	120.44
21	N	614	ASN	CA-CB-CG	-5.33	107.27	112.60
21	N	737	SER	N-CA-C	5.33	118.00	111.82
24	Q	52	ASN	CA-C-N	5.33	127.95	120.28
24	Q	52	ASN	C-N-CA	5.33	127.95	120.28
9	2	105	VAL	N-CA-CB	5.32	120.40	110.77
13	6	39	THR	N-CA-C	-5.32	99.42	108.26
20	Z	786	SER	O-C-N	5.32	128.22	122.15
21	N	230	VAL	O-C-N	-5.32	116.35	121.83
32	M	216	LYS	N-CA-CB	5.32	117.73	110.01
32	M	283	LEU	O-C-N	-5.32	115.80	122.35
2	B	130	PHE	N-CA-CB	5.32	117.83	110.17
20	Z	849	ARG	N-CA-C	-5.32	100.64	108.99
1	A	84	ASN	N-CA-C	-5.32	100.73	109.40
3	C	59	GLN	N-CA-C	-5.32	105.76	113.21
7	G	21	ASN	CB-CA-C	5.32	118.96	109.65
7	G	182	HIS	CA-CB-CG	-5.32	108.48	113.80
22	S	147	TRP	CE2-CD2-CE3	5.32	124.12	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	242	ILE	CB-CA-C	5.32	118.01	111.25
28	H	295	PHE	CA-C-N	5.32	127.41	120.28
28	H	295	PHE	C-N-CA	5.32	127.41	120.28
29	I	365	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
31	L	62	ARG	O-C-N	-5.32	116.48	122.12
5	e	24	VAL	CA-C-N	5.32	127.36	120.44
5	e	24	VAL	C-N-CA	5.32	127.36	120.44
7	G	183	HIS	CG-CD2-NE2	5.32	112.52	107.20
15	W	34	GLU	N-CA-C	-5.32	105.48	111.28
20	Z	959	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
21	N	602	VAL	CB-CA-C	-5.32	108.71	114.35
23	P	30	ASN	N-CA-CB	5.32	117.78	110.07
26	U	34	VAL	N-CA-C	-5.32	100.66	108.11
26	U	138	VAL	CA-C-O	5.32	125.92	120.39
31	L	376	PHE	N-CA-C	5.32	119.03	112.54
1	a	113	PRO	CA-N-CD	-5.32	104.56	112.00
10	j	50	PHE	CA-C-O	5.32	126.35	120.71
1	A	21	PRO	CA-C-N	5.32	131.95	121.58
1	A	21	PRO	C-N-CA	5.32	131.95	121.58
7	G	244	GLN	CA-C-N	5.32	127.72	120.54
7	G	244	GLN	C-N-CA	5.32	127.72	120.54
18	X	87	PHE	N-CA-C	-5.32	99.74	108.41
23	P	368	LEU	CB-CG-CD2	5.32	126.65	110.70
25	R	335	ARG	CD-NE-CZ	-5.32	116.95	124.40
2	b	35	LEU	N-CA-CB	5.32	119.80	111.56
14	n	36	GLN	O-C-N	-5.32	117.40	121.55
19	Y	10	ALA	N-CA-CB	5.32	118.03	110.16
20	Z	108	ASP	CA-C-O	-5.32	112.88	120.16
20	Z	900	LEU	N-CA-C	-5.32	101.21	109.72
33	J	14	THR	CA-CB-OG1	5.32	117.57	109.60
33	J	76	ILE	CB-CG1-CD1	5.32	124.96	113.80
33	J	162	GLU	CB-CA-C	-5.32	102.50	110.90
7	G	52	LYS	N-CA-C	-5.31	98.72	108.02
31	L	57	LEU	CB-CA-C	-5.31	101.97	110.79
11	4	5	LEU	N-CA-C	-5.31	101.00	109.23
14	7	218	TYR	CA-C-N	5.31	127.35	120.44
14	7	218	TYR	C-N-CA	5.31	127.35	120.44
21	N	323	GLY	O-C-N	5.31	129.61	122.70
25	R	245	SER	CA-C-N	5.31	127.40	120.28
25	R	245	SER	C-N-CA	5.31	127.40	120.28
27	O	253	GLN	CG-CD-NE2	-5.31	108.43	116.40
28	H	399	GLU	CA-C-O	5.31	126.92	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	138	PHE	N-CA-C	-5.31	101.81	110.20
22	S	26	ALA	CA-C-N	5.31	128.13	120.38
22	S	26	ALA	C-N-CA	5.31	128.13	120.38
22	S	204	ASP	CA-C-N	5.31	127.83	120.29
22	S	204	ASP	C-N-CA	5.31	127.83	120.29
22	S	205	ASN	CB-CG-ND2	-5.31	108.43	116.40
26	U	135	ASP	O-C-N	-5.31	116.79	123.27
27	O	239	MET	N-CA-C	-5.31	107.17	113.97
29	I	421	GLU	CA-C-N	5.31	127.34	120.44
29	I	421	GLU	C-N-CA	5.31	127.34	120.44
10	j	150	CYS	CA-C-N	5.31	127.83	120.29
10	j	150	CYS	C-N-CA	5.31	127.83	120.29
4	D	222	VAL	O-C-N	5.31	129.05	123.00
9	2	81	THR	CA-C-O	-5.31	114.79	120.42
23	P	421	GLU	CA-C-N	5.31	127.83	120.29
23	P	421	GLU	C-N-CA	5.31	127.83	120.29
27	O	60	ARG	CD-NE-CZ	-5.31	116.97	124.40
30	K	78	GLU	N-CA-CB	5.31	119.06	110.40
31	L	85	GLU	O-C-N	-5.31	116.10	122.15
31	L	418	ALA	O-C-N	5.31	127.75	122.12
33	J	240	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	A	190	LYS	N-CA-C	-5.31	105.60	113.40
6	F	173	GLU	N-CA-C	-5.31	105.39	111.07
6	F	187	ASP	CB-CA-C	-5.31	101.98	110.79
9	2	189	GLN	CA-C-O	5.31	126.17	120.55
11	4	27	VAL	N-CA-C	-5.31	99.03	107.15
12	5	188	TYR	CA-C-N	5.31	128.38	120.95
12	5	188	TYR	C-N-CA	5.31	128.38	120.95
12	5	238	ALA	CA-C-N	5.31	127.83	120.29
12	5	238	ALA	C-N-CA	5.31	127.83	120.29
20	Z	593	HIS	ND1-CE1-NE2	5.31	113.71	108.40
21	N	503	THR	CA-CB-OG1	5.31	117.56	109.60
23	P	28	ALA	O-C-N	-5.31	116.49	122.12
23	P	57	GLU	CA-C-N	5.31	127.73	120.46
23	P	57	GLU	C-N-CA	5.31	127.73	120.46
27	O	219	ILE	CB-CA-C	5.31	119.54	112.22
29	I	196	GLU	CB-CA-C	-5.31	101.83	110.85
14	7	164	ASN	N-CA-CB	5.31	119.62	111.24
21	N	600	THR	N-CA-C	5.31	118.92	112.23
1	a	149	GLU	N-CA-CB	5.30	118.20	110.88
7	g	194	LYS	CA-C-O	-5.30	114.80	120.42
1	A	63	LEU	N-CA-C	-5.30	106.81	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	882	LEU	CA-C-N	5.30	129.58	120.72
20	Z	882	LEU	C-N-CA	5.30	129.58	120.72
23	P	115	ARG	NE-CZ-NH2	5.30	123.97	119.20
28	H	309	ASP	CA-C-O	-5.30	115.12	121.11
33	J	80	SER	CA-C-O	5.30	126.21	119.95
5	e	159	GLU	N-CA-C	-5.30	102.31	110.32
11	k	130	TYR	N-CA-CB	5.30	119.72	110.65
14	n	35	GLN	CG-CD-OE1	-5.30	110.19	120.80
32	M	139	LYS	CB-CA-C	-5.30	102.90	111.28
32	M	425	ARG	NE-CZ-NH2	-5.30	114.43	119.20
33	J	257	ARG	O-C-N	-5.30	115.98	122.34
2	b	107	THR	CA-C-N	5.30	127.70	120.54
2	b	107	THR	C-N-CA	5.30	127.70	120.54
4	d	231	GLN	CA-C-N	5.30	127.38	120.28
4	d	231	GLN	C-N-CA	5.30	127.38	120.28
6	f	143	HIS	O-C-N	5.30	129.42	123.27
7	g	232	LYS	N-CA-C	-5.30	100.86	108.60
11	k	146	HIS	CB-CG-CD2	-5.30	124.31	131.20
13	m	46	ARG	CD-NE-CZ	-5.30	116.98	124.40
1	A	124	LEU	N-CA-C	-5.30	105.50	111.28
2	B	75	TYR	CB-CG-CD1	5.30	128.75	120.80
6	F	105	VAL	CA-C-N	5.30	127.82	120.29
6	F	105	VAL	C-N-CA	5.30	127.82	120.29
8	1	129	HIS	CA-C-N	5.30	128.37	120.95
8	1	129	HIS	C-N-CA	5.30	128.37	120.95
10	3	145	GLN	CG-CD-NE2	-5.30	108.45	116.40
20	Z	116	ALA	N-CA-CB	5.30	117.92	110.12
21	N	613	HIS	N-CA-C	-5.30	106.79	113.20
13	m	115	VAL	CA-C-O	5.30	126.57	120.90
11	4	159	ASP	O-C-N	-5.30	116.50	122.12
24	Q	340	ASP	CB-CA-C	-5.30	101.99	110.79
27	O	112	LYS	N-CA-C	5.30	117.86	111.40
31	L	313	ASP	CA-CB-CG	5.30	117.90	112.60
33	J	361	VAL	N-CA-CB	5.30	118.53	110.58
5	e	31	ILE	CA-C-N	5.30	128.36	120.31
5	e	31	ILE	C-N-CA	5.30	128.36	120.31
2	B	4	ARG	N-CA-C	-5.30	104.76	113.50
15	W	74	ALA	CA-C-N	5.30	127.02	120.34
15	W	74	ALA	C-N-CA	5.30	127.02	120.34
21	N	162	ARG	NE-CZ-NH2	-5.30	114.43	119.20
32	M	16	ASP	CA-CB-CG	-5.30	107.30	112.60
12	5	194	GLY	N-CA-C	-5.30	107.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	83	ASN	CA-C-N	5.30	127.64	120.44
17	T	83	ASN	C-N-CA	5.30	127.64	120.44
17	T	161	TRP	CD2-CE2-CZ2	-5.30	117.10	122.40
20	Z	49	LEU	CA-C-O	5.30	126.38	120.82
20	Z	769	ASN	O-C-N	-5.30	116.34	122.86
21	N	174	LEU	CA-C-N	5.30	131.66	121.54
21	N	174	LEU	C-N-CA	5.30	131.66	121.54
22	S	382	ARG	NE-CZ-NH2	-5.30	114.43	119.20
24	Q	252	HIS	CG-CD2-NE2	5.30	112.50	107.20
30	K	395	VAL	CA-C-O	-5.30	115.44	120.95
33	J	260	GLY	CA-C-O	-5.30	115.36	122.24
2	B	204	PHE	N-CA-C	-5.29	100.10	108.73
9	2	39	ASN	CA-CB-CG	-5.29	107.31	112.60
27	O	159	LYS	CA-C-N	5.29	128.99	121.42
27	O	159	LYS	C-N-CA	5.29	128.99	121.42
28	H	228	PRO	N-CA-C	-5.29	107.12	114.27
1	a	124	LEU	CA-C-N	5.29	127.37	120.28
1	a	124	LEU	C-N-CA	5.29	127.37	120.28
6	F	32	GLY	N-CA-C	5.29	118.15	112.33
20	Z	867	PHE	CA-C-N	5.29	127.81	120.29
20	Z	867	PHE	C-N-CA	5.29	127.81	120.29
27	O	313	ILE	CA-C-N	5.29	127.37	120.28
27	O	313	ILE	C-N-CA	5.29	127.37	120.28
28	H	73	ASP	CA-C-O	5.29	123.44	119.68
28	H	461	SER	N-CA-CB	5.29	119.44	110.49
31	L	134	SER	CA-C-O	-5.29	113.02	119.43
31	L	215	PRO	N-CA-C	-5.29	102.27	111.32
32	M	177	THR	N-CA-CB	5.29	117.69	109.48
3	c	217	ARG	N-CA-C	5.29	118.06	109.06
13	m	165	LYS	CA-C-O	-5.29	115.18	121.16
14	n	184	ALA	O-C-N	5.29	129.87	122.36
1	A	233	PHE	N-CA-C	-5.29	100.68	108.99
7	G	192	ALA	CA-C-N	5.29	127.33	120.56
7	G	192	ALA	C-N-CA	5.29	127.33	120.56
24	Q	322	GLU	CA-C-N	5.29	127.37	120.28
24	Q	322	GLU	C-N-CA	5.29	127.37	120.28
28	H	404	TRP	CE2-CD2-CE3	5.29	124.09	118.80
28	H	413	ASN	CA-CB-CG	-5.29	107.31	112.60
28	H	452	SER	N-CA-C	-5.29	105.62	111.71
29	I	90	GLU	CA-C-N	5.29	127.32	120.44
29	I	90	GLU	C-N-CA	5.29	127.32	120.44
1	a	33	LYS	N-CA-C	-5.29	105.14	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	73	HIS	CG-CD2-NE2	5.29	112.49	107.20
6	F	152	ASN	CA-CB-CG	5.29	117.89	112.60
11	4	40	PRO	CA-C-N	5.29	128.32	120.17
11	4	40	PRO	C-N-CA	5.29	128.32	120.17
11	4	106	GLY	O-C-N	-5.29	118.94	123.23
13	6	95	ASN	N-CA-C	5.29	117.96	111.82
27	O	100	ASP	O-C-N	-5.29	116.12	122.15
31	L	54	ASN	CB-CA-C	-5.29	102.58	110.88
5	e	60	GLU	CB-CG-CD	-5.29	103.61	112.60
11	k	55	GLN	CA-C-N	5.29	127.80	120.29
11	k	55	GLN	C-N-CA	5.29	127.80	120.29
14	n	37	PRO	N-CA-CB	5.29	108.25	103.33
12	5	266	HIS	CA-CB-CG	-5.29	108.51	113.80
20	Z	445	PRO	O-C-N	5.29	129.78	122.64
23	P	12	ASP	O-C-N	5.29	127.73	122.12
23	P	86	HIS	ND1-CE1-NE2	5.29	113.69	108.40
32	M	244	LEU	N-CA-C	-5.29	101.35	109.76
32	M	412	HIS	CA-CB-CG	5.29	119.09	113.80
1	a	48	LYS	N-CA-C	-5.29	105.97	112.90
14	n	136	ARG	CA-C-N	5.29	128.34	120.31
14	n	136	ARG	C-N-CA	5.29	128.34	120.31
11	4	138	PHE	CA-CB-CG	5.29	119.08	113.80
21	N	590	ALA	N-CA-C	5.29	118.83	112.38
24	Q	166	LYS	N-CA-C	-5.29	106.67	113.23
29	I	158	GLY	CA-C-N	5.29	130.29	122.94
29	I	158	GLY	C-N-CA	5.29	130.29	122.94
31	L	290	ARG	CG-CD-NE	-5.29	100.37	112.00
3	c	136	ILE	N-CA-C	-5.28	100.28	107.99
5	e	200	VAL	CB-CA-C	-5.28	105.01	112.14
8	1	95	CYS	CA-C-O	-5.28	114.13	120.10
16	V	93	ASP	CB-CA-C	-5.28	102.02	110.79
22	S	274	PHE	CA-C-N	5.28	127.31	120.44
22	S	274	PHE	C-N-CA	5.28	127.31	120.44
22	S	346	TYR	CB-CG-CD2	-5.28	112.88	120.80
28	H	306	ILE	N-CA-CB	-5.28	105.24	111.90
30	K	351	LEU	O-C-N	-5.28	116.52	122.12
2	b	245	ASP	CA-C-N	5.28	128.34	120.31
2	b	245	ASP	C-N-CA	5.28	128.34	120.31
4	D	26	ALA	CA-C-O	-5.28	114.95	120.55
18	X	8	ILE	N-CA-CB	5.28	118.51	111.64
10	j	173	ASN	O-C-N	-5.28	114.86	122.36
2	b	8	SER	N-CA-C	-5.28	101.27	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	186	GLU	CA-C-N	5.28	127.30	120.44
13	m	186	GLU	C-N-CA	5.28	127.30	120.44
3	C	67	TYR	CA-C-N	5.28	129.38	121.72
3	C	67	TYR	C-N-CA	5.28	129.38	121.72
8	1	20	GLY	O-C-N	-5.28	117.66	124.15
32	M	35	LYS	N-CA-C	-5.28	105.70	111.82
10	j	15	MET	O-C-N	-5.28	117.03	123.10
7	G	109	ILE	N-CA-CB	5.28	113.83	110.50
20	Z	241	THR	N-CA-CB	5.28	117.88	110.12
20	Z	317	GLN	OE1-CD-NE2	5.28	127.88	122.60
27	O	263	PHE	CA-C-N	5.28	127.62	120.44
27	O	263	PHE	C-N-CA	5.28	127.62	120.44
30	K	334	LEU	N-CA-CB	5.28	119.41	110.49
31	L	425	VAL	CG1-CB-CG2	5.28	122.41	110.80
33	J	261	SER	N-CA-CB	5.28	119.47	110.50
33	J	278	GLN	CA-C-O	-5.28	113.56	119.79
1	A	191	ILE	N-CA-C	-5.28	100.25	108.95
4	D	32	CYS	CA-C-N	5.28	130.99	122.29
4	D	32	CYS	C-N-CA	5.28	130.99	122.29
8	1	48	ASP	CA-CB-CG	-5.28	107.33	112.60
17	T	75	PHE	O-C-N	5.28	127.50	122.07
21	N	276	GLU	O-C-N	5.28	127.71	122.12
22	S	470	GLN	CA-C-O	5.28	126.01	120.42
23	P	257	TRP	CD2-CE2-CZ2	-5.28	117.12	122.40
24	Q	208	ILE	N-CA-C	-5.28	107.61	112.83
31	L	219	LEU	O-C-N	5.28	129.39	123.27
4	d	104	VAL	CA-C-N	5.27	128.26	120.82
4	d	104	VAL	C-N-CA	5.27	128.26	120.82
13	m	112	PRO	CA-C-O	-5.27	115.15	121.48
7	G	99	PHE	CA-C-N	5.27	127.78	120.29
7	G	99	PHE	C-N-CA	5.27	127.78	120.29
11	4	83	PHE	CB-CA-C	5.27	119.16	110.88
12	5	212	TYR	N-CA-C	-5.27	105.53	111.28
21	N	832	HIS	N-CA-CB	5.27	119.40	110.49
4	d	68	ASP	N-CA-C	-5.27	101.39	108.19
6	F	208	VAL	CB-CA-C	-5.27	105.13	111.88
24	Q	54	GLN	CB-CG-CD	-5.27	103.64	112.60
25	R	322	LEU	CA-C-N	5.27	127.35	120.28
25	R	322	LEU	C-N-CA	5.27	127.35	120.28
27	O	369	ARG	NE-CZ-NH1	-5.27	116.23	121.50
33	J	390	MET	CA-C-N	5.27	127.34	120.28
33	J	390	MET	C-N-CA	5.27	127.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	65	LYS	N-CA-CB	5.27	122.09	111.60
29	I	332	GLU	N-CA-C	-5.27	106.53	113.17
30	K	392	LEU	CB-CA-C	5.27	119.81	110.85
1	a	41	ASN	CB-CG-ND2	5.27	124.31	116.40
10	j	135	ASP	CA-CB-CG	-5.27	107.33	112.60
3	C	93	ILE	CA-C-N	5.27	127.77	120.29
3	C	93	ILE	C-N-CA	5.27	127.77	120.29
6	F	81	ALA	O-C-N	5.27	128.16	122.15
7	G	33	ASN	N-CA-CB	5.27	118.41	110.30
16	V	251	TYR	CB-CG-CD1	5.27	128.70	120.80
18	X	19	GLU	N-CA-C	-5.27	106.08	112.88
25	R	231	LEU	CA-C-N	5.27	129.03	121.55
25	R	231	LEU	C-N-CA	5.27	129.03	121.55
26	U	90	ILE	CB-CA-C	5.27	115.92	110.70
27	O	285	SER	CA-C-N	5.27	127.77	120.29
27	O	285	SER	C-N-CA	5.27	127.77	120.29
29	I	373	GLU	CB-CG-CD	-5.27	103.64	112.60
30	K	215	PRO	N-CA-C	5.27	123.33	112.47
33	J	60	ASP	CA-C-N	5.27	127.61	120.44
33	J	60	ASP	C-N-CA	5.27	127.61	120.44
14	7	148	ILE	N-CA-C	-5.27	99.97	107.77
20	Z	534	PHE	CA-CB-CG	-5.27	108.53	113.80
23	P	172	GLU	N-CA-C	-5.27	102.95	110.59
24	Q	428	GLU	O-C-N	5.27	128.15	122.15
26	U	32	ARG	NE-CZ-NH1	-5.27	116.23	121.50
26	U	238	ASN	N-CA-CB	5.27	118.84	110.57
30	K	378	LEU	CA-C-O	-5.27	114.60	120.66
11	k	2	ASP	N-CA-CB	5.27	119.39	110.49
12	l	284	ASN	CB-CA-C	-5.27	100.92	109.13
21	N	662	MET	N-CA-CB	5.27	118.05	110.20
22	S	367	TYR	CA-CB-CG	-5.27	104.42	113.90
32	M	115	LYS	CA-CB-CG	-5.27	103.57	114.10
1	a	104	PHE	N-CA-C	5.26	116.70	111.07
24	Q	221	MET	CA-C-N	5.26	127.28	120.44
24	Q	221	MET	C-N-CA	5.26	127.28	120.44
24	Q	222	SER	CA-C-N	5.26	125.94	119.99
24	Q	222	SER	C-N-CA	5.26	125.94	119.99
25	R	70	TYR	O-C-N	-5.26	116.61	122.09
28	H	460	THR	O-C-N	5.26	128.98	123.03
32	M	417	GLU	CA-C-N	5.26	125.82	119.98
32	M	417	GLU	C-N-CA	5.26	125.82	119.98
33	J	306	ARG	CA-C-O	-5.26	112.95	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	179	GLU	CB-CA-C	-5.26	102.05	110.79
12	5	138	CYS	CB-CA-C	-5.26	102.62	110.88
26	U	86	LYS	N-CA-C	-5.26	105.52	112.94
28	H	432	ARG	O-C-N	5.26	127.70	122.12
33	J	142	VAL	CA-CB-CG1	-5.26	101.45	110.40
1	a	98	LYS	CA-C-O	-5.26	114.84	120.42
12	l	125	ALA	O-C-N	5.26	127.77	122.09
6	F	148	GLN	OE1-CD-NE2	5.26	127.86	122.60
20	Z	486	SER	CA-C-N	5.26	127.33	120.28
20	Z	486	SER	C-N-CA	5.26	127.33	120.28
3	c	234	GLU	CA-C-O	5.26	126.00	119.79
4	d	147	LEU	O-C-N	-5.26	116.97	123.44
5	e	116	VAL	CA-C-O	-5.26	115.28	120.85
13	m	50	LYS	CA-C-O	-5.26	113.28	119.48
4	D	216	LYS	N-CA-C	-5.26	99.70	109.06
7	G	32	GLU	CA-C-N	5.26	129.62	120.68
7	G	32	GLU	C-N-CA	5.26	129.62	120.68
7	G	103	TYR	CA-CB-CG	-5.26	104.43	113.90
14	7	142	PRO	O-C-N	5.26	129.56	123.14
20	Z	356	ASP	N-CA-C	5.26	117.01	111.28
21	N	394	ARG	NE-CZ-NH2	5.26	123.93	119.20
23	P	316	LYS	O-C-N	-5.26	116.65	122.07
28	H	307	PHE	CA-C-N	-5.26	115.78	122.77
28	H	307	PHE	C-N-CA	-5.26	115.78	122.77
29	I	53	THR	CA-CB-OG1	5.26	117.49	109.60
31	L	77	ARG	CA-C-N	5.26	128.31	120.31
31	L	77	ARG	C-N-CA	5.26	128.31	120.31
32	M	69	ILE	CB-CA-C	-5.26	104.96	112.22
33	J	219	VAL	CB-CA-C	5.26	119.48	112.22
6	f	171	TYR	CA-C-N	5.26	127.76	120.29
6	f	171	TYR	C-N-CA	5.26	127.76	120.29
20	Z	541	ASP	N-CA-C	-5.26	104.18	111.28
2	b	58	SER	N-CA-C	-5.26	106.10	112.88
10	j	199	TYR	CB-CG-CD2	5.26	128.69	120.80
11	k	7	ILE	CB-CA-C	5.26	119.80	110.71
2	B	117	ILE	CA-C-O	-5.26	115.48	120.95
2	B	135	LEU	N-CA-C	-5.26	100.83	109.40
12	5	120	MET	CA-C-N	5.26	130.73	122.21
12	5	120	MET	C-N-CA	5.26	130.73	122.21
17	T	207	ALA	CB-CA-C	-5.26	102.06	110.79
20	Z	398	LYS	CA-C-O	-5.26	115.28	120.90
21	N	794	LYS	CA-CB-CG	-5.26	103.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	210	LEU	O-C-N	-5.26	116.55	122.12
23	P	87	GLY	CA-C-N	5.26	129.60	122.19
23	P	87	GLY	C-N-CA	5.26	129.60	122.19
25	R	170	VAL	CA-C-O	5.26	126.42	120.95
28	H	302	LYS	N-CA-CB	5.26	120.51	111.00
30	K	165	GLU	N-CA-C	-5.26	102.70	110.48
31	L	62	ARG	NE-CZ-NH2	5.26	123.93	119.20
6	f	40	SER	N-CA-C	-5.25	101.45	108.86
24	Q	13	ARG	N-CA-CB	5.25	117.84	110.12
25	R	132	GLN	N-CA-C	5.25	117.92	111.82
25	R	235	LEU	N-CA-C	-5.25	104.48	112.04
28	H	93	GLU	CA-C-O	-5.25	115.70	121.58
4	d	245	GLU	N-CA-CB	5.25	117.93	110.16
1	A	126	GLN	O-C-N	5.25	127.69	122.12
4	D	213	THR	CA-CB-CG2	5.25	119.43	110.50
12	5	143	LEU	N-CA-C	5.25	117.08	111.36
12	5	278	GLU	N-CA-C	5.25	117.08	111.36
20	Z	732	ILE	N-CA-C	-5.25	105.26	110.62
25	R	169	ASP	CA-CB-CG	5.25	117.85	112.60
21	N	788	TYR	N-CA-C	-5.25	105.54	112.94
26	U	269	THR	CA-C-N	5.25	127.75	120.29
26	U	269	THR	C-N-CA	5.25	127.75	120.29
1	a	64	LEU	N-CA-CB	5.25	119.63	110.81
1	a	203	VAL	CA-CB-CG1	5.25	119.32	110.40
4	d	139	ASP	N-CA-C	-5.25	99.72	109.06
9	i	249	ILE	CA-C-N	5.25	130.39	122.99
9	i	249	ILE	C-N-CA	5.25	130.39	122.99
11	k	57	ALA	CA-C-N	5.25	127.74	120.29
11	k	57	ALA	C-N-CA	5.25	127.74	120.29
23	P	158	ASP	N-CA-CB	5.25	117.62	110.01
24	Q	231	ASP	CB-CA-C	-5.25	102.29	110.74
25	R	21	VAL	N-CA-C	5.25	120.22	112.61
27	O	312	ASP	CA-C-N	5.25	127.87	120.42
27	O	312	ASP	C-N-CA	5.25	127.87	120.42
29	I	93	LYS	O-C-N	5.25	127.68	122.12
29	I	320	GLY	N-CA-C	-5.25	100.74	113.18
30	K	360	MET	N-CA-CB	5.25	118.84	110.65
12	l	134	LEU	CA-C-N	5.25	126.70	120.14
12	l	134	LEU	C-N-CA	5.25	126.70	120.14
20	Z	779	ALA	N-CA-CB	5.25	117.83	110.12
22	S	265	SER	N-CA-CB	5.25	120.12	111.62
23	P	144	VAL	O-C-N	5.25	127.23	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	95	LYS	CB-CA-C	-5.25	102.61	110.90
30	K	293	GLN	CG-CD-NE2	-5.25	108.53	116.40
31	L	108	VAL	O-C-N	-5.25	116.76	122.64
14	n	200	LYS	CB-CA-C	-5.25	101.86	110.72
5	E	143	LEU	N-CA-C	-5.25	100.62	108.96
23	P	47	ARG	N-CA-CB	5.25	119.35	110.49
30	K	83	GLN	CB-CA-C	-5.25	101.93	110.85
11	k	143	LEU	N-CA-CB	5.24	117.83	110.12
2	B	87	ASP	N-CA-CB	5.24	117.92	110.16
7	G	228	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
14	7	214	MET	CA-C-O	5.24	126.11	120.55
20	Z	151	HIS	CB-CA-C	-5.24	99.82	109.15
21	N	116	GLN	N-CA-CB	5.24	118.62	110.44
21	N	236	GLY	CA-C-N	5.24	127.73	120.29
21	N	236	GLY	C-N-CA	5.24	127.73	120.29
3	C	105	ASP	CA-C-N	5.24	129.82	120.70
3	C	105	ASP	C-N-CA	5.24	129.82	120.70
5	E	188	HIS	CB-CG-ND1	5.24	130.56	122.70
14	7	218	TYR	N-CA-C	-5.24	105.48	111.14
16	V	279	HIS	ND1-CE1-NE2	5.24	113.64	108.40
33	J	312	ARG	NE-CZ-NH2	5.24	123.92	119.20
10	j	31	SER	N-CA-C	-5.24	98.85	108.02
12	5	121	ALA	N-CA-C	-5.24	101.33	109.24
13	6	218	ASP	CA-CB-CG	-5.24	107.36	112.60
30	K	90	GLN	N-CA-C	5.24	117.74	111.71
30	K	140	HIS	ND1-CE1-NE2	5.24	113.64	108.40
3	c	171	ALA	CA-C-N	5.24	127.73	120.29
3	c	171	ALA	C-N-CA	5.24	127.73	120.29
4	d	223	ALA	CA-C-N	-5.24	115.80	122.77
4	d	223	ALA	C-N-CA	-5.24	115.80	122.77
9	i	204	VAL	O-C-N	-5.24	117.03	123.00
10	j	179	ALA	CA-C-N	5.24	130.77	122.60
10	j	179	ALA	C-N-CA	5.24	130.77	122.60
9	2	218	ASN	OD1-CG-ND2	-5.24	117.36	122.60
21	N	479	GLU	CA-C-N	5.24	127.30	120.28
21	N	479	GLU	C-N-CA	5.24	127.30	120.28
28	H	332	THR	CA-C-N	5.24	127.25	120.44
28	H	332	THR	C-N-CA	5.24	127.25	120.44
30	K	322	ASP	CA-C-N	5.24	130.88	122.86
30	K	322	ASP	C-N-CA	5.24	130.88	122.86
32	M	390	GLN	CB-CG-CD	-5.24	103.69	112.60
3	C	160	TRP	CZ3-CH2-CZ2	-5.24	114.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	44	PHE	CA-CB-CG	-5.24	108.56	113.80
11	4	176	PHE	CA-C-N	5.24	129.80	122.36
11	4	176	PHE	C-N-CA	5.24	129.80	122.36
23	P	157	ALA	CA-C-N	5.24	127.25	120.44
23	P	157	ALA	C-N-CA	5.24	127.25	120.44
6	f	7	ASP	CA-CB-CG	5.24	117.84	112.60
16	V	152	VAL	N-CA-CB	5.24	119.87	111.23
17	T	243	ALA	CA-C-O	-5.24	115.00	120.55
20	Z	888	LEU	N-CA-CB	5.24	120.50	111.13
21	N	674	GLN	OE1-CD-NE2	5.24	127.84	122.60
23	P	126	THR	CA-C-O	5.24	126.02	120.10
28	H	63	ILE	CA-C-O	-5.24	115.30	120.85
3	c	117	ASP	CA-C-N	5.23	127.26	120.56
3	c	117	ASP	C-N-CA	5.23	127.26	120.56
9	i	192	ILE	O-C-N	5.23	127.22	121.83
11	k	189	ILE	O-C-N	5.23	128.83	123.18
14	n	257	ASP	CA-CB-CG	-5.23	107.37	112.60
11	4	95	ARG	N-CA-C	5.23	117.39	111.11
20	Z	447	VAL	CB-CA-C	-5.23	103.78	112.26
1	A	193	HIS	ND1-CE1-NE2	5.23	113.63	108.40
5	E	94	THR	CA-C-N	5.23	127.72	120.29
5	E	94	THR	C-N-CA	5.23	127.72	120.29
20	Z	796	LEU	CA-C-O	-5.23	114.87	120.42
21	N	657	MET	CB-CA-C	-5.23	102.10	110.79
22	S	347	HIS	CA-C-N	5.23	127.72	120.29
22	S	347	HIS	C-N-CA	5.23	127.72	120.29
23	P	413	ASN	CB-CA-C	-5.23	102.67	110.88
25	R	96	GLN	CA-C-N	5.23	127.29	120.28
25	R	96	GLN	C-N-CA	5.23	127.29	120.28
4	d	209	ASN	CA-CB-CG	-5.23	107.37	112.60
7	g	111	ALA	CA-C-N	5.23	127.29	120.28
7	g	111	ALA	C-N-CA	5.23	127.29	120.28
8	h	78	GLN	CB-CA-C	-5.23	100.23	110.11
8	h	191	GLY	O-C-N	5.23	129.50	122.70
12	l	220	LYS	CB-CA-C	-5.23	100.50	109.65
10	3	147	PHE	O-C-N	5.23	127.67	122.12
20	Z	133	ASP	O-C-N	5.23	127.66	122.12
28	H	277	SER	N-CA-C	-5.23	104.34	111.56
32	M	382	SER	N-CA-CB	5.23	117.81	110.12
4	D	4	TYR	N-CA-C	-5.23	104.64	112.54
14	7	217	LEU	CA-C-N	5.23	127.55	120.44
14	7	217	LEU	C-N-CA	5.23	127.55	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	642	ASP	CA-CB-CG	-5.23	107.37	112.60
6	f	33	SER	CA-C-N	5.23	127.50	120.50
6	f	33	SER	C-N-CA	5.23	127.50	120.50
8	h	188	THR	CA-C-O	5.23	126.90	121.31
13	m	86	ASP	CA-CB-CG	-5.23	107.37	112.60
13	6	99	ARG	CB-CG-CD	5.23	123.32	111.30
14	7	174	THR	CA-CB-OG1	5.23	117.44	109.60
22	S	185	PHE	O-C-N	-5.23	116.44	122.09
28	H	296	GLU	CA-C-N	5.23	127.71	120.29
28	H	296	GLU	C-N-CA	5.23	127.71	120.29
31	L	58	ASN	CB-CA-C	-5.23	101.96	110.85
32	M	293	SER	O-C-N	-5.23	117.10	123.16
2	b	33	THR	N-CA-CB	5.23	118.95	110.43
8	1	46	VAL	CA-C-O	5.23	123.68	118.98
21	N	870	ASN	N-CA-CB	5.23	118.05	109.95
28	H	439	THR	CA-CB-CG2	-5.23	101.62	110.50
4	d	175	LEU	CA-C-O	-5.22	115.32	120.70
1	A	148	GLU	N-CA-C	-5.22	106.75	113.02
4	D	160	SER	N-CA-C	-5.22	105.48	111.07
13	6	121	GLY	CA-C-O	5.22	125.17	121.04
14	7	210	ILE	CA-CB-CG1	5.22	119.28	110.40
15	W	136	ASN	CB-CG-ND2	-5.22	108.56	116.40
26	U	84	ASN	OD1-CG-ND2	5.22	127.83	122.60
28	H	117	THR	N-CA-C	-5.22	105.24	113.02
32	M	405	ASN	OD1-CG-ND2	5.22	127.83	122.60
4	d	205	THR	O-C-N	-5.22	116.58	123.21
5	e	132	ARG	N-CA-CB	5.22	119.92	110.83
20	Z	852	GLN	N-CA-C	-5.22	105.48	111.07
20	Z	908	ILE	CA-CB-CG1	5.22	119.28	110.40
21	N	214	LEU	CA-C-N	5.22	128.25	120.31
21	N	214	LEU	C-N-CA	5.22	128.25	120.31
28	H	289	ARG	CB-CG-CD	5.22	123.31	111.30
33	J	36	SER	N-CA-C	5.22	117.05	111.36
6	F	43	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
11	4	98	TYR	N-CA-CB	5.22	118.89	110.85
21	N	296	CYS	O-C-N	-5.22	116.20	122.15
9	i	189	GLN	CA-C-N	5.22	127.28	120.28
9	i	189	GLN	C-N-CA	5.22	127.28	120.28
3	C	222	ASP	CA-CB-CG	5.22	117.82	112.60
17	T	123	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
24	Q	67	THR	O-C-N	-5.22	115.65	122.59
8	h	182	ILE	CB-CA-C	-5.22	104.00	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	58	LYS	CB-CA-C	-5.22	102.66	110.90
18	X	99	PHE	CA-CB-CG	-5.22	108.58	113.80
23	P	326	ASP	N-CA-C	-5.22	102.74	110.46
4	d	249	LYS	N-CA-C	5.22	117.71	111.71
10	j	151	GLU	N-CA-C	-5.22	105.67	111.36
13	m	153	LEU	O-C-N	5.22	127.44	122.07
14	n	135	GLN	N-CA-C	5.22	116.97	111.28
5	E	157	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
9	2	237	GLY	CA-C-N	5.22	130.27	121.14
9	2	237	GLY	C-N-CA	5.22	130.27	121.14
22	S	212	SER	CA-C-N	5.22	127.70	120.29
22	S	212	SER	C-N-CA	5.22	127.70	120.29
22	S	246	GLU	O-C-N	5.22	129.44	123.02
23	P	289	ASN	OD1-CG-ND2	5.22	127.82	122.60
32	M	58	MET	CA-C-N	5.22	127.27	120.28
32	M	58	MET	C-N-CA	5.22	127.27	120.28
33	J	24	GLU	O-C-N	5.22	128.10	122.15
6	f	224	ILE	N-CA-CB	5.21	118.34	111.25
6	F	125	GLY	N-CA-C	-5.21	100.82	113.18
8	1	41	ASP	CA-C-O	5.21	127.97	120.51
9	2	161	LEU	N-CA-CB	5.21	117.88	110.16
20	Z	428	TRP	N-CA-CB	5.21	119.30	110.49
25	R	157	SER	N-CA-C	-5.21	105.77	111.82
26	U	161	ILE	CA-C-N	5.21	130.59	121.52
26	U	161	ILE	C-N-CA	5.21	130.59	121.52
32	M	393	ALA	O-C-N	-5.21	116.70	122.07
1	a	240	ASN	CA-CB-CG	5.21	117.81	112.60
3	c	97	ASN	CA-C-N	5.21	127.27	120.28
3	c	97	ASN	C-N-CA	5.21	127.27	120.28
14	n	164	ASN	CA-C-N	5.21	128.23	120.31
14	n	164	ASN	C-N-CA	5.21	128.23	120.31
28	H	400	ARG	CB-CG-CD	5.21	123.29	111.30
12	l	213	GLY	CA-C-N	5.21	127.23	120.56
12	l	213	GLY	C-N-CA	5.21	127.23	120.56
12	5	81	PHE	O-C-N	-5.21	117.44	123.33
17	T	128	TYR	CB-CG-CD1	5.21	128.62	120.80
21	N	219	ASN	CA-CB-CG	-5.21	107.39	112.60
28	H	199	THR	N-CA-C	-5.21	105.68	111.36
29	I	262	ARG	NE-CZ-NH2	5.21	123.89	119.20
31	L	72	ASP	CA-C-O	-5.21	115.03	120.55
20	Z	223	LEU	CA-C-N	5.21	127.26	120.28
20	Z	223	LEU	C-N-CA	5.21	127.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	336	HIS	CA-C-O	5.21	125.66	119.56
4	d	102	ASP	CA-CB-CG	-5.21	107.39	112.60
6	f	213	ILE	O-C-N	5.21	128.82	123.20
1	A	108	TYR	CA-CB-CG	-5.21	104.53	113.90
1	A	173	PRO	CA-C-N	5.21	130.95	122.67
1	A	173	PRO	C-N-CA	5.21	130.95	122.67
1	A	197	GLU	N-CA-CB	5.21	118.80	110.73
10	3	203	ARG	N-CA-C	5.21	117.84	110.50
15	W	80	GLN	CA-C-N	5.21	130.79	122.56
15	W	80	GLN	C-N-CA	5.21	130.79	122.56
22	S	310	LEU	CB-CA-C	-5.21	102.00	110.85
25	R	211	LYS	N-CA-CB	5.21	117.78	110.12
3	c	135	PHE	CA-CB-CG	-5.21	108.59	113.80
3	c	192	LEU	N-CA-C	5.21	117.04	111.36
10	j	57	ALA	N-CA-C	5.21	116.96	111.28
10	j	152	SER	N-CA-CB	5.21	117.77	110.12
1	A	51	THR	O-C-N	-5.21	116.84	123.24
4	D	9	SER	N-CA-C	-5.21	105.60	112.94
4	D	188	VAL	CA-C-N	5.21	127.26	120.28
4	D	188	VAL	C-N-CA	5.21	127.26	120.28
5	E	218	GLN	N-CA-CB	5.21	119.29	110.49
10	3	145	GLN	CA-C-O	-5.21	115.35	120.82
20	Z	234	PRO	O-C-N	5.21	129.67	122.64
23	P	228	SER	CA-C-O	5.21	125.94	120.42
25	R	132	GLN	CA-C-N	5.21	128.22	120.31
25	R	132	GLN	C-N-CA	5.21	128.22	120.31
26	U	275	VAL	CA-CB-CG2	-5.21	101.55	110.40
32	M	301	VAL	CB-CA-C	5.21	119.41	112.22
1	a	133	TYR	CA-C-N	5.21	132.49	122.03
1	a	133	TYR	C-N-CA	5.21	132.49	122.03
1	A	51	THR	CA-C-O	5.21	127.20	121.11
7	G	56	SER	N-CA-C	-5.21	101.00	108.60
17	T	10	SER	CA-C-N	5.21	127.68	120.29
17	T	10	SER	C-N-CA	5.21	127.68	120.29
23	P	27	LEU	CA-C-N	5.21	127.25	120.28
23	P	27	LEU	C-N-CA	5.21	127.25	120.28
25	R	234	SER	N-CA-CB	5.21	118.89	110.40
32	M	350	PRO	CA-C-N	5.21	129.60	121.17
32	M	350	PRO	C-N-CA	5.21	129.60	121.17
4	d	137	GLY	CA-C-N	5.20	130.69	122.36
4	d	137	GLY	C-N-CA	5.20	130.69	122.36
6	f	81	ALA	N-CA-C	-5.20	105.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	127	SER	N-CA-CB	5.20	119.28	110.49
3	C	53	THR	N-CA-C	-5.20	99.72	110.80
14	7	191	VAL	O-C-N	5.20	127.30	121.94
20	Z	871	HIS	CA-C-O	5.20	125.73	119.59
29	I	176	SER	N-CA-CB	5.20	118.70	110.11
31	L	128	ILE	N-CA-CB	5.20	118.33	111.25
9	2	54	ILE	CA-CB-CG2	-5.20	101.66	110.50
25	R	208	ASN	CA-C-N	5.20	127.25	120.28
25	R	208	ASN	C-N-CA	5.20	127.25	120.28
31	L	196	VAL	CA-CB-CG1	5.20	119.24	110.40
3	c	220	ALA	N-CA-C	-5.20	99.48	108.69
7	g	61	PRO	N-CD-CG	5.20	111.00	103.20
9	i	113	LYS	N-CA-C	5.20	116.95	111.28
2	B	44	VAL	CA-C-O	-5.20	114.80	121.40
12	5	226	GLU	CA-CB-CG	5.20	124.50	114.10
13	6	162	VAL	CB-CA-C	-5.20	105.66	111.80
21	N	582	ASP	CA-C-O	5.20	126.06	120.70
23	P	351	ARG	NE-CZ-NH2	-5.20	114.52	119.20
24	Q	51	ARG	CD-NE-CZ	-5.20	117.12	124.40
30	K	136	SER	CA-C-O	-5.20	116.04	121.55
32	M	30	LEU	CA-C-N	5.20	127.67	120.29
32	M	30	LEU	C-N-CA	5.20	127.67	120.29
33	J	321	VAL	CA-C-N	5.20	127.67	120.29
33	J	321	VAL	C-N-CA	5.20	127.67	120.29
1	a	89	ASP	CA-C-N	5.20	127.51	120.44
1	a	89	ASP	C-N-CA	5.20	127.51	120.44
11	k	83	PHE	CA-C-N	5.20	127.58	120.46
11	k	83	PHE	C-N-CA	5.20	127.58	120.46
20	Z	914	LEU	N-CA-CB	5.20	118.19	110.29
21	N	573	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
24	Q	128	GLU	CA-C-N	5.20	130.73	122.62
24	Q	128	GLU	C-N-CA	5.20	130.73	122.62
24	Q	319	LYS	N-CA-CB	5.20	117.85	110.16
28	H	234	ARG	CA-C-N	5.20	127.67	120.29
28	H	234	ARG	C-N-CA	5.20	127.67	120.29
33	J	257	ARG	N-CA-CB	-5.20	102.97	110.56
20	Z	228	GLU	CB-CA-C	-5.20	100.69	110.67
22	S	227	ASN	N-CA-C	-5.20	105.30	111.69
26	U	232	VAL	CB-CA-C	-5.20	105.23	111.88
3	c	152	ASN	CA-C-O	-5.20	115.29	120.64
4	D	207	ALA	O-C-N	-5.20	115.85	122.34
5	E	131	GLU	CB-CG-CD	-5.20	103.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	3	ARG	CA-C-N	5.20	131.05	121.70
6	F	3	ARG	C-N-CA	5.20	131.05	121.70
15	W	17	ARG	CB-CA-C	-5.20	100.61	109.65
22	S	77	THR	CA-C-N	5.20	128.68	120.47
22	S	77	THR	C-N-CA	5.20	128.68	120.47
22	S	382	ARG	O-C-N	-5.20	114.85	122.43
27	O	237	PRO	CA-C-N	5.20	127.86	120.53
27	O	237	PRO	C-N-CA	5.20	127.86	120.53
29	I	368	LYS	N-CA-CB	5.20	118.39	110.44
30	K	411	TYR	CB-CG-CD1	-5.20	113.01	120.80
27	O	366	MET	CG-SD-CE	-5.19	89.47	100.90
31	L	219	LEU	CB-CA-C	5.19	118.78	110.16
2	b	181	ASP	N-CA-C	-5.19	105.70	111.36
8	h	18	LYS	O-C-N	-5.19	115.30	122.46
10	j	104	PHE	CB-CA-C	-5.19	103.01	111.68
13	m	90	LYS	CA-C-O	-5.19	115.29	121.16
13	6	108	LYS	N-CA-C	-5.19	101.78	109.83
20	Z	420	ALA	CA-C-N	5.19	128.20	120.31
20	Z	420	ALA	C-N-CA	5.19	128.20	120.31
20	Z	738	TYR	CD1-CE1-CZ	5.19	128.95	119.60
21	N	304	LEU	CB-CA-C	-5.19	102.73	110.88
27	O	389	GLN	CB-CG-CD	-5.19	103.77	112.60
33	J	105	LYS	N-CA-C	-5.19	106.97	113.72
1	A	12	TYR	CB-CG-CD2	-5.19	113.02	120.80
9	2	182	LYS	N-CA-CB	5.19	117.75	110.12
11	4	132	ALA	CA-C-O	5.19	127.93	120.51
18	X	117	LYS	N-CA-C	-5.19	99.93	108.49
20	Z	630	LYS	CG-CD-CE	5.19	123.24	111.30
26	U	55	PRO	CB-CA-C	5.19	118.17	110.85
26	U	252	HIS	CG-CD2-NE2	5.19	112.39	107.20
26	U	260	ASN	CA-C-N	5.19	127.24	120.28
26	U	260	ASN	C-N-CA	5.19	127.24	120.28
29	I	81	ILE	CA-C-N	5.19	127.23	120.28
29	I	81	ILE	C-N-CA	5.19	127.23	120.28
7	g	127	ASN	OD1-CG-ND2	5.19	127.79	122.60
9	i	225	ARG	CA-CB-CG	5.19	124.48	114.10
2	B	159	TRP	CB-CA-C	-5.19	98.89	109.94
12	5	206	SER	CA-C-N	5.19	131.58	121.41
12	5	206	SER	C-N-CA	5.19	131.58	121.41
16	V	293	VAL	CA-CB-CG2	-5.19	101.58	110.40
20	Z	199	ASP	N-CA-C	5.19	117.02	111.36
22	S	264	VAL	N-CA-CB	5.19	119.52	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	67	THR	N-CA-CB	5.19	119.26	110.49
27	O	214	ALA	CA-C-N	5.19	127.23	120.28
27	O	214	ALA	C-N-CA	5.19	127.23	120.28
3	c	26	LEU	CA-C-N	5.19	128.19	120.31
3	c	26	LEU	C-N-CA	5.19	128.19	120.31
9	i	48	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	31	ALA	CA-C-O	-5.19	113.67	119.79
3	C	42	ASP	N-CA-C	-5.19	106.19	112.88
4	D	214	VAL	CA-C-N	5.19	130.20	122.99
4	D	214	VAL	C-N-CA	5.19	130.20	122.99
18	X	55	LYS	CA-C-N	5.19	125.64	120.04
18	X	55	LYS	C-N-CA	5.19	125.64	120.04
20	Z	226	GLU	CB-CG-CD	-5.19	103.78	112.60
20	Z	740	VAL	N-CA-C	5.19	115.96	110.72
21	N	808	ALA	O-C-N	5.19	127.41	122.07
22	S	128	ILE	CA-C-N	5.19	129.51	121.26
22	S	128	ILE	C-N-CA	5.19	129.51	121.26
31	L	170	MET	N-CA-CB	5.19	117.75	110.12
20	Z	386	VAL	O-C-N	5.19	127.11	121.87
22	S	207	ASN	CA-CB-CG	-5.19	107.41	112.60
7	g	154	SER	O-C-N	5.18	127.61	122.12
8	h	108	VAL	CA-C-N	5.18	130.72	122.94
8	h	108	VAL	C-N-CA	5.18	130.72	122.94
9	2	61	ALA	N-CA-CB	5.18	118.45	110.21
20	Z	225	LEU	CA-C-N	5.18	127.18	120.44
20	Z	225	LEU	C-N-CA	5.18	127.18	120.44
21	N	325	PHE	CA-C-N	5.18	127.65	120.29
21	N	325	PHE	C-N-CA	5.18	127.65	120.29
25	R	220	ALA	N-CA-C	5.18	116.93	111.28
30	K	144	ASN	N-CA-CB	5.18	119.25	110.49
30	K	273	GLU	CA-C-N	5.18	131.30	121.97
30	K	273	GLU	C-N-CA	5.18	131.30	121.97
4	D	156	TYR	N-CA-C	-5.18	101.31	109.50
8	1	192	VAL	N-CA-CB	5.18	118.38	111.64
20	Z	857	LEU	CB-CA-C	-5.18	101.44	110.09
21	N	672	ASN	CB-CG-ND2	5.18	124.17	116.40
21	N	904	VAL	CA-C-O	5.18	126.73	120.67
24	Q	21	ASN	O-C-N	5.18	127.48	122.09
32	M	60	GLU	CA-C-N	5.18	128.19	120.31
32	M	60	GLU	C-N-CA	5.18	128.19	120.31
1	A	110	TYR	CA-C-O	-5.18	115.19	120.99
6	F	205	SER	N-CA-C	-5.18	100.25	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	87	HIS	ND1-CE1-NE2	5.18	113.58	108.40
3	c	90	THR	CA-C-N	5.18	127.65	120.29
3	c	90	THR	C-N-CA	5.18	127.65	120.29
6	F	39	ARG	CA-CB-CG	5.18	124.46	114.10
8	1	45	ARG	NH1-CZ-NH2	5.18	126.03	119.30
11	4	122	LEU	CB-CA-C	-5.18	102.05	110.85
20	Z	726	GLU	N-CA-C	5.18	116.73	111.14
22	S	79	ASN	N-CA-C	5.18	116.92	111.28
25	R	326	ALA	CB-CA-C	-5.18	102.75	110.88
5	e	139	GLY	N-CA-C	-5.18	100.91	113.18
5	e	142	LEU	CA-C-O	-5.18	115.05	121.11
13	m	160	ASN	CA-CB-CG	-5.18	107.42	112.60
14	7	179	PHE	CB-CG-CD1	-5.18	111.90	120.70
32	M	166	ARG	CA-C-N	5.18	127.56	120.46
32	M	166	ARG	C-N-CA	5.18	127.56	120.46
4	d	157	SER	O-C-N	-5.18	116.91	123.17
13	m	56	ASP	CA-C-N	5.18	129.91	122.35
13	m	56	ASP	C-N-CA	5.18	129.91	122.35
15	W	191	ILE	CA-C-O	5.18	123.50	119.46
21	N	44	PRO	N-CA-C	5.18	120.64	113.65
21	N	419	THR	CA-C-O	5.18	125.91	120.42
23	P	247	THR	CA-C-N	5.18	127.22	120.28
23	P	247	THR	C-N-CA	5.18	127.22	120.28
24	Q	358	GLU	CA-C-N	5.18	127.55	120.46
24	Q	358	GLU	C-N-CA	5.18	127.55	120.46
25	R	316	LEU	CA-C-O	5.18	126.26	120.82
5	e	65	GLU	CB-CG-CD	-5.17	103.80	112.60
7	G	58	LEU	N-CA-C	-5.17	106.81	113.23
14	7	56	ALA	CA-C-O	-5.17	115.74	121.33
16	V	109	HIS	N-CA-CB	5.17	119.58	111.56
20	Z	819	GLY	N-CA-C	-5.17	106.23	112.49
23	P	115	ARG	CA-C-O	-5.17	115.36	120.90
23	P	239	GLN	O-C-N	-5.17	115.91	122.27
24	Q	426	LEU	CA-C-O	-5.17	115.06	120.55
28	H	342	GLY	CA-C-N	5.17	127.73	120.28
28	H	342	GLY	C-N-CA	5.17	127.73	120.28
31	L	82	ARG	CB-CA-C	-5.17	102.05	110.85
31	L	315	PHE	O-C-N	-5.17	115.71	122.59
32	M	209	ASP	CA-CB-CG	5.17	117.77	112.60
33	J	2	THR	N-CA-C	-5.17	101.32	109.50
33	J	366	GLY	CA-C-N	5.17	127.48	120.44
33	J	366	GLY	C-N-CA	5.17	127.48	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	76	GLY	CA-C-N	5.17	128.68	121.02
6	f	76	GLY	C-N-CA	5.17	128.68	121.02
11	k	115	GLU	CB-CA-C	-5.17	102.17	110.14
14	7	240	THR	CA-C-O	5.17	125.92	120.33
17	T	177	PHE	N-CA-CB	5.17	118.13	110.53
1	a	185	HIS	CB-CG-CD2	-5.17	124.48	131.20
7	g	209	GLU	N-CA-CB	5.17	119.23	110.49
8	h	98	ASN	CA-C-N	5.17	131.68	122.06
8	h	98	ASN	C-N-CA	5.17	131.68	122.06
8	h	126	GLY	CA-C-O	-5.17	117.21	122.59
14	n	225	SER	O-C-N	5.17	129.43	123.17
6	F	41	ASN	CA-CB-CG	-5.17	107.43	112.60
17	T	171	ILE	CA-CB-CG1	5.17	119.19	110.40
20	Z	260	GLU	CA-CB-CG	-5.17	103.76	114.10
23	P	164	GLN	CG-CD-NE2	-5.17	108.64	116.40
24	Q	422	VAL	CA-CB-CG1	5.17	119.19	110.40
27	O	326	HIS	CG-CD2-NE2	5.17	112.37	107.20
28	H	432	ARG	CA-C-O	-5.17	115.07	120.55
29	I	341	PRO	N-CA-CB	5.17	108.68	103.25
5	e	224	LYS	N-CA-C	-5.17	105.72	111.36
23	P	312	PRO	CA-C-O	-5.17	112.39	118.90
27	O	154	GLU	CA-C-N	5.17	127.63	120.29
27	O	154	GLU	C-N-CA	5.17	127.63	120.29
4	d	7	ALA	CA-C-N	5.17	131.74	122.38
4	d	7	ALA	C-N-CA	5.17	131.74	122.38
10	j	28	ARG	N-CA-CB	5.17	118.29	109.87
17	T	186	ARG	NE-CZ-NH1	-5.17	116.33	121.50
20	Z	792	VAL	CA-C-N	5.17	127.63	120.29
20	Z	792	VAL	C-N-CA	5.17	127.63	120.29
20	Z	801	HIS	CG-CD2-NE2	5.17	112.37	107.20
21	N	498	ILE	CA-C-O	-5.17	115.69	121.17
25	R	355	SER	N-CA-CB	5.17	117.72	110.12
1	a	124	LEU	O-C-N	5.17	127.60	122.12
12	l	82	ARG	O-C-N	-5.17	117.12	122.96
2	B	112	SER	CB-CA-C	-5.17	100.75	110.67
3	C	41	SER	CA-C-N	-5.17	114.54	122.60
3	C	41	SER	C-N-CA	-5.17	114.54	122.60
7	G	238	GLU	N-CA-CB	5.17	117.71	110.12
10	3	15	MET	CG-SD-CE	-5.17	89.53	100.90
13	6	204	ILE	CA-CB-CG1	5.17	119.18	110.40
22	S	92	LEU	CA-C-N	5.17	127.20	120.28
22	S	92	LEU	C-N-CA	5.17	127.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	407	ASN	N-CA-C	-5.17	102.25	109.69
25	R	308	LEU	CA-C-N	5.17	127.63	120.29
25	R	308	LEU	C-N-CA	5.17	127.63	120.29
26	U	129	GLY	CA-C-N	5.17	128.82	120.55
26	U	129	GLY	C-N-CA	5.17	128.82	120.55
2	B	244	ASN	CA-CB-CG	-5.17	107.44	112.60
16	V	142	ASP	CA-CB-CG	-5.17	107.44	112.60
17	T	42	PRO	CA-C-N	5.17	129.95	122.36
17	T	42	PRO	C-N-CA	5.17	129.95	122.36
8	h	184	MET	CA-C-N	5.16	130.31	122.98
8	h	184	MET	C-N-CA	5.16	130.31	122.98
13	6	46	ARG	CB-CA-C	-5.16	99.81	109.72
14	7	232	ILE	N-CA-CB	5.16	118.27	111.25
17	T	164	LEU	CA-C-N	5.16	127.62	120.29
17	T	164	LEU	C-N-CA	5.16	127.62	120.29
20	Z	899	GLN	CA-C-N	5.16	130.91	122.81
20	Z	899	GLN	C-N-CA	5.16	130.91	122.81
21	N	207	LEU	N-CA-C	5.16	116.99	111.36
10	j	204	GLN	O-C-N	-5.16	117.19	123.13
20	Z	734	ASP	N-CA-CB	5.16	117.80	110.16
29	I	345	ASP	CB-CA-C	-5.16	102.33	111.05
33	J	282	PHE	CA-C-O	5.16	124.49	118.97
1	A	210	MET	O-C-N	5.16	128.03	122.15
5	E	244	LYS	CB-CA-C	-5.16	102.22	110.79
24	Q	297	ASP	N-CA-C	-5.16	105.73	111.36
9	2	63	LEU	N-CA-C	-5.16	99.88	108.34
21	N	325	PHE	CA-C-O	-5.16	114.79	120.36
22	S	239	ARG	CB-CA-C	-5.16	102.23	110.79
23	P	223	LEU	O-C-N	5.16	127.59	122.12
23	P	319	GLU	CA-C-O	-5.16	113.09	120.16
25	R	254	SER	CA-C-O	-5.16	115.40	120.82
29	I	150	HIS	ND1-CE1-NE2	5.16	113.56	108.40
32	M	333	LEU	CA-C-N	5.16	128.52	120.68
32	M	333	LEU	C-N-CA	5.16	128.52	120.68
3	c	50	ARG	CB-CG-CD	5.16	123.16	111.30
12	l	208	GLN	CA-C-N	5.16	127.45	120.44
12	l	208	GLN	C-N-CA	5.16	127.45	120.44
4	D	119	ARG	NE-CZ-NH2	5.16	123.84	119.20
12	5	268	VAL	CB-CA-C	-5.16	105.18	112.14
20	Z	625	THR	CA-C-N	5.16	124.60	119.24
20	Z	625	THR	C-N-CA	5.16	124.60	119.24
28	H	286	GLU	O-C-N	5.16	128.94	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	283	ASP	CA-CB-CG	-5.16	107.44	112.60
4	d	47	GLU	O-C-N	-5.16	117.01	123.04
7	g	243	ALA	CA-C-N	5.16	127.45	120.44
7	g	243	ALA	C-N-CA	5.16	127.45	120.44
5	E	98	THR	N-CA-CB	5.16	118.27	110.28
13	6	134	ASP	N-CA-C	-5.16	103.28	109.83
18	X	97	TYR	N-CA-CB	5.16	120.41	111.39
20	Z	142	ASP	CA-C-N	5.16	131.25	121.97
20	Z	142	ASP	C-N-CA	5.16	131.25	121.97
20	Z	458	SER	N-CA-C	-5.16	105.74	111.36
21	N	782	PHE	CA-CB-CG	-5.16	108.64	113.80
22	S	302	HIS	CB-CG-CD2	-5.16	124.50	131.20
24	Q	264	TYR	CB-CG-CD2	-5.16	113.07	120.80
25	R	404	VAL	CA-C-N	5.16	127.19	120.28
25	R	404	VAL	C-N-CA	5.16	127.19	120.28
26	U	162	GLU	N-CA-C	-5.16	108.25	114.75
27	O	270	ILE	CA-C-O	-5.16	115.05	120.57
21	N	17	GLN	N-CA-CB	5.15	119.20	110.49
22	S	26	ALA	CA-C-O	-5.15	115.09	120.55
22	S	109	GLU	CA-C-N	5.15	130.67	121.75
22	S	109	GLU	C-N-CA	5.15	130.67	121.75
13	m	64	GLY	N-CA-C	-5.15	100.97	113.18
3	C	225	VAL	CB-CA-C	-5.15	104.43	111.33
8	1	181	VAL	N-CA-C	5.15	116.23	109.58
16	V	188	LEU	O-C-N	5.15	127.38	122.07
21	N	60	MET	CA-CB-CG	-5.15	103.80	114.10
22	S	144	LEU	N-CA-C	5.15	116.90	111.28
29	I	184	ILE	N-CA-C	-5.15	100.99	108.36
32	M	158	THR	CA-CB-CG2	-5.15	101.74	110.50
33	J	128	ASN	N-CA-C	-5.15	100.77	108.96
1	a	62	LYS	O-C-N	-5.15	116.16	122.34
13	m	87	HIS	CA-C-N	5.15	129.50	122.34
13	m	87	HIS	C-N-CA	5.15	129.50	122.34
16	V	248	ALA	N-CA-CB	5.15	118.55	110.46
20	Z	766	HIS	ND1-CE1-NE2	5.15	113.55	108.40
21	N	697	PHE	O-C-N	5.15	127.37	122.07
30	K	214	PRO	CA-C-N	5.15	126.28	119.84
30	K	214	PRO	C-N-CA	5.15	126.28	119.84
5	e	137	PRO	CA-C-O	-5.15	115.66	121.43
14	n	190	LYS	CA-C-O	-5.15	115.41	120.82
22	S	432	ILE	O-C-N	5.15	128.59	121.90
27	O	142	ASP	CA-C-N	5.15	127.60	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	142	ASP	C-N-CA	5.15	127.60	120.29
27	O	147	ARG	CB-CA-C	5.15	120.56	110.67
4	d	243	GLN	CA-C-N	5.15	127.60	120.29
4	d	243	GLN	C-N-CA	5.15	127.60	120.29
6	f	69	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
10	j	84	PRO	CA-N-CD	-5.15	104.79	112.00
12	l	100	TRP	N-CA-C	-5.15	102.44	110.42
1	A	164	VAL	CA-C-O	-5.15	115.89	121.19
5	E	221	CYS	N-CA-CB	5.15	120.51	111.55
15	W	105	VAL	CB-CA-C	-5.15	105.37	111.65
16	V	190	HIS	ND1-CE1-NE2	5.15	113.55	108.40
22	S	334	HIS	CA-C-O	5.15	126.01	120.55
25	R	109	LYS	CA-C-O	-5.15	115.40	120.70
26	U	105	LYS	N-CA-CB	5.15	117.78	110.16
29	I	302	ILE	CB-CA-C	5.15	119.09	112.14
29	I	340	ARG	CA-C-N	5.15	126.27	119.84
29	I	340	ARG	C-N-CA	5.15	126.27	119.84
31	L	432	ILE	CA-C-N	5.15	128.02	120.71
31	L	432	ILE	C-N-CA	5.15	128.02	120.71
11	k	58	GLU	CA-C-N	5.15	127.60	120.29
11	k	58	GLU	C-N-CA	5.15	127.60	120.29
2	B	23	TYR	CB-CG-CD2	-5.15	113.08	120.80
19	Y	67	VAL	N-CA-CB	5.15	119.72	111.23
22	S	88	PHE	N-CA-C	-5.15	105.75	111.36
4	d	146	LYS	CA-C-N	5.14	130.84	121.89
4	d	146	LYS	C-N-CA	5.14	130.84	121.89
12	l	78	THR	N-CA-C	-5.14	101.49	109.72
12	l	150	SER	N-CA-C	-5.14	103.61	110.55
14	7	137	ARG	NE-CZ-NH2	-5.14	114.57	119.20
16	V	84	ASP	CB-CA-C	5.14	118.13	110.62
16	V	111	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
20	Z	159	LEU	O-C-N	5.14	127.57	122.12
20	Z	706	LYS	CA-C-N	5.14	127.17	120.28
20	Z	706	LYS	C-N-CA	5.14	127.17	120.28
21	N	263	SER	CA-C-N	5.14	129.30	120.71
21	N	263	SER	C-N-CA	5.14	129.30	120.71
21	N	747	HIS	CB-CG-CD2	-5.14	124.51	131.20
22	S	393	ARG	N-CA-C	5.14	116.89	111.28
33	J	43	ARG	CB-CA-C	-5.14	101.29	110.70
8	1	120	TYR	N-CA-CB	5.14	119.15	110.77
9	2	90	SER	N-CA-CB	5.14	118.14	110.22
14	7	179	PHE	CA-C-O	-5.14	115.10	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	227	ILE	CB-CA-C	-5.14	105.20	112.14
27	O	48	PHE	N-CA-C	-5.14	105.57	111.07
32	M	47	GLU	CA-C-N	5.14	127.17	120.28
32	M	47	GLU	C-N-CA	5.14	127.17	120.28
1	a	133	TYR	CD1-CG-CD2	-5.14	110.39	118.10
3	C	28	SER	N-CA-C	5.14	117.62	111.71
26	U	77	ASN	N-CA-CB	5.14	117.77	110.16
5	e	241	LYS	N-CA-C	5.14	116.57	111.07
6	f	75	ALA	N-CA-C	-5.14	99.85	110.80
6	f	110	HIS	CA-CB-CG	-5.14	108.66	113.80
11	k	53	THR	CA-CB-OG1	5.14	117.31	109.60
13	m	72	LEU	CA-C-N	5.14	127.50	120.46
13	m	72	LEU	C-N-CA	5.14	127.50	120.46
5	E	33	LEU	CA-C-N	5.14	126.04	120.44
5	E	33	LEU	C-N-CA	5.14	126.04	120.44
19	Y	84	TYR	CB-CA-C	-5.14	102.26	110.79
28	H	169	GLU	CA-C-O	-5.14	115.81	121.31
30	K	69	LYS	CA-C-N	5.14	129.37	120.58
30	K	69	LYS	C-N-CA	5.14	129.37	120.58
31	L	209	ARG	CA-CB-CG	5.14	124.38	114.10
33	J	200	ARG	CA-C-N	5.14	127.17	120.28
33	J	200	ARG	C-N-CA	5.14	127.17	120.28
7	g	123	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
24	Q	109	ASP	CA-CB-CG	5.14	117.74	112.60
30	K	252	ARG	CA-C-N	5.14	127.17	120.28
30	K	252	ARG	C-N-CA	5.14	127.17	120.28
2	b	160	LYS	CA-C-O	-5.14	113.89	120.31
9	i	101	ARG	CA-C-N	5.14	127.78	120.49
9	i	101	ARG	C-N-CA	5.14	127.78	120.49
14	n	215	ARG	O-C-N	-5.14	116.67	122.12
8	1	71	HIS	CB-CG-ND1	5.14	130.41	122.70
11	4	135	TYR	N-CA-C	-5.14	106.79	113.16
16	V	202	ASP	N-CA-C	-5.14	102.46	110.42
20	Z	46	LYS	CA-C-N	5.14	127.12	120.44
20	Z	46	LYS	C-N-CA	5.14	127.12	120.44
23	P	353	ILE	CA-CB-CG1	-5.14	101.67	110.40
32	M	425	ARG	CA-C-N	5.14	128.85	121.50
32	M	425	ARG	C-N-CA	5.14	128.85	121.50
33	J	298	ASP	CA-C-O	5.14	125.68	119.31
33	J	402	LYS	N-CA-CB	5.14	119.14	110.77
1	a	163	TYR	CB-CG-CD2	-5.13	113.10	120.80
20	Z	926	ASN	CA-C-N	5.13	130.13	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	926	ASN	C-N-CA	5.13	130.13	122.99
24	Q	68	MET	CG-SD-CE	-5.13	89.60	100.90
30	K	96	ILE	N-CA-C	-5.13	102.47	109.55
32	M	277	ILE	O-C-N	-5.13	117.84	123.18
32	M	408	SER	CA-C-N	5.13	130.63	121.75
32	M	408	SER	C-N-CA	5.13	130.63	121.75
10	j	57	ALA	N-CA-CB	-5.13	102.58	110.12
4	D	50	SER	N-CA-CB	5.13	118.64	110.84
6	F	146	GLU	CA-C-N	5.13	130.30	122.65
6	F	146	GLU	C-N-CA	5.13	130.30	122.65
16	V	206	THR	CA-C-O	-5.13	115.21	121.88
26	U	279	SER	CA-C-N	5.13	127.16	120.28
26	U	279	SER	C-N-CA	5.13	127.16	120.28
29	I	370	ASN	CA-C-N	5.13	131.34	121.54
29	I	370	ASN	C-N-CA	5.13	131.34	121.54
30	K	345	ASP	O-C-N	-5.13	117.20	123.10
32	M	327	THR	O-C-N	-5.13	117.93	123.42
33	J	335	MET	CA-C-N	5.13	130.97	121.94
33	J	335	MET	C-N-CA	5.13	130.97	121.94
1	a	181	ASN	CA-C-O	5.13	125.99	120.55
12	l	231	LEU	O-C-N	-5.13	116.30	122.15
4	D	67	ILE	O-C-N	5.13	127.24	121.90
6	F	211	LEU	CA-C-O	5.13	126.18	120.43
7	G	89	VAL	N-CA-C	-5.13	105.41	111.00
7	G	147	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
16	V	57	PHE	CA-C-O	-5.13	114.84	120.43
16	V	72	PRO	CA-C-N	5.13	128.50	120.75
16	V	72	PRO	C-N-CA	5.13	128.50	120.75
23	P	346	ILE	CA-CB-CG2	-5.13	101.78	110.50
26	U	135	ASP	N-CA-C	-5.13	100.67	109.24
26	U	193	GLN	CA-C-N	5.13	127.58	120.29
26	U	193	GLN	C-N-CA	5.13	127.58	120.29
9	i	158	SER	CA-C-O	5.13	125.86	120.42
3	c	8	SER	N-CA-C	5.13	116.68	111.14
7	g	136	THR	CA-C-N	5.13	129.40	121.71
7	g	136	THR	C-N-CA	5.13	129.40	121.71
17	T	224	ARG	O-C-N	-5.13	115.93	122.34
20	Z	756	MET	CB-CA-C	-5.13	102.13	110.85
23	P	47	ARG	NE-CZ-NH2	5.13	123.82	119.20
25	R	381	ILE	O-C-N	-5.13	117.36	123.05
28	H	73	ASP	CA-CB-CG	-5.13	107.47	112.60
1	a	23	GLY	N-CA-C	-5.13	108.15	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	191	GLU	CA-C-N	5.13	127.57	120.29
3	c	191	GLU	C-N-CA	5.13	127.57	120.29
7	g	177	GLU	CA-C-N	5.13	127.15	120.28
7	g	177	GLU	C-N-CA	5.13	127.15	120.28
12	5	139	ARG	O-C-N	5.13	127.56	122.12
20	Z	15	GLN	N-CA-C	-5.13	105.77	111.36
31	L	160	PRO	O-C-N	5.13	128.84	123.10
1	A	183	GLU	CA-C-N	5.12	127.15	120.28
1	A	183	GLU	C-N-CA	5.12	127.15	120.28
16	V	233	LYS	CB-CA-C	-5.12	102.14	110.85
27	O	67	SER	N-CA-C	-5.12	106.88	112.72
33	J	338	THR	CA-CB-OG1	5.12	117.29	109.60
33	J	352	GLY	O-C-N	5.12	127.87	122.59
33	J	367	MET	CG-SD-CE	-5.12	89.62	100.90
3	c	134	SER	CB-CA-C	-5.12	101.65	110.16
3	c	187	ASP	N-CA-CB	5.12	117.74	110.16
1	A	33	LYS	CA-C-O	5.12	124.58	118.69
22	S	225	HIS	N-CA-C	5.12	118.27	111.30
26	U	125	VAL	N-CA-CB	-5.12	105.65	112.26
32	M	378	GLU	CB-CG-CD	-5.12	103.89	112.60
4	D	81	ASP	CA-CB-CG	-5.12	107.48	112.60
17	T	161	TRP	CE2-CD2-CE3	5.12	123.92	118.80
22	S	357	LEU	CA-C-N	5.12	129.34	120.58
22	S	357	LEU	C-N-CA	5.12	129.34	120.58
22	S	468	ALA	CA-C-N	5.12	127.14	120.28
22	S	468	ALA	C-N-CA	5.12	127.14	120.28
23	P	385	ASN	CB-CA-C	-5.12	102.14	110.85
24	Q	312	LEU	N-CA-C	-5.12	105.78	111.36
4	d	14	ASP	CA-CB-CG	5.12	117.72	112.60
9	2	224	VAL	O-C-N	5.12	128.36	122.93
12	5	105	THR	CA-CB-OG1	5.12	117.28	109.60
13	6	73	VAL	CA-C-N	5.12	127.14	120.28
13	6	73	VAL	C-N-CA	5.12	127.14	120.28
23	P	118	VAL	N-CA-CB	5.12	117.50	110.54
6	F	101	ARG	CG-CD-NE	-5.12	100.74	112.00
8	1	166	HIS	N-CA-C	5.12	116.55	111.07
9	2	39	ASN	CA-C-N	-5.12	112.46	120.55
9	2	39	ASN	C-N-CA	-5.12	112.46	120.55
20	Z	590	ALA	CB-CA-C	-5.12	102.62	110.81
25	R	74	ASN	CA-CB-CG	-5.12	107.48	112.60
30	K	35	ASN	CA-CB-CG	-5.12	107.48	112.60
33	J	385	ALA	N-CA-C	5.12	116.94	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	HIS	CA-CB-CG	-5.12	108.68	113.80
2	B	189	ILE	CA-C-O	5.12	126.05	120.57
15	W	135	ASN	CA-CB-CG	5.12	117.72	112.60
16	V	286	GLU	O-C-N	5.12	127.34	122.07
20	Z	927	VAL	N-CA-C	-5.12	100.75	108.12
32	M	215	PRO	CB-CA-C	-5.12	105.06	111.71
2	b	228	PRO	N-CD-CG	5.12	110.87	103.20
13	m	95	ASN	CA-CB-CG	5.12	117.72	112.60
4	D	218	ASP	CA-C-N	5.12	129.45	122.34
4	D	218	ASP	C-N-CA	5.12	129.45	122.34
23	P	354	SER	N-CA-C	5.12	116.94	111.36
23	P	361	THR	N-CA-CB	5.12	117.54	110.17
24	Q	288	LYS	N-CA-C	-5.12	105.33	112.03
26	U	82	LYS	O-C-N	5.12	127.61	122.09
28	H	192	ASP	CA-CB-CG	-5.12	107.48	112.60
32	M	60	GLU	N-CA-C	5.12	116.86	111.28
32	M	87	ASP	CA-C-O	5.12	125.89	120.36
2	b	202	GLY	N-CA-C	-5.11	108.17	115.64
11	k	60	ILE	CA-CB-CG2	5.11	119.19	110.50
2	B	11	THR	CA-CB-OG1	5.11	117.27	109.60
12	5	254	HIS	CG-CD2-NE2	5.11	112.31	107.20
21	N	396	SER	CA-C-N	-5.11	112.90	121.75
21	N	396	SER	C-N-CA	-5.11	112.90	121.75
21	N	457	SER	N-CA-CB	5.11	118.61	111.15
21	N	652	VAL	CA-C-O	5.11	126.27	120.85
23	P	269	VAL	CA-CB-CG2	-5.11	101.71	110.40
28	H	135	ASP	CB-CA-C	-5.11	102.16	110.85
31	L	410	ILE	N-CA-CB	5.11	116.83	111.00
32	M	63	LYS	CA-C-N	5.11	127.55	120.29
32	M	63	LYS	C-N-CA	5.11	127.55	120.29
21	N	767	ALA	CA-C-O	-5.11	115.78	121.51
29	I	357	THR	CA-C-N	5.11	130.09	121.14
29	I	357	THR	C-N-CA	5.11	130.09	121.14
10	j	104	PHE	CA-C-N	5.11	127.83	122.11
10	j	104	PHE	C-N-CA	5.11	127.83	122.11
21	N	345	ASP	CA-C-N	5.11	130.57	122.60
21	N	345	ASP	C-N-CA	5.11	130.57	122.60
3	c	30	SER	N-CA-CB	5.11	117.61	110.56
21	N	223	LEU	CA-C-N	5.11	127.54	120.29
21	N	223	LEU	C-N-CA	5.11	127.54	120.29
31	L	145	ARG	N-CA-CB	5.11	117.48	109.97
32	M	186	LEU	CA-C-N	5.11	127.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	186	LEU	C-N-CA	5.11	127.13	120.28
33	J	286	LYS	CB-CA-C	-5.11	102.86	110.88
1	a	110	TYR	O-C-N	-5.11	116.55	123.19
6	f	145	LEU	CA-C-O	5.11	126.93	121.16
5	E	207	VAL	O-C-N	-5.11	117.19	122.14
14	7	218	TYR	O-C-N	5.11	127.61	122.09
21	N	29	ASN	OD1-CG-ND2	5.11	127.71	122.60
21	N	237	LEU	N-CA-CB	5.11	117.72	110.16
23	P	49	ALA	N-CA-C	5.11	116.85	111.28
23	P	109	SER	CB-CA-C	-5.11	102.83	110.90
23	P	369	LEU	N-CA-C	-5.11	106.73	113.17
23	P	419	VAL	CA-CB-CG1	5.11	119.08	110.40
32	M	356	SER	CB-CA-C	-5.11	100.86	110.67
2	b	48	GLU	N-CA-C	-5.11	101.78	109.85
4	D	193	LYS	N-CA-C	5.11	116.84	111.28
6	F	96	SER	CB-CA-C	-5.11	102.17	110.85
10	3	103	TYR	CA-CB-CG	-5.11	104.71	113.90
20	Z	495	ILE	O-C-N	5.11	127.21	121.90
21	N	524	ILE	N-CA-C	5.11	115.83	110.62
22	S	379	LEU	N-CA-C	-5.11	105.90	111.82
25	R	40	ILE	CA-C-N	5.11	127.08	120.44
25	R	40	ILE	C-N-CA	5.11	127.08	120.44
25	R	329	PHE	O-C-N	-5.11	116.33	122.15
27	O	89	SER	O-C-N	5.11	129.15	122.87
31	L	384	ASP	N-CA-CB	5.11	117.86	109.95
13	m	130	VAL	N-CA-CB	5.10	118.97	111.52
14	n	122	PRO	CA-C-N	5.10	127.54	120.29
14	n	122	PRO	C-N-CA	5.10	127.54	120.29
22	S	398	THR	N-CA-CB	5.10	117.80	110.20
25	R	73	ASN	OD1-CG-ND2	-5.10	117.50	122.60
25	R	359	VAL	CA-CB-CG1	-5.10	101.72	110.40
7	g	182	HIS	ND1-CE1-NE2	5.10	113.50	108.40
10	j	5	SER	N-CA-C	-5.10	105.72	111.28
14	7	259	LYS	N-CA-C	-5.10	106.74	113.17
16	V	262	THR	N-CA-CB	5.10	119.11	110.49
24	Q	330	LEU	CA-C-N	5.10	127.12	120.28
24	Q	330	LEU	C-N-CA	5.10	127.12	120.28
28	H	344	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	191	ILE	CA-C-N	5.10	127.11	120.28
2	B	191	ILE	C-N-CA	5.10	127.11	120.28
7	G	48	PHE	CB-CA-C	-5.10	99.63	109.37
23	P	123	ARG	NE-CZ-NH1	-5.10	116.40	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	106	ASN	CA-CB-CG	-5.10	107.50	112.60
28	H	86	GLY	CA-C-O	-5.10	114.69	120.30
28	H	198	MET	CA-C-N	5.10	127.53	120.29
28	H	198	MET	C-N-CA	5.10	127.53	120.29
31	L	118	ILE	O-C-N	5.10	128.69	123.03
1	A	24	ARG	CA-C-O	-5.10	115.06	120.92
5	E	241	LYS	O-C-N	-5.10	116.34	122.15
19	Y	80	GLU	CB-CG-CD	-5.10	103.93	112.60
20	Z	392	LEU	CD1-CG-CD2	5.10	122.02	110.80
24	Q	35	SER	N-CA-C	5.10	117.58	111.71
4	d	246	GLN	N-CA-CB	5.10	117.70	110.16
9	i	151	GLY	CA-C-N	5.10	131.86	122.79
9	i	151	GLY	C-N-CA	5.10	131.86	122.79
11	k	195	PHE	CB-CG-CD2	-5.10	112.03	120.70
4	D	117	GLN	CA-C-O	-5.10	115.15	120.55
21	N	224	THR	CA-CB-CG2	-5.10	101.83	110.50
22	S	184	TRP	CE3-CZ3-CH2	-5.10	114.47	121.10
29	I	312	GLN	CA-C-N	5.10	127.37	120.44
29	I	312	GLN	C-N-CA	5.10	127.37	120.44
8	1	129	HIS	ND1-CE1-NE2	5.10	113.50	108.40
2	b	90	ARG	CA-C-N	5.09	127.06	120.44
2	b	90	ARG	C-N-CA	5.09	127.06	120.44
8	h	44	THR	N-CA-CB	5.09	119.61	110.80
9	i	112	LEU	CA-C-N	5.09	127.11	120.28
9	i	112	LEU	C-N-CA	5.09	127.11	120.28
10	j	3	ASP	CA-C-N	5.09	124.88	119.28
10	j	3	ASP	C-N-CA	5.09	124.88	119.28
4	D	42	VAL	N-CA-C	-5.09	100.87	108.46
8	1	99	LYS	N-CA-CB	5.09	117.70	110.16
13	6	79	SER	N-CA-CB	5.09	118.06	110.22
16	V	233	LYS	N-CA-CB	5.09	117.70	110.16
20	Z	870	ALA	N-CA-CB	-5.09	101.88	110.49
21	N	119	LYS	CB-CG-CD	5.09	123.02	111.30
22	S	466	LYS	N-CA-CB	5.09	117.70	110.16
30	K	350	ARG	O-C-N	5.09	127.96	122.15
7	g	6	THR	CB-CA-C	5.09	118.56	111.63
11	k	146	HIS	CA-C-O	5.09	125.95	120.70
21	N	6	ALA	CA-C-N	5.09	127.30	120.58
21	N	6	ALA	C-N-CA	5.09	127.30	120.58
21	N	773	MET	CG-SD-CE	5.09	112.11	100.90
29	I	158	GLY	N-CA-C	-5.09	103.18	110.46
30	K	131	LEU	N-CA-C	-5.09	107.45	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	50	ASP	CA-CB-CG	5.09	117.69	112.60
8	1	42	LYS	CA-C-O	5.09	124.78	119.03
14	7	214	MET	N-CA-CB	5.09	117.61	110.12
21	N	53	ASP	CB-CA-C	-5.09	102.59	111.35
21	N	250	ASP	CA-C-O	-5.09	114.90	120.70
23	P	316	LYS	CA-C-N	5.09	127.10	120.28
23	P	316	LYS	C-N-CA	5.09	127.10	120.28
24	Q	407	ALA	N-CA-CB	5.09	117.61	110.12
27	O	217	LEU	CA-C-N	5.09	127.52	120.29
27	O	217	LEU	C-N-CA	5.09	127.52	120.29
29	I	204	HIS	ND1-CE1-NE2	5.09	113.49	108.40
30	K	290	ARG	CB-CA-C	-5.09	102.34	110.79
31	L	345	ARG	NE-CZ-NH2	-5.09	114.62	119.20
9	i	215	TYR	O-C-N	5.09	128.98	123.13
13	m	127	LYS	N-CA-C	-5.09	100.41	109.06
10	3	103	TYR	CA-C-O	-5.09	116.09	121.94
19	Y	54	VAL	CA-C-N	5.09	131.26	121.54
19	Y	54	VAL	C-N-CA	5.09	131.26	121.54
25	R	179	PHE	CA-C-O	5.09	125.82	120.42
28	H	54	ASN	O-C-N	5.09	127.95	122.15
32	M	412	HIS	ND1-CE1-NE2	5.09	113.49	108.40
33	J	266	SER	N-CA-C	5.09	117.56	111.71
3	C	7	ASP	O-C-N	5.09	128.52	122.26
16	V	209	GLU	CA-C-N	5.09	127.05	120.44
16	V	209	GLU	C-N-CA	5.09	127.05	120.44
23	P	211	PRO	N-CA-CB	5.09	108.19	103.46
23	P	364	ARG	N-CA-CB	5.09	117.78	110.20
1	A	56	GLN	CG-CD-NE2	-5.09	108.77	116.40
1	A	120	ARG	NE-CZ-NH2	-5.09	114.62	119.20
20	Z	326	VAL	CA-C-N	5.09	128.04	120.31
20	Z	326	VAL	C-N-CA	5.09	128.04	120.31
20	Z	546	ILE	CB-CA-C	-5.09	105.20	112.22
23	P	257	TRP	N-CA-C	-5.09	106.58	112.89
27	O	98	TYR	CB-CA-C	-5.09	102.20	110.85
29	I	362	LEU	CA-C-N	5.09	126.50	120.14
29	I	362	LEU	C-N-CA	5.09	126.50	120.14
32	M	181	SER	O-C-N	5.08	129.63	122.41
1	a	110	TYR	N-CA-C	-5.08	101.59	109.72
10	j	170	ALA	CA-C-N	5.08	127.51	120.29
10	j	170	ALA	C-N-CA	5.08	127.51	120.29
20	Z	524	ALA	CA-C-N	5.08	130.44	120.99
20	Z	524	ALA	C-N-CA	5.08	130.44	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	748	PHE	CA-C-O	5.08	125.30	119.35
30	K	412	ALA	CB-CA-C	-5.08	101.23	110.63
31	L	344	ASP	CA-CB-CG	-5.08	107.52	112.60
1	a	66	PRO	N-CA-C	-5.08	106.91	113.57
6	f	91	GLN	N-CA-CB	5.08	117.68	110.16
6	f	179	PHE	CA-C-N	5.08	127.64	120.42
6	f	179	PHE	C-N-CA	5.08	127.64	120.42
12	l	181	ARG	NE-CZ-NH1	5.08	126.58	121.50
2	B	242	GLU	CA-C-N	5.08	127.42	120.46
2	B	242	GLU	C-N-CA	5.08	127.42	120.46
12	5	199	GLY	CA-C-O	5.08	126.16	121.38
12	5	211	ALA	CA-C-N	5.08	127.09	120.28
12	5	211	ALA	C-N-CA	5.08	127.09	120.28
13	6	163	ASN	CA-C-N	5.08	129.35	122.19
13	6	163	ASN	C-N-CA	5.08	129.35	122.19
23	P	282	HIS	CA-C-N	5.08	127.50	120.29
23	P	282	HIS	C-N-CA	5.08	127.50	120.29
27	O	355	PRO	N-CD-CG	5.08	110.82	103.20
28	H	116	THR	CA-C-O	-5.08	115.67	121.00
28	H	311	ILE	N-CA-CB	5.08	119.61	111.23
2	B	21	ILE	O-C-N	5.08	127.18	121.90
20	Z	885	ALA	CA-C-N	5.08	127.41	120.35
20	Z	885	ALA	C-N-CA	5.08	127.41	120.35
24	Q	116	PHE	N-CA-C	-5.08	105.82	111.36
31	L	312	MET	CB-CA-C	-5.08	102.36	110.79
32	M	377	GLN	CB-CA-C	5.08	118.93	110.90
1	a	38	THR	N-CA-C	-5.08	106.93	113.23
4	d	157	SER	CA-C-O	5.08	127.14	121.40
5	e	111	SER	CA-C-O	5.08	125.78	119.79
9	i	194	ASN	CA-CB-CG	-5.08	107.52	112.60
14	7	124	TYR	CG-CD1-CE1	-5.08	113.58	121.20
20	Z	164	VAL	CA-CB-CG2	5.08	119.03	110.40
21	N	322	ASP	CB-CA-C	-5.08	100.39	111.71
23	P	222	ASN	CB-CA-C	-5.08	102.22	110.85
31	L	330	PRO	CA-C-N	5.08	128.03	120.31
31	L	330	PRO	C-N-CA	5.08	128.03	120.31
15	W	177	GLY	CA-C-N	5.08	127.92	120.46
15	W	177	GLY	C-N-CA	5.08	127.92	120.46
16	V	44	GLY	N-CA-C	-5.08	101.15	113.18
21	N	187	ASN	CA-C-N	5.08	127.50	120.29
21	N	187	ASN	C-N-CA	5.08	127.50	120.29
33	J	367	MET	CA-C-N	5.08	127.04	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	367	MET	C-N-CA	5.08	127.04	120.44
12	l	200	ASP	N-CA-C	-5.08	99.99	110.80
7	G	56	SER	O-C-N	-5.08	117.93	123.26
15	W	137	VAL	N-CA-C	-5.08	101.17	108.48
23	P	230	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
28	H	205	ASP	CA-C-N	5.08	130.04	122.99
28	H	205	ASP	C-N-CA	5.08	130.04	122.99
29	I	303	GLN	OE1-CD-NE2	-5.08	117.52	122.60
33	J	134	VAL	CB-CA-C	-5.08	105.29	112.14
33	J	398	ILE	O-C-N	5.08	128.91	122.57
1	a	168	ALA	CA-C-O	5.07	126.66	121.23
12	l	212	TYR	N-CA-C	5.07	116.81	111.28
15	W	124	GLU	CA-C-N	5.07	129.19	120.72
15	W	124	GLU	C-N-CA	5.07	129.19	120.72
17	T	110	LEU	CA-C-N	5.07	127.50	120.29
17	T	110	LEU	C-N-CA	5.07	127.50	120.29
20	Z	195	PHE	CA-CB-CG	-5.07	108.73	113.80
20	Z	258	PRO	CB-CA-C	5.07	117.11	110.92
22	S	205	ASN	N-CA-CB	5.07	117.67	110.16
23	P	3	ARG	NE-CZ-NH2	-5.07	114.63	119.20
24	Q	227	CYS	O-C-N	5.07	127.50	122.12
29	I	115	ASP	CA-CB-CG	5.07	117.67	112.60
32	M	66	LYS	CG-CD-CE	5.07	122.97	111.30
32	M	125	GLN	CA-C-O	5.07	127.46	121.58
13	m	92	LEU	CA-C-O	5.07	126.01	120.58
14	7	102	ASP	CB-CA-C	-5.07	99.82	110.17
1	a	62	LYS	N-CA-C	-5.07	106.68	112.92
2	B	54	PRO	N-CA-C	-5.07	106.93	113.57
2	B	164	ILE	N-CA-CB	5.07	119.60	111.23
3	C	162	ALA	N-CA-C	-5.07	100.75	108.76
20	Z	909	ARG	CA-C-N	5.07	124.68	119.05
20	Z	909	ARG	C-N-CA	5.07	124.68	119.05
21	N	365	PHE	N-CA-C	5.07	116.89	111.36
21	N	715	ILE	N-CA-CB	5.07	117.14	111.21
24	Q	115	ILE	N-CA-C	-5.07	105.55	110.42
25	R	242	GLU	CA-C-N	5.07	130.19	121.87
25	R	242	GLU	C-N-CA	5.07	130.19	121.87
30	K	384	ALA	N-CA-C	5.07	116.81	111.28
1	a	15	HIS	O-C-N	5.07	128.93	123.10
27	O	126	ILE	CA-C-N	5.07	127.03	120.44
27	O	126	ILE	C-N-CA	5.07	127.03	120.44
28	H	136	ALA	N-CA-CB	5.07	119.06	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	199	GLU	N-CA-CB	5.07	117.66	110.16
4	d	186	ALA	CA-C-O	-5.07	115.05	120.42
5	e	136	ARG	CG-CD-NE	-5.07	100.85	112.00
9	i	171	TRP	CB-CG-CD1	5.07	134.50	126.90
12	l	101	VAL	O-C-N	5.07	129.03	123.10
14	n	115	ASP	N-CA-CB	5.07	118.25	110.95
4	D	67	ILE	CA-C-O	-5.07	115.43	121.05
7	G	68	GLN	OE1-CD-NE2	5.07	127.67	122.60
7	G	223	GLU	N-CA-C	-5.07	106.51	113.30
9	2	70	ILE	N-CA-C	-5.07	100.35	107.75
9	2	91	ASN	OD1-CG-ND2	5.07	127.67	122.60
20	Z	898	HIS	ND1-CE1-NE2	5.07	113.47	108.40
23	P	53	ALA	CA-C-O	5.07	125.80	119.97
28	H	409	ARG	CA-C-N	5.07	127.48	120.29
28	H	409	ARG	C-N-CA	5.07	127.48	120.29
33	J	373	ARG	CB-CG-CD	5.07	122.95	111.30
4	d	148	TYR	N-CA-CB	5.07	119.83	111.62
11	k	151	ASP	N-CA-CB	5.07	118.96	110.85
4	D	57	THR	N-CA-C	-5.07	108.84	114.62
9	2	97	LEU	CB-CA-C	-5.07	102.38	110.79
9	2	114	GLN	CG-CD-NE2	-5.07	108.80	116.40
10	3	55	GLY	CA-C-N	5.07	128.52	121.02
10	3	55	GLY	C-N-CA	5.07	128.52	121.02
14	7	219	TYR	CB-CA-C	-5.07	102.93	110.88
20	Z	435	GLN	CA-C-N	5.07	127.07	120.28
20	Z	435	GLN	C-N-CA	5.07	127.07	120.28
21	N	242	PHE	CA-CB-CG	-5.07	108.73	113.80
26	U	210	TYR	N-CA-C	-5.07	105.67	111.14
32	M	198	VAL	CB-CA-C	-5.07	105.23	112.22
8	1	66	ASP	CB-CA-C	-5.06	102.38	110.79
21	N	753	PHE	CA-CB-CG	-5.06	108.74	113.80
22	S	279	ILE	N-CA-C	5.06	115.29	110.53
23	P	60	ALA	N-CA-CB	5.06	117.66	110.16
26	U	45	THR	CA-C-O	5.06	126.36	120.49
28	H	351	VAL	N-CA-C	-5.06	100.36	107.75
7	g	65	VAL	N-CA-C	-5.06	98.81	109.34
10	j	75	LYS	N-CA-CB	5.06	117.56	110.12
4	D	74	SER	CA-C-O	-5.06	115.54	121.46
15	W	30	ILE	CA-C-N	5.06	127.48	120.29
15	W	30	ILE	C-N-CA	5.06	127.48	120.29
21	N	324	LYS	N-CA-C	-5.06	106.95	113.02
21	N	681	ASN	N-CA-C	-5.06	105.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	97	ILE	CA-C-O	-5.06	115.48	120.85
23	P	302	LEU	N-CA-C	-5.06	105.95	111.82
32	M	357	ARG	NE-CZ-NH2	-5.06	114.64	119.20
4	d	74	SER	N-CA-C	-5.06	101.85	109.85
1	A	114	CYS	CA-C-N	5.06	127.48	120.29
1	A	114	CYS	C-N-CA	5.06	127.48	120.29
17	T	32	ILE	N-CA-C	5.06	115.83	110.72
21	N	17	GLN	CA-CB-CG	5.06	124.22	114.10
24	Q	240	PHE	CA-C-O	5.06	126.13	120.82
28	H	148	ASN	O-C-N	5.06	129.23	123.31
31	L	376	PHE	CA-C-N	5.06	127.37	120.54
31	L	376	PHE	C-N-CA	5.06	127.37	120.54
3	c	96	GLN	OE1-CD-NE2	5.06	127.66	122.60
5	e	99	HIS	O-C-N	5.06	127.48	122.12
6	F	114	ASP	CA-C-N	5.06	127.06	120.28
6	F	114	ASP	C-N-CA	5.06	127.06	120.28
6	F	163	ALA	CB-CA-C	-5.06	101.77	110.22
20	Z	807	VAL	CA-C-O	5.06	126.21	120.85
21	N	713	VAL	N-CA-CB	5.06	118.11	112.34
22	S	32	GLN	O-C-N	-5.06	116.76	122.12
22	S	173	LEU	CA-C-O	-5.06	115.62	121.19
27	O	216	ASP	CA-CB-CG	-5.06	107.54	112.60
28	H	379	LEU	CA-C-O	-5.06	115.46	119.71
11	4	78	GLN	OE1-CD-NE2	-5.06	117.54	122.60
13	6	127	LYS	CA-C-O	-5.06	115.19	121.11
20	Z	87	LYS	CA-C-N	5.06	124.55	119.19
20	Z	87	LYS	C-N-CA	5.06	124.55	119.19
24	Q	361	HIS	CG-CD2-NE2	5.06	112.26	107.20
30	K	237	VAL	N-CA-C	5.06	119.86	109.34
30	K	241	GLU	CA-C-N	5.06	128.69	120.60
30	K	241	GLU	C-N-CA	5.06	128.69	120.60
30	K	402	ILE	N-CA-C	-5.06	101.20	108.53
6	F	203	ASP	N-CA-C	-5.06	105.97	113.40
11	4	48	GLY	N-CA-C	-5.06	103.53	110.20
20	Z	336	SER	CB-CA-C	-5.06	102.25	110.85
27	O	72	LYS	CB-CG-CD	5.06	122.93	111.30
2	b	51	SER	CA-C-O	-5.05	115.06	120.42
6	f	130	VAL	N-CA-C	-5.05	100.62	108.81
6	f	174	ARG	N-CA-C	5.05	116.87	111.36
11	k	98	TYR	N-CA-C	-5.05	99.75	108.69
16	V	249	GLU	O-C-N	-5.05	116.39	122.15
20	Z	243	GLN	OE1-CD-NE2	5.05	127.65	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	260	GLN	CA-C-N	5.05	127.60	120.42
24	Q	260	GLN	C-N-CA	5.05	127.60	120.42
24	Q	290	THR	N-CA-C	-5.05	105.85	111.36
25	R	238	PHE	CA-CB-CG	5.05	118.85	113.80
5	e	209	GLU	N-CA-C	-5.05	106.43	112.59
13	m	58	ILE	N-CA-C	-5.05	100.29	107.77
4	D	209	ASN	N-CA-CB	-5.05	103.18	110.56
11	4	121	TYR	CA-C-N	5.05	127.47	120.29
11	4	121	TYR	C-N-CA	5.05	127.47	120.29
4	d	36	VAL	CA-CB-CG2	-5.05	101.81	110.40
9	i	145	HIS	CA-C-O	5.05	125.48	119.67
2	B	151	ASP	CA-CB-CG	-5.05	107.55	112.60
4	D	146	LYS	CA-C-O	5.05	126.66	120.60
16	V	245	VAL	N-CA-CB	5.05	117.04	110.57
16	V	274	GLN	N-CA-CB	5.05	119.03	110.49
21	N	826	GLU	CA-C-N	5.05	127.46	120.29
21	N	826	GLU	C-N-CA	5.05	127.46	120.29
29	I	431	ASN	OD1-CG-ND2	5.05	127.65	122.60
30	K	334	LEU	O-C-N	5.05	129.31	122.59
32	M	33	ARG	CD-NE-CZ	-5.05	117.33	124.40
14	n	206	ALA	O-C-N	5.05	127.47	122.12
12	5	133	TRP	CE2-CD2-CE3	5.05	123.85	118.80
19	Y	41	ASP	N-CA-C	-5.05	107.17	113.38
21	N	477	SER	CB-CA-C	-5.05	99.90	109.95
25	R	170	VAL	N-CA-CB	-5.05	103.67	110.54
30	K	121	ARG	N-CA-CB	5.05	117.78	109.95
32	M	101	THR	CA-CB-OG1	5.05	117.17	109.60
3	c	142	ASP	N-CA-C	-5.05	107.62	112.97
6	F	180	ILE	N-CA-C	5.05	115.82	110.72
9	2	138	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
20	Z	230	ILE	CB-CA-C	-5.05	105.25	112.22
21	N	47	GLU	N-CA-C	-5.05	105.78	111.28
29	I	78	ASN	CB-CA-C	-5.05	102.41	110.79
4	d	129	PHE	N-CA-CB	5.05	117.46	110.04
7	g	178	LYS	CA-C-N	5.05	127.04	120.28
7	g	178	LYS	C-N-CA	5.05	127.04	120.28
14	n	91	SER	CA-C-O	5.05	125.90	120.55
21	N	482	ALA	CB-CA-C	-5.05	102.41	110.79
22	S	135	ASN	N-CA-C	5.05	116.86	111.36
22	S	208	ILE	CA-CB-CG1	-5.05	101.82	110.40
24	Q	135	HIS	CA-CB-CG	5.05	118.85	113.80
25	R	216	ILE	CA-C-O	5.05	125.92	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	349	SER	N-CA-CB	5.05	118.62	110.85
27	O	200	GLU	CB-CG-CD	-5.05	104.02	112.60
28	H	46	ALA	CB-CA-C	-5.05	102.96	110.88
28	H	134	THR	N-CA-C	-5.05	107.12	113.28
30	K	353	PHE	CA-C-N	5.05	126.45	120.14
30	K	353	PHE	C-N-CA	5.05	126.45	120.14
32	M	410	VAL	N-CA-CB	-5.05	102.22	111.91
32	M	427	SER	N-CA-C	5.05	116.86	111.36
7	G	96	ALA	N-CA-C	-5.04	105.78	111.28
24	Q	100	LEU	N-CA-C	5.04	116.47	111.07
33	J	70	SER	N-CA-C	-5.04	101.62	109.24
6	f	80	ASP	CA-CB-CG	-5.04	107.56	112.60
11	k	47	ALA	O-C-N	-5.04	117.96	123.26
12	l	113	ASN	CA-CB-CG	-5.04	107.56	112.60
12	l	228	ALA	CA-C-N	5.04	127.00	120.44
12	l	228	ALA	C-N-CA	5.04	127.00	120.44
2	B	80	PRO	CB-CA-C	-5.04	104.98	112.55
10	3	68	ARG	CA-C-N	5.04	127.00	120.44
10	3	68	ARG	C-N-CA	5.04	127.00	120.44
11	4	31	SER	CA-C-O	-5.04	112.69	120.81
14	7	210	ILE	N-CA-CB	5.04	116.45	110.55
16	V	196	TYR	CB-CG-CD1	-5.04	113.24	120.80
20	Z	739	ALA	N-CA-C	5.04	116.78	111.28
24	Q	274	LEU	CA-C-O	-5.04	114.91	120.36
28	H	467	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	a	68	THR	CA-CB-OG1	5.04	117.16	109.60
3	c	52	VAL	N-CA-CB	5.04	121.69	112.36
11	k	41	HIS	CB-CG-CD2	-5.04	124.65	131.20
5	E	165	TYR	CB-CG-CD2	5.04	128.36	120.80
22	S	427	ILE	N-CA-C	-5.04	108.06	112.90
23	P	390	TYR	N-CA-C	-5.04	100.24	108.76
27	O	236	HIS	CA-C-N	5.04	126.14	119.84
27	O	236	HIS	C-N-CA	5.04	126.14	119.84
27	O	286	PHE	CA-CB-CG	-5.04	108.76	113.80
5	E	151	ASP	CA-CB-CG	-5.04	107.56	112.60
11	4	88	LEU	CA-C-N	5.04	127.45	120.29
11	4	88	LEU	C-N-CA	5.04	127.45	120.29
13	6	216	THR	N-CA-C	-5.04	101.75	109.41
19	Y	5	VAL	CB-CA-C	5.04	116.67	111.23
22	S	117	SER	CA-C-N	5.04	131.17	121.54
22	S	117	SER	C-N-CA	5.04	131.17	121.54
24	Q	129	LYS	CB-CA-C	-5.04	98.85	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	79	SER	O-C-N	-5.04	116.06	122.26
30	K	225	ALA	N-CA-C	-5.04	105.87	111.36
9	i	41	VAL	CB-CA-C	5.04	118.81	111.80
2	B	170	ALA	CA-C-O	-5.04	115.08	120.42
8	1	82	PRO	CA-C-N	5.04	132.16	122.03
8	1	82	PRO	C-N-CA	5.04	132.16	122.03
20	Z	883	THR	N-CA-CB	5.04	118.75	110.39
22	S	55	ARG	NE-CZ-NH2	5.04	123.73	119.20
22	S	60	LEU	CB-CA-C	-5.04	102.94	110.90
24	Q	416	VAL	O-C-N	5.04	127.02	121.83
26	U	252	HIS	CA-C-N	5.04	127.44	120.29
26	U	252	HIS	C-N-CA	5.04	127.44	120.29
30	K	74	HIS	CA-C-O	5.04	125.89	120.55
31	L	426	LYS	CB-CA-C	-5.04	102.94	110.90
33	J	386	VAL	CA-C-O	-5.04	115.71	120.95
7	g	68	GLN	OE1-CD-NE2	-5.04	117.56	122.60
21	N	102	VAL	CA-C-N	5.04	126.99	120.44
21	N	102	VAL	C-N-CA	5.04	126.99	120.44
23	P	117	SER	CA-C-O	-5.04	115.21	120.55
28	H	272	ILE	CB-CA-C	5.04	117.22	110.42
29	I	230	THR	N-CA-C	-5.04	107.08	113.18
30	K	298	GLU	CA-C-O	-5.04	114.18	119.97
30	K	300	LEU	CB-CA-C	-5.04	102.43	110.79
1	a	247	ALA	N-CA-CB	5.04	117.31	110.01
1	A	212	ASP	O-C-N	5.04	127.26	122.07
14	7	208	GLU	CA-CB-CG	5.04	124.17	114.10
16	V	291	ASN	N-CA-C	-5.04	106.99	113.23
24	Q	270	ILE	O-C-N	5.04	127.02	121.83
27	O	214	ALA	CB-CA-C	-5.04	102.12	110.68
29	I	432	LEU	N-CA-CB	5.04	117.37	110.07
2	b	88	LYS	CB-CA-C	-5.03	101.00	110.67
5	e	136	ARG	CA-C-N	5.03	125.02	119.89
5	e	136	ARG	C-N-CA	5.03	125.02	119.89
6	f	69	HIS	CA-C-O	-5.03	113.31	120.51
13	6	19	THR	CA-C-N	5.03	130.63	122.68
13	6	19	THR	C-N-CA	5.03	130.63	122.68
14	7	118	GLU	N-CA-C	-5.03	104.88	112.99
19	Y	86	ARG	CA-C-N	5.03	127.53	120.28
19	Y	86	ARG	C-N-CA	5.03	127.53	120.28
20	Z	442	VAL	O-C-N	-5.03	117.36	122.95
20	Z	542	ILE	CA-C-O	-5.03	115.84	121.23
21	N	88	ARG	N-CA-CB	5.03	119.00	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	194	SER	N-CA-CB	5.03	119.00	110.49
2	b	137	ALA	N-CA-CB	5.03	119.59	110.83
20	Z	501	LYS	CA-C-N	5.03	127.86	120.71
20	Z	501	LYS	C-N-CA	5.03	127.86	120.71
23	P	246	GLN	CA-C-O	5.03	125.57	119.38
10	j	192	LYS	N-CA-CB	5.03	118.99	110.49
13	m	178	LYS	N-CA-C	-5.03	101.98	109.42
3	C	70	ASN	N-CA-C	-5.03	100.49	108.14
10	3	21	VAL	N-CA-C	-5.03	100.65	108.95
19	Y	65	ASP	N-CA-C	-5.03	107.16	113.15
21	N	228	VAL	N-CA-C	-5.03	105.64	110.72
31	L	124	GLY	CA-C-N	5.03	125.02	119.89
31	L	124	GLY	C-N-CA	5.03	125.02	119.89
4	d	188	VAL	N-CA-C	-5.03	105.94	110.82
20	Z	635	ALA	CB-CA-C	-5.03	102.96	110.50
25	R	217	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
18	X	105	ASN	OD1-CG-ND2	5.03	127.63	122.60
20	Z	218	GLU	N-CA-CB	5.03	118.73	110.39
21	N	459	ASN	CA-CB-CG	-5.03	107.57	112.60
23	P	380	ILE	CA-C-N	5.03	127.43	120.29
23	P	380	ILE	C-N-CA	5.03	127.43	120.29
32	M	230	LEU	CA-C-N	5.03	127.43	120.29
32	M	230	LEU	C-N-CA	5.03	127.43	120.29
32	M	231	LEU	CA-C-N	5.03	127.28	120.44
32	M	231	LEU	C-N-CA	5.03	127.28	120.44
32	M	335	PRO	CA-C-N	5.03	127.43	120.29
32	M	335	PRO	C-N-CA	5.03	127.43	120.29
32	M	383	THR	N-CA-C	-5.03	103.02	110.46
33	J	251	ASP	O-C-N	-5.03	116.99	122.67
6	f	203	ASP	CA-CB-CG	-5.03	107.57	112.60
9	i	202	VAL	N-CA-C	-5.03	101.17	108.36
3	C	199	LYS	CA-C-O	5.03	125.75	120.42
4	D	34	VAL	N-CA-C	-5.03	101.01	108.45
6	F	76	GLY	CA-C-N	5.03	128.24	121.05
6	F	76	GLY	C-N-CA	5.03	128.24	121.05
7	G	64	ASN	O-C-N	-5.03	117.06	123.24
10	3	188	TYR	CA-CB-CG	-5.03	104.85	113.90
13	6	176	VAL	N-CA-CB	5.03	119.68	111.44
20	Z	771	HIS	CA-CB-CG	-5.03	108.78	113.80
20	Z	827	LEU	CA-C-N	5.03	127.01	120.28
20	Z	827	LEU	C-N-CA	5.03	127.01	120.28
21	N	473	ASP	N-CA-CB	5.03	118.98	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	133	LEU	O-C-N	5.03	127.25	122.07
12	l	100	TRP	CA-CB-CG	5.02	123.14	113.60
2	B	239	THR	CA-C-N	5.02	127.01	120.28
2	B	239	THR	C-N-CA	5.02	127.01	120.28
17	T	143	SER	CA-C-N	5.02	127.21	120.58
17	T	143	SER	C-N-CA	5.02	127.21	120.58
20	Z	606	CYS	CA-C-N	5.02	127.01	120.28
20	Z	606	CYS	C-N-CA	5.02	127.01	120.28
21	N	476	THR	CA-C-O	5.02	124.35	118.77
22	S	388	ILE	N-CA-C	-5.02	105.81	110.53
30	K	77	ARG	CA-C-O	-5.02	114.19	119.97
9	i	194	ASN	OD1-CG-ND2	-5.02	117.58	122.60
3	C	130	PRO	N-CA-C	-5.02	103.88	111.41
6	F	183	ASP	CA-C-N	5.02	130.06	121.07
6	F	183	ASP	C-N-CA	5.02	130.06	121.07
8	1	182	ILE	N-CA-CB	5.02	117.49	111.31
9	2	235	PRO	CA-C-N	5.02	128.00	120.87
9	2	235	PRO	C-N-CA	5.02	128.00	120.87
17	T	148	LEU	O-C-N	5.02	127.24	122.07
24	Q	311	LEU	CA-C-N	5.02	127.42	120.29
24	Q	311	LEU	C-N-CA	5.02	127.42	120.29
26	U	248	ASP	N-CA-C	5.02	116.75	111.28
7	g	34	GLY	CA-C-N	5.02	128.60	121.42
7	g	34	GLY	C-N-CA	5.02	128.60	121.42
12	l	284	ASN	CA-CB-CG	-5.02	107.58	112.60
3	C	133	VAL	CA-C-O	5.02	125.90	120.43
10	3	49	VAL	CA-C-O	-5.02	115.00	120.72
2	b	71	ILE	CA-CB-CG1	5.02	118.93	110.40
3	c	158	THR	N-CA-CB	5.02	120.22	111.13
4	d	77	GLY	N-CA-C	-5.02	103.86	110.29
4	d	113	VAL	CA-C-O	5.02	126.17	120.85
4	d	192	VAL	CB-CA-C	-5.02	105.29	112.22
2	B	27	ALA	CA-C-N	5.02	127.07	120.60
2	B	27	ALA	C-N-CA	5.02	127.07	120.60
14	7	87	SER	O-C-N	-5.02	115.81	122.74
20	Z	110	ASN	CA-C-O	5.02	125.74	120.42
26	U	16	LEU	CA-C-N	5.02	129.16	120.58
26	U	16	LEU	C-N-CA	5.02	129.16	120.58
27	O	114	GLN	CA-C-N	5.02	127.01	120.28
27	O	114	GLN	C-N-CA	5.02	127.01	120.28
27	O	118	GLY	N-CA-C	-5.02	108.32	115.30
27	O	282	GLN	OE1-CD-NE2	5.02	127.62	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	53	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
3	c	185	LYS	CA-C-N	5.02	127.33	120.46
3	c	185	LYS	C-N-CA	5.02	127.33	120.46
4	d	58	ARG	O-C-N	5.02	128.11	122.19
7	g	56	SER	CA-C-N	-5.02	114.62	122.65
7	g	56	SER	C-N-CA	-5.02	114.62	122.65
5	E	61	SER	CA-C-O	5.02	125.22	119.35
10	3	90	LEU	CA-C-N	5.02	126.88	120.56
10	3	90	LEU	C-N-CA	5.02	126.88	120.56
16	V	215	ASN	N-CA-CB	5.02	117.42	110.04
16	V	290	ASN	CA-C-O	-5.02	115.23	120.55
17	T	190	ALA	CA-C-O	-5.02	115.21	120.63
31	L	279	PHE	CA-C-N	5.02	130.30	122.17
31	L	279	PHE	C-N-CA	5.02	130.30	122.17
1	A	114	CYS	N-CA-C	-5.02	105.26	111.33
4	D	10	ILE	N-CA-C	-5.02	100.90	108.12
8	1	187	LEU	CB-CA-C	-5.02	102.66	110.74
13	6	96	SER	CA-C-O	-5.02	115.10	120.42
21	N	607	GLN	CA-C-N	5.02	127.41	120.29
21	N	607	GLN	C-N-CA	5.02	127.41	120.29
21	N	849	THR	CA-C-N	5.02	130.76	122.33
21	N	849	THR	C-N-CA	5.02	130.76	122.33
24	Q	132	PHE	N-CA-CB	5.02	117.41	109.94
30	K	382	VAL	O-C-N	-5.02	117.00	121.87
32	M	50	ARG	CD-NE-CZ	5.02	131.42	124.40
7	g	246	GLU	CB-CG-CD	-5.01	104.08	112.60
10	j	167	ILE	CA-C-O	5.01	125.89	120.47
14	n	43	SER	N-CA-CB	5.01	118.96	110.49
1	A	160	ALA	CA-C-O	5.01	125.71	119.79
6	F	176	LEU	N-CA-C	5.01	117.40	111.33
8	1	166	HIS	CA-C-N	5.01	127.00	120.28
8	1	166	HIS	C-N-CA	5.01	127.00	120.28
11	4	190	ARG	CA-C-N	5.01	130.06	122.99
11	4	190	ARG	C-N-CA	5.01	130.06	122.99
20	Z	34	GLU	O-C-N	-5.01	116.63	123.15
20	Z	360	SER	CB-CA-C	-5.01	102.32	110.85
22	S	102	SER	O-C-N	5.01	129.13	122.41
23	P	395	ARG	CA-C-N	5.01	126.11	119.84
23	P	395	ARG	C-N-CA	5.01	126.11	119.84
25	R	147	LYS	N-CA-C	-5.01	106.33	112.90
28	H	62	ARG	CA-C-N	5.01	127.54	120.42
28	H	62	ARG	C-N-CA	5.01	127.54	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	202	GLU	N-CA-C	-5.01	101.52	109.59
2	B	241	GLN	CG-CD-NE2	5.01	123.92	116.40
29	I	396	CYS	CA-C-O	-5.01	115.11	120.42
8	h	105	GLY	CA-C-O	-5.01	116.50	120.81
12	l	286	ILE	N-CA-CB	5.01	118.30	112.33
2	B	71	ILE	O-C-N	5.01	127.48	122.97
3	C	156	ASN	OD1-CG-ND2	5.01	127.61	122.60
17	T	138	ASP	CB-CA-C	-5.01	110.82	116.63
20	Z	345	GLU	N-CA-C	5.01	116.55	111.14
20	Z	523	ALA	CA-C-N	5.01	127.00	120.28
20	Z	523	ALA	C-N-CA	5.01	127.00	120.28
21	N	17	GLN	OE1-CD-NE2	5.01	127.61	122.60
22	S	106	GLY	CA-C-N	5.01	128.87	120.70
22	S	106	GLY	C-N-CA	5.01	128.87	120.70
22	S	391	GLY	O-C-N	5.01	127.74	122.28
23	P	103	TYR	CA-C-O	-5.01	115.56	120.82
24	Q	244	GLU	CA-C-N	5.01	126.96	120.44
24	Q	244	GLU	C-N-CA	5.01	126.96	120.44
27	O	203	THR	N-CA-C	5.01	116.80	110.33
31	L	309	LEU	N-CA-CB	5.01	117.49	110.12
7	g	120	VAL	O-C-N	-5.01	116.67	121.83
14	n	237	THR	N-CA-C	-5.01	108.44	114.75
2	B	35	LEU	CA-C-O	-5.01	115.87	121.23
2	B	158	PRO	O-C-N	-5.01	116.82	123.13
6	F	10	THR	N-CA-C	-5.01	106.09	113.61
7	G	24	VAL	CB-CA-C	-5.01	104.15	112.26
7	G	37	SER	N-CA-C	-5.01	100.55	109.06
20	Z	564	ARG	CA-C-O	5.01	125.80	120.24
21	N	866	TYR	CA-C-O	-5.01	115.74	121.40
25	R	64	LYS	CB-CA-C	-5.01	102.47	110.79
25	R	67	CYS	CA-C-N	5.01	126.95	120.44
25	R	67	CYS	C-N-CA	5.01	126.95	120.44
33	J	253	ILE	CA-C-N	5.01	129.92	122.05
33	J	253	ILE	C-N-CA	5.01	129.92	122.05
5	e	92	ALA	CB-CA-C	-5.01	101.06	110.67
30	K	400	TYR	N-CA-CB	5.01	119.21	110.65
31	L	71	ASP	O-C-N	-5.01	116.81	122.12
3	c	170	SER	N-CA-C	5.01	116.74	111.28
4	d	141	ARG	N-CA-C	-5.01	106.76	112.92
5	e	100	ASN	N-CA-CB	5.01	117.93	110.22
5	e	223	THR	CA-C-N	5.01	127.40	120.29
5	e	223	THR	C-N-CA	5.01	127.40	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	165	GLU	CA-C-N	5.01	127.25	120.44
10	j	165	GLU	C-N-CA	5.01	127.25	120.44
11	k	46	PHE	CD1-CG-CD2	5.01	126.11	118.60
4	D	184	PRO	CA-C-N	5.01	125.79	119.98
4	D	184	PRO	C-N-CA	5.01	125.79	119.98
4	D	226	SER	N-CA-CB	5.01	118.04	110.28
12	5	113	ASN	N-CA-CB	5.01	119.28	110.37
12	5	279	GLU	N-CA-C	-5.01	107.22	113.38
17	T	52	LEU	CA-C-N	5.01	127.40	120.29
17	T	52	LEU	C-N-CA	5.01	127.40	120.29
20	Z	24	THR	CA-CB-OG1	-5.01	102.09	109.60
20	Z	51	LEU	CA-C-N	5.01	126.95	120.44
20	Z	51	LEU	C-N-CA	5.01	126.95	120.44
20	Z	207	ILE	CA-C-O	5.01	124.51	119.20
26	U	223	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
29	I	343	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
29	I	394	ALA	CA-C-O	-5.01	115.56	120.82
30	K	137	VAL	CB-CA-C	5.01	118.46	111.40
8	h	87	ALA	O-C-N	5.00	127.22	122.07
4	D	141	ARG	O-C-N	5.00	129.64	122.13
12	5	84	GLN	OE1-CD-NE2	5.00	127.61	122.60
15	W	176	PRO	CA-C-N	5.00	129.73	121.87
15	W	176	PRO	C-N-CA	5.00	129.73	121.87
17	T	94	HIS	CA-C-N	5.00	129.66	122.40
17	T	94	HIS	C-N-CA	5.00	129.66	122.40
32	M	49	GLN	O-C-N	-5.00	116.11	122.27
11	k	133	HIS	ND1-CE1-NE2	5.00	113.40	108.40
13	m	141	ARG	CA-C-O	-5.00	114.69	120.49
5	E	35	SER	CA-C-O	5.00	126.75	121.05
16	V	237	ASN	OD1-CG-ND2	-5.00	117.60	122.60
17	T	40	LEU	CA-C-N	5.00	131.39	122.13
17	T	40	LEU	C-N-CA	5.00	131.39	122.13
31	L	204	PRO	CA-C-N	5.00	126.98	120.28
31	L	204	PRO	C-N-CA	5.00	126.98	120.28
2	b	90	ARG	NE-CZ-NH2	5.00	123.70	119.20
6	f	135	ILE	O-C-N	5.00	128.28	123.03
14	n	248	GLU	CA-C-O	5.00	127.38	121.58
7	G	135	SER	N-CA-C	-5.00	102.67	110.42
14	7	155	ASN	CA-C-O	5.00	124.32	118.97
18	X	78	ILE	N-CA-C	-5.00	101.28	108.48
24	Q	246	TYR	CA-C-O	5.00	125.72	120.42
25	R	32	LEU	O-C-N	5.00	127.42	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	176	SER	N-CA-C	-5.00	103.41	110.31
30	K	74	HIS	N-CA-CB	5.00	117.47	110.12
32	M	205	ASP	O-C-N	5.00	127.22	122.07
33	J	130	ALA	CA-C-N	5.00	131.03	122.38
33	J	130	ALA	C-N-CA	5.00	131.03	122.38

There are no chirality outliers.

All (353) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	111	TYR	Sidechain
8	1	17	PHE	Sidechain
8	1	198	TYR	Sidechain
8	1	202	TYR	Sidechain
8	1	34	TYR	Sidechain
8	1	79	TYR	Sidechain
9	2	101	ARG	Sidechain
9	2	104	ARG	Sidechain
9	2	117	PHE	Sidechain
9	2	215	TYR	Sidechain
9	2	225	ARG	Sidechain
9	2	236	ARG	Sidechain
10	3	154	TYR	Sidechain
10	3	177	ARG	Sidechain
10	3	28	ARG	Sidechain
10	3	50	PHE	Sidechain
10	3	69	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	147	HIS	Sidechain
11	4	176	PHE	Sidechain
11	4	23	ARG	Sidechain
11	4	70	ARG	Sidechain
11	4	73	TYR	Sidechain
11	4	95	ARG	Sidechain
12	5	179	TYR	Sidechain
12	5	202	PHE	Sidechain
12	5	210	PHE	Sidechain
12	5	242	ARG	Sidechain
13	6	13	TYR	Sidechain
13	6	131	TYR	Sidechain
13	6	182	TYR	Sidechain
13	6	221	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	6	225	TYR	Sidechain
13	6	41	TYR	Sidechain
13	6	83	TYR	Sidechain
14	7	124	TYR	Sidechain
14	7	126	PHE	Sidechain
14	7	194	ARG	Sidechain
14	7	226	ARG	Sidechain
14	7	261	TYR	Sidechain
14	7	49	TYR	Sidechain
1	A	105	ARG	Sidechain
1	A	106	TYR	Sidechain
1	A	11	GLY	Peptide
1	A	12	TYR	Sidechain,Peptide
1	A	131	ARG	Sidechain
1	A	186	PHE	Sidechain
1	A	30	TYR	Sidechain
1	A	46	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	156	TYR	Sidechain
2	B	204	PHE	Sidechain
2	B	23	TYR	Sidechain
2	B	235	PHE	Sidechain
2	B	236	ARG	Sidechain
2	B	4	ARG	Sidechain
2	B	75	TYR	Sidechain
3	C	149	TYR	Sidechain
3	C	230	PHE	Sidechain
4	D	108	TYR	Sidechain
4	D	120	TYR	Sidechain
4	D	127	ARG	Sidechain
4	D	166	ARG	Sidechain
4	D	232	TYR	Sidechain
4	D	48	ARG	Sidechain
4	D	83	ARG	Sidechain
5	E	136	ARG	Sidechain
5	E	166	ARG	Sidechain
5	E	167	TYR	Sidechain
5	E	53	ARG	Sidechain
5	E	8	TYR	Sidechain
6	F	123	TYR	Sidechain
6	F	128	TYR	Sidechain
6	F	137	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	F	174	ARG	Sidechain
6	F	225	TYR	Sidechain
6	F	4	ASN	Peptide
6	F	82	ARG	Sidechain
6	F	94	TYR	Sidechain
7	G	242	PHE	Sidechain
28	H	145	TYR	Sidechain
28	H	181	TYR	Sidechain
28	H	208	TYR	Sidechain
28	H	266	ARG	Sidechain
28	H	283	TYR	Sidechain
28	H	292	ARG	Sidechain
28	H	331	ARG	Sidechain
28	H	344	ASP	Peptide
28	H	377	PHE	Sidechain
28	H	403	ARG	Sidechain
28	H	435	ARG	Sidechain
28	H	72	SER	Peptide
28	H	95	HIS	Sidechain
29	I	222	TYR	Sidechain
29	I	245	LEU	Peptide
29	I	246	ARG	Peptide
29	I	316	PHE	Sidechain
29	I	339	ILE	Peptide
29	I	340	ARG	Peptide
29	I	342	GLY	Peptide
29	I	345	ASP	Peptide
29	I	350	PHE	Sidechain
29	I	426	ASN	Peptide
29	I	64	ARG	Sidechain
33	J	116	ARG	Sidechain
33	J	210	PHE	Sidechain,Peptide
33	J	231	ARG	Sidechain
33	J	238	ARG	Sidechain
33	J	260	GLY	Peptide
33	J	282	PHE	Peptide
33	J	309	ARG	Sidechain,Peptide
33	J	333	ARG	Sidechain
33	J	344	ARG	Sidechain
33	J	368	TYR	Sidechain
33	J	373	ARG	Sidechain
33	J	42	ARG	Sidechain

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Mol	Chain	Res	Type	Group
33	J	56	ARG	Sidechain
33	J	63	ARG	Sidechain
33	J	94	TYR	Sidechain
30	K	128	ARG	Sidechain
30	K	233	ALA	Peptide
30	K	234	PHE	Peptide
30	K	236	ARG	Peptide
30	K	252	ARG	Sidechain
30	K	259	ARG	Sidechain
30	K	281	ARG	Sidechain
30	K	303	MET	Peptide
30	K	329	LEU	Peptide
30	K	330	ARG	Sidechain
30	K	332	GLY	Peptide
30	K	333	ARG	Peptide
30	K	411	TYR	Sidechain
30	K	412	ALA	Peptide
30	K	427	TYR	Sidechain
30	K	58	TYR	Sidechain
30	K	67	TYR	Sidechain
30	K	77	ARG	Sidechain
31	L	126	ARG	Sidechain
31	L	161	ARG	Sidechain
31	L	191	ARG	Sidechain
31	L	221	TYR	Sidechain
31	L	243	PHE	Sidechain
31	L	255	TYR	Sidechain
31	L	269	TYR	Sidechain
31	L	290	ARG	Sidechain
31	L	312	MET	Peptide
31	L	314	GLY	Peptide
31	L	315	PHE	Peptide
31	L	316	ASP	Peptide
31	L	338	LEU	Peptide
31	L	339	ARG	Sidechain,Peptide
31	L	342	ARG	Peptide
31	L	386	PHE	Sidechain
31	L	407	ARG	Sidechain
31	L	62	ARG	Sidechain
31	L	77	ARG	Sidechain
31	L	78	ARG	Sidechain
32	M	172	VAL	Peptide

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Mol	Chain	Res	Type	Group
32	M	213	ARG	Sidechain
32	M	267	PHE	Sidechain
32	M	292	ASP	Mainchain
32	M	342	ARG	Sidechain
32	M	381	ARG	Sidechain
32	M	425	ARG	Sidechain
21	N	109	TYR	Sidechain
21	N	188	TYR	Sidechain
21	N	222	TYR	Sidechain
21	N	242	PHE	Sidechain
21	N	340	HIS	Sidechain
21	N	422	TYR	Sidechain
21	N	463	TYR	Sidechain
21	N	471	TYR	Sidechain
21	N	504	TYR	Sidechain
21	N	559	TYR	Sidechain
21	N	70	TYR	Sidechain
21	N	739	PHE	Sidechain
21	N	743	PHE	Sidechain
21	N	776	TYR	Sidechain
21	N	777	ALA	Peptide
21	N	813	ARG	Sidechain
21	N	861	TYR	Sidechain
21	N	88	ARG	Sidechain
21	N	881	TYR	Sidechain
21	N	889	ARG	Sidechain
21	N	896	PHE	Sidechain
27	O	137	TYR	Sidechain
27	O	178	TYR	Sidechain
27	O	33	TYR	Sidechain
27	O	62	TYR	Sidechain
27	O	98	TYR	Sidechain
23	P	193	TYR	Sidechain
23	P	213	TYR	Sidechain
23	P	220	TYR	Sidechain
23	P	221	TYR	Sidechain
23	P	230	HIS	Sidechain
23	P	232	ARG	Sidechain
23	P	234	TYR	Sidechain
23	P	3	ARG	Sidechain
23	P	318	TYR	Sidechain
23	P	356	TYR	Sidechain

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Mol	Chain	Res	Type	Group
23	P	364	ARG	Sidechain
24	Q	116	PHE	Sidechain
24	Q	145	HIS	Sidechain
24	Q	146	TYR	Sidechain
24	Q	20	TYR	Sidechain
24	Q	209	TYR	Sidechain
24	Q	243	PHE	Sidechain
24	Q	246	TYR	Sidechain
24	Q	27	TYR	Sidechain
24	Q	286	TYR	Sidechain
24	Q	294	ARG	Sidechain
24	Q	306	TYR	Sidechain
24	Q	332	ARG	Sidechain
24	Q	339	TYR	Sidechain
24	Q	400	TYR	Sidechain
25	R	140	TYR	Sidechain
25	R	179	PHE	Sidechain
25	R	181	TYR	Sidechain
25	R	207	ARG	Sidechain
25	R	210	TYR	Sidechain
25	R	246	TYR	Sidechain
25	R	297	TYR	Sidechain
25	R	304	TYR	Sidechain
25	R	321	TYR	Sidechain
25	R	338	TYR	Sidechain
25	R	345	TYR	Sidechain
25	R	400	TYR	Sidechain
25	R	70	TYR	Peptide
22	S	119	TYR	Sidechain
22	S	145	PHE	Sidechain
22	S	185	PHE	Sidechain
22	S	239	ARG	Sidechain
22	S	259	TYR	Sidechain
22	S	346	TYR	Sidechain
22	S	377	TYR	Sidechain
22	S	399	TYR	Sidechain
22	S	421	TYR	Sidechain
22	S	467	PHE	Sidechain
22	S	82	TYR	Sidechain
17	T	186	ARG	Sidechain
17	T	234	TYR	Sidechain
17	T	251	HIS	Peptide

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Mol	Chain	Res	Type	Group
26	U	137	TYR	Sidechain
26	U	254	ARG	Sidechain
26	U	288	PHE	Sidechain
26	U	72	TYR	Sidechain
26	U	93	TYR	Sidechain
16	V	100	ARG	Sidechain
16	V	20	ARG	Sidechain
16	V	251	TYR	Sidechain
16	V	273	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	61	TYR	Sidechain
15	W	148	GLU	Mainchain
15	W	163	ASN	Peptide
15	W	179	ARG	Sidechain
15	W	23	ARG	Sidechain
18	X	17	TYR	Sidechain
18	X	22	ARG	Sidechain
18	X	27	ILE	Peptide
18	X	96	ARG	Sidechain
19	Y	84	TYR	Sidechain
20	Z	103	TYR	Sidechain
20	Z	136	ARG	Sidechain
20	Z	138	ARG	Sidechain
20	Z	195	PHE	Sidechain
20	Z	210	TYR	Sidechain
20	Z	236	PHE	Sidechain
20	Z	323	TYR	Sidechain
20	Z	341	TYR	Sidechain
20	Z	394	TYR	Sidechain
20	Z	441	TYR	Sidechain
20	Z	477	TYR	Sidechain
20	Z	55	ARG	Sidechain
20	Z	608	TYR	Sidechain
20	Z	766	HIS	Sidechain
20	Z	902	TYR	Sidechain
1	a	106	TYR	Sidechain
1	a	11	GLY	Peptide
1	a	12	TYR	Sidechain,Peptide
1	a	135	ARG	Sidechain
1	a	14	ARG	Sidechain
1	a	166	TYR	Sidechain
1	a	19	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	b	128	ARG	Sidechain
2	b	224	TYR	Sidechain
2	b	4	ARG	Sidechain
2	b	6	SER	Peptide
2	b	99	ARG	Sidechain
3	c	113	ARG	Sidechain
3	c	114	ARG	Sidechain
3	c	129	ARG	Peptide
3	c	144	TYR	Sidechain
3	c	180	TYR	Sidechain
3	c	20	TYR	Sidechain
3	c	9	ARG	Sidechain
4	d	111	ARG	Sidechain
4	d	120	TYR	Sidechain
4	d	172	ARG	Sidechain
4	d	174	PHE	Sidechain
4	d	232	TYR	Sidechain
4	d	29	ARG	Sidechain
5	e	156	PHE	Sidechain
5	e	231	TYR	Sidechain
5	e	72	ARG	Sidechain
6	f	126	ARG	Sidechain
6	f	128	TYR	Sidechain
6	f	137	TYR	Sidechain
6	f	171	TYR	Sidechain
6	f	18	ARG	Peptide
6	f	4	ASN	Peptide
6	f	59	TYR	Sidechain
6	f	6	TYR	Sidechain
7	g	112	PHE	Sidechain
7	g	132	PHE	Sidechain
8	h	133	TYR	Sidechain
8	h	183	ARG	Sidechain
8	h	198	TYR	Sidechain
8	h	70	TYR	Sidechain
8	h	75	TYR	Sidechain
9	i	119	TYR	Sidechain
9	i	126	TYR	Sidechain
9	i	152	TYR	Sidechain
9	i	215	TYR	Sidechain
10	j	203	ARG	Sidechain
10	j	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	j	40	PHE	Sidechain
10	j	46	TYR	Sidechain
10	j	99	ARG	Sidechain
11	k	107	TYR	Sidechain
11	k	171	ARG	Sidechain
11	k	195	PHE	Sidechain
11	k	59	TYR	Sidechain
11	k	85	ARG	Sidechain
12	l	139	ARG	Sidechain
12	l	148	ARG	Sidechain
12	l	212	TYR	Sidechain
12	l	230	TYR	Sidechain
12	l	245	TYR	Sidechain
12	l	272	PHE	Sidechain
13	m	103	HIS	Sidechain
13	m	111	PHE	Sidechain
13	m	13	TYR	Sidechain
13	m	41	TYR	Sidechain
14	n	109	TYR	Sidechain
14	n	261	TYR	Sidechain
14	n	63	TYR	Sidechain
14	n	74	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1924	0	1916	8	0
1	a	1924	0	1916	7	0
2	B	1900	0	1910	3	0
2	b	1900	0	1910	3	0
3	C	1884	0	1880	6	0
3	c	1884	0	1880	7	0
4	D	1863	0	1878	8	0
4	d	1986	0	1996	7	0
5	E	1889	0	1856	6	0
5	e	1889	0	1856	6	0
6	F	1784	0	1788	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	1784	0	1788	3	0
7	G	1905	0	1897	6	0
7	g	1905	0	1897	2	0
8	1	1512	0	1478	3	0
8	h	1512	0	1478	3	0
9	2	1720	0	1716	6	0
9	i	1720	0	1716	1	0
10	3	1581	0	1571	6	0
10	j	1581	0	1571	5	0
11	4	1562	0	1569	3	0
11	k	1562	0	1569	6	0
12	5	1644	0	1592	5	0
12	l	1644	0	1592	1	0
13	6	1757	0	1708	5	0
13	m	1757	0	1708	7	0
14	7	1790	0	1790	2	0
14	n	1816	0	1818	6	0
15	W	1535	0	1542	3	0
16	V	2274	0	2273	4	0
17	T	2193	0	2161	6	0
18	X	1033	0	1017	4	0
19	Y	731	0	675	3	0
20	Z	7006	0	6932	44	0
21	N	7158	0	7226	21	0
22	S	3895	0	3938	7	0
23	P	3609	0	3694	8	0
24	Q	3499	0	3524	5	0
25	R	3259	0	3263	8	0
26	U	2427	0	2462	6	0
27	O	3186	0	3213	10	0
28	H	3313	0	3320	11	0
29	I	3022	0	3091	27	0
30	K	3113	0	3168	12	0
31	L	3083	0	3156	7	0
32	M	3285	0	3323	10	0
33	J	3171	0	3312	47	0
34	H	31	0	12	0	0
34	I	31	0	12	0	0
34	J	31	0	12	0	0
34	K	31	0	12	2	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	L	27	0	12	0	0
36	M	27	0	12	0	0
All	All	110555	0	110606	329	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 1.

All (329) 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)
33:J:234:PHE:CE1	33:J:234:PHE:CZ	1.76	1.67
33:J:234:PHE:CZ	33:J:234:PHE:CE2	1.77	1.62
33:J:234:PHE:CE2	33:J:234:PHE:CD2	1.81	1.62
33:J:234:PHE:CD2	33:J:234:PHE:CG	1.81	1.62
33:J:234:PHE:CG	33:J:234:PHE:CD1	1.80	1.62
20:Z:948:TRP:CH2	20:Z:948:TRP:CZ3	2.06	1.40
20:Z:948:TRP:CH2	20:Z:948:TRP:CZ2	2.16	1.31
33:J:234:PHE:CD2	33:J:286:LYS:CD	2.38	1.06
20:Z:738:TYR:CZ	29:I:69:LEU:HB3	1.90	1.06
33:J:234:PHE:CZ	33:J:286:LYS:CD	2.39	1.05
33:J:234:PHE:CG	33:J:286:LYS:CD	2.39	1.05
33:J:234:PHE:CE1	33:J:286:LYS:CD	2.40	1.05
33:J:234:PHE:CE2	33:J:286:LYS:CD	2.40	1.04
33:J:234:PHE:CZ	33:J:286:LYS:CE	2.40	1.04
33:J:234:PHE:CD1	33:J:286:LYS:CD	2.41	1.04
33:J:234:PHE:CE1	33:J:286:LYS:CE	2.41	1.03
33:J:234:PHE:CD2	33:J:286:LYS:CE	2.42	1.03
33:J:234:PHE:CD1	33:J:286:LYS:CE	2.42	1.02
33:J:234:PHE:CG	33:J:286:LYS:CE	2.43	1.02
33:J:234:PHE:CE2	33:J:286:LYS:CE	2.46	0.98
20:Z:738:TYR:OH	29:I:69:LEU:CB	2.15	0.95
20:Z:738:TYR:CZ	29:I:66:LYS:O	2.19	0.95
20:Z:738:TYR:CZ	29:I:66:LYS:HA	2.02	0.94
33:J:234:PHE:CZ	33:J:286:LYS:HD3	2.04	0.89
20:Z:738:TYR:OH	29:I:66:LYS:O	1.90	0.89
33:J:234:PHE:CD2	33:J:286:LYS:HD2	2.07	0.89
20:Z:738:TYR:OH	29:I:65:ILE:O	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:738:TYR:OH	29:I:66:LYS:C	2.18	0.86
33:J:234:PHE:CE1	33:J:286:LYS:HE3	2.11	0.82
20:Z:738:TYR:OH	29:I:69:LEU:HB3	1.79	0.82
20:Z:738:TYR:CE2	29:I:66:LYS:HA	2.14	0.81
33:J:234:PHE:CZ	33:J:286:LYS:HE2	2.16	0.80
33:J:234:PHE:CE2	33:J:286:LYS:HD2	2.20	0.77
33:J:234:PHE:CE2	33:J:286:LYS:HE2	2.20	0.77
20:Z:738:TYR:CZ	20:Z:738:TYR:OH	2.40	0.75
20:Z:738:TYR:CZ	29:I:69:LEU:HD23	2.22	0.75
20:Z:738:TYR:OH	29:I:69:LEU:N	2.21	0.73
33:J:234:PHE:CD1	33:J:286:LYS:HE3	2.20	0.73
20:Z:738:TYR:CZ	29:I:66:LYS:CA	2.74	0.69
33:J:234:PHE:CE1	33:J:286:LYS:HD3	2.28	0.68
20:Z:738:TYR:OH	29:I:69:LEU:HB2	1.94	0.67
1:A:205:PHE:CE2	1:A:209:HIS:CE1	2.83	0.67
20:Z:611:THR:HA	21:N:813:ARG:HH21	1.62	0.65
20:Z:738:TYR:CZ	29:I:69:LEU:CB	2.75	0.65
32:M:263:VAL:HG12	32:M:267:PHE:CZ	2.32	0.65
33:J:234:PHE:CD1	33:J:286:LYS:CG	2.80	0.65
7:g:107:ILE:HD12	7:g:107:ILE:H	1.61	0.64
20:Z:738:TYR:CZ	29:I:66:LYS:C	2.76	0.64
26:U:94:HIS:HB2	26:U:120:LEU:HD11	1.80	0.64
15:W:103:ASN:HB2	15:W:106:GLN:HE21	1.62	0.63
4:d:42:VAL:HG11	4:d:136:ALA:HB1	1.81	0.61
22:S:151:GLU:HB3	22:S:155:LEU:HD23	1.82	0.60
14:7:160:LEU:HG	14:7:175:LEU:HD12	1.83	0.60
20:Z:738:TYR:CE1	29:I:69:LEU:HB3	2.36	0.60
11:k:186:LYS:H	11:k:186:LYS:HD2	1.66	0.59
31:L:141:LYS:O	31:L:144:VAL:HG12	2.02	0.59
30:K:362:LEU:HD23	30:K:362:LEU:H	1.66	0.59
32:M:136:ASP:HB3	32:M:137:PRO:HD2	1.84	0.59
12:5:88:ILE:HG13	12:5:228:ALA:HB1	1.84	0.58
20:Z:738:TYR:CE1	29:I:66:LYS:O	2.56	0.58
3:C:52:VAL:HG12	33:J:401:ALA:HA	1.87	0.57
4:d:54:LEU:H	4:d:54:LEU:HD22	1.71	0.56
12:5:210:PHE:CD1	12:5:242:ARG:HG3	2.41	0.56
20:Z:738:TYR:CE2	29:I:69:LEU:HD23	2.41	0.55
3:C:67:TYR:CD2	3:C:88:ILE:HD13	2.42	0.55
30:K:352:ILE:HD12	34:K:501:ATP:H2	1.71	0.55
23:P:3:ARG:H	23:P:3:ARG:HD3	1.71	0.55
9:2:161:LEU:H	9:2:161:LEU:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:8:THR:HA	17:T:30:ILE:HD11	1.89	0.54
1:A:192:ASP:OD2	1:A:193:HIS:CD2	2.61	0.54
33:J:196:THR:HG23	33:J:246:PHE:CE1	2.42	0.54
6:F:121:GLN:HE22	7:G:87:HIS:CE1	2.26	0.54
32:M:96:ASN:H	32:M:106:VAL:HG12	1.72	0.54
13:6:145:ARG:HG3	13:6:155:MET:HE2	1.90	0.54
14:n:165:LEU:HD23	14:n:165:LEU:H	1.73	0.53
33:J:234:PHE:CG	33:J:286:LYS:CG	2.91	0.53
22:S:37:VAL:HA	22:S:54:TRP:HE1	1.73	0.53
13:6:102:GLN:HE22	13:6:137:GLY:HA2	1.73	0.53
2:B:143:ASN:HD21	10:3:80:ARG:HH12	1.57	0.53
8:1:47:HIS:CG	8:1:48:ASP:H	2.26	0.53
17:T:151:TRP:HE1	17:T:163:LEU:HD22	1.74	0.53
33:J:234:PHE:CG	33:J:286:LYS:HG3	2.44	0.52
33:J:349:LYS:HG2	33:J:386:VAL:HG21	1.91	0.52
22:S:404:LEU:HB2	22:S:405:ARG:HH11	1.73	0.52
20:Z:738:TYR:CZ	29:I:69:LEU:CD2	2.93	0.51
1:a:81:MET:HE3	1:a:83:VAL:HG22	1.92	0.51
14:n:245:LEU:H	14:n:245:LEU:HD12	1.75	0.51
1:a:199:TRP:CE3	1:a:227:VAL:HG11	2.46	0.51
17:T:215:LYS:H	17:T:215:LYS:HD2	1.76	0.51
25:R:208:ASN:HD22	33:J:339:ARG:HH22	1.57	0.51
32:M:155:ILE:HD12	32:M:155:ILE:H	1.74	0.51
4:D:161:ALA:HB1	4:D:175:LEU:HD21	1.93	0.51
28:H:148:ASN:HD21	28:H:152:ILE:HA	1.76	0.51
13:6:102:GLN:HE22	13:6:137:GLY:CA	2.25	0.50
11:k:63:ASN:HD22	11:k:83:PHE:HE2	1.60	0.50
14:7:42:THR:HG23	14:7:43:SER:H	1.75	0.50
5:E:102:TYR:HA	13:6:103:HIS:CE1	2.47	0.50
14:n:50:ASP:HB3	14:n:199:PRO:HA	1.93	0.50
20:Z:153:TYR:HA	20:Z:156:HIS:CD2	2.46	0.50
27:O:189:TYR:CE1	27:O:193:LEU:HD11	2.47	0.49
3:c:201:THR:HG22	3:c:203:SER:H	1.77	0.49
24:Q:267:LEU:HD11	24:Q:334:HIS:HB2	1.94	0.49
9:2:82:GLU:CD	10:3:130:ILE:HD12	2.37	0.49
33:J:333:ARG:HH21	33:J:337:LEU:HD11	1.78	0.49
18:X:67:ILE:HD13	18:X:67:ILE:H	1.78	0.49
19:Y:9:GLN:HA	25:R:416:LYS:HZ3	1.78	0.49
16:V:32:ILE:HD12	16:V:32:ILE:H	1.77	0.49
33:J:234:PHE:CG	33:J:286:LYS:NZ	2.80	0.49
10:3:149:MET:HE3	10:3:153:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:100:ALA:HB2	28:H:149:LEU:HD23	1.95	0.49
18:X:11:ARG:HH21	18:X:104:LYS:H	1.60	0.48
21:N:373:VAL:HG13	21:N:750:SER:HB3	1.94	0.48
25:R:98:LEU:HD12	25:R:98:LEU:H	1.77	0.48
3:c:86:ILE:HG23	3:c:87:LEU:HG	1.96	0.48
5:e:88:MET:HE3	5:e:116:VAL:CG1	2.43	0.48
21:N:55:PHE:HB3	21:N:57:ASP:H	1.77	0.48
9:2:164:MET:SD	9:2:168:GLU:HG3	2.54	0.48
19:Y:54:VAL:HG21	19:Y:63:ASN:HD22	1.79	0.48
25:R:62:TYR:HB2	25:R:145:GLY:HA2	1.95	0.48
6:F:72:LEU:HD23	6:F:132:LEU:HD22	1.96	0.48
21:N:371:LEU:O	21:N:375:HIS:CD2	2.67	0.48
13:m:9:GLN:HE21	14:n:34:THR:HB	1.79	0.47
4:D:54:LEU:H	4:D:54:LEU:HD22	1.79	0.47
4:D:199:LEU:HD13	4:D:210:ILE:HG23	1.96	0.47
31:L:197:ILE:HG13	31:L:324:ILE:HD11	1.95	0.47
9:2:201:ASN:HD22	9:2:218:ASN:CG	2.22	0.47
20:Z:233:LEU:H	20:Z:234:PRO:HD2	1.79	0.47
33:J:234:PHE:CD2	33:J:286:LYS:NZ	2.82	0.47
2:b:11:THR:HG21	3:c:7:ASP:HB2	1.97	0.47
20:Z:233:LEU:H	20:Z:234:PRO:CD	2.27	0.47
30:K:248:GLY:HA3	33:J:218:LEU:HD12	1.95	0.47
13:m:131:TYR:CE2	13:m:141:ARG:HD3	2.49	0.47
21:N:680:LYS:HA	21:N:683:LEU:HD12	1.97	0.47
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.97	0.47
15:W:12:ASN:HB2	15:W:55:ALA:HB2	1.97	0.47
17:T:26:LEU:O	17:T:30:ILE:HG22	2.15	0.47
24:Q:220:LEU:HD13	24:Q:261:VAL:HG22	1.96	0.47
28:H:108:GLY:HA3	28:H:144:LYS:HG3	1.95	0.47
1:A:87:ILE:N	1:A:88:PRO:HD2	2.29	0.47
2:b:217:GLU:H	2:b:234:ARG:HH11	1.61	0.47
1:A:163:TYR:O	2:B:61:LEU:HD21	2.15	0.47
6:F:171:TYR:HB2	6:F:199:GLN:HE22	1.80	0.47
9:2:42:VAL:HG11	9:2:180:ALA:HB1	1.96	0.47
27:O:29:PHE:CZ	27:O:45:LEU:HD23	2.50	0.47
8:h:22:ILE:HD12	8:h:160:THR:HB	1.97	0.46
13:m:30:VAL:HG12	13:m:214:ILE:HG13	1.97	0.46
21:N:482:ALA:HB1	21:N:517:LEU:HD23	1.97	0.46
29:I:313:LEU:HD13	29:I:324:VAL:HG11	1.98	0.46
1:A:205:PHE:O	1:A:209:HIS:CD2	2.68	0.46
6:F:173:GLU:HB2	7:G:58:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:M:97:SER:H	32:M:112:ALA:HB1	1.80	0.46
23:P:173:MET:O	23:P:177:ILE:HG13	2.16	0.46
32:M:197:ILE:HG21	32:M:277:ILE:HD11	1.96	0.46
16:V:230:TYR:CD2	23:P:412:LEU:HB3	2.51	0.46
28:H:357:ARG:HE	28:H:357:ARG:HA	1.81	0.46
4:d:207:ALA:HB3	4:d:230:ASN:HD22	1.81	0.46
1:A:178:ILE:HD11	1:A:214:LEU:HD21	1.97	0.46
2:b:24:ALA:O	2:b:28:VAL:HG23	2.15	0.46
14:n:207:GLU:O	14:n:211:VAL:HG23	2.16	0.46
4:D:103:PRO:HD2	4:D:141:ARG:HH22	1.80	0.46
4:D:216:LYS:HB3	4:D:217:PRO:HD2	1.98	0.46
15:W:33:VAL:HG11	15:W:76:LEU:HD21	1.98	0.46
17:T:55:LEU:HD11	17:T:93:ASN:HA	1.98	0.46
21:N:718:GLU:HB3	21:N:725:LEU:HA	1.97	0.46
23:P:384:VAL:HG11	24:Q:353:PRO:HB3	1.97	0.45
27:O:110:ASP:HB2	27:O:122:HIS:HB2	1.98	0.45
5:e:85:ALA:HB2	5:e:140:VAL:HG21	1.97	0.45
5:E:41:ALA:HA	5:E:46:VAL:HG22	1.96	0.45
24:Q:174:LEU:O	24:Q:178:HIS:CD2	2.69	0.45
3:C:54:SER:HB2	3:C:57:LEU:HB2	1.98	0.45
5:E:113:THR:HG22	5:E:164:PHE:HB3	1.98	0.45
21:N:688:ASN:HB3	21:N:690:HIS:CE1	2.52	0.45
5:e:101:LEU:O	13:m:103:HIS:HE1	2.00	0.45
26:U:228:LYS:O	26:U:232:VAL:HG23	2.16	0.45
22:S:351:ALA:HA	22:S:359:LYS:HD3	1.98	0.45
29:I:361:ILE:HG22	29:I:365:HIS:CE1	2.51	0.45
32:M:96:ASN:H	32:M:106:VAL:CG1	2.29	0.45
4:D:151:GLU:HB3	4:D:152:PRO:HD2	1.99	0.45
30:K:324:LEU:HD22	30:K:329:LEU:HD12	1.98	0.45
2:B:143:ASN:HD21	10:3:80:ARG:NH1	2.15	0.45
11:4:42:THR:HG21	11:4:80:VAL:HG11	1.99	0.45
20:Z:738:TYR:OH	29:I:69:LEU:CA	2.64	0.45
4:D:97:ARG:O	4:D:101:GLU:HA	2.17	0.44
10:3:138:VAL:HG11	10:3:146:LEU:HB3	1.99	0.44
20:Z:531:ALA:HB1	20:Z:572:ILE:HG22	1.99	0.44
32:M:58:MET:O	32:M:62:ILE:HG13	2.18	0.44
20:Z:948:TRP:HA	20:Z:948:TRP:CE3	2.52	0.44
1:a:211:ILE:HG23	1:a:217:GLU:HA	1.98	0.44
11:4:23:ARG:HA	11:4:23:ARG:HH21	1.82	0.44
25:R:64:LYS:HE3	25:R:99:TYR:CE2	2.52	0.44
8:1:47:HIS:CG	8:1:48:ASP:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:105:ASN:HD21	18:X:116:ALA:H	1.63	0.44
20:Z:146:PHE:CZ	20:Z:148:GLY:HA3	2.52	0.44
21:N:579:SER:H	26:U:176:ARG:NH2	2.16	0.44
6:f:137:TYR:CE1	6:f:141:GLY:HA2	2.53	0.43
24:Q:141:LEU:HG	24:Q:145:HIS:CE1	2.54	0.43
10:j:38:ASN:HB3	10:j:183:TRP:CE2	2.53	0.43
7:G:13:SER:HB2	7:G:127:ASN:HD21	1.83	0.43
27:O:70:TYR:CD1	27:O:109:LEU:HD22	2.53	0.43
30:K:58:TYR:CE1	33:J:34:ILE:HD11	2.52	0.43
12:5:79:LEU:C	12:5:79:LEU:HD22	2.44	0.43
17:T:34:LEU:HD13	17:T:61:ILE:HG21	2.00	0.43
33:J:188:TYR:CZ	33:J:315:GLU:HB2	2.54	0.43
7:G:107:ILE:H	7:G:107:ILE:HD12	1.83	0.43
20:Z:802:ASP:CG	20:Z:803:ALA:H	2.24	0.43
33:J:261:SER:H	33:J:269:GLN:HE22	1.66	0.43
6:f:213:ILE:HD12	6:f:230:VAL:HG12	2.00	0.43
7:g:50:VAL:HG21	7:g:66:LYS:HB2	2.01	0.43
30:K:297:ILE:HG23	33:J:250:ILE:HD12	2.00	0.43
3:C:108:VAL:O	3:C:112:VAL:HG23	2.18	0.43
25:R:235:LEU:HD23	25:R:235:LEU:HA	1.92	0.43
30:K:68:ILE:HD12	33:J:44:LEU:HB2	2.00	0.43
5:e:101:LEU:O	13:m:103:HIS:CE1	2.72	0.43
6:f:190:ILE:HG23	6:f:213:ILE:HD13	1.99	0.43
13:6:35:THR:HB	13:6:48:GLU:H	1.83	0.43
21:N:149:GLU:HG2	21:N:152:LEU:HG	2.01	0.43
21:N:490:LEU:HD11	21:N:731:VAL:HG21	2.00	0.43
21:N:762:ARG:HH11	21:N:916:LEU:HD21	1.84	0.43
22:S:383:LEU:HD23	22:S:383:LEU:HA	1.93	0.43
28:H:104:LYS:NZ	32:M:145:LEU:HD13	2.33	0.43
30:K:99:PHE:HA	30:K:110:VAL:HG12	2.00	0.43
19:Y:52:ASN:HB3	19:Y:55:THR:HA	2.01	0.43
21:N:32:VAL:HG21	21:N:64:ILE:HA	2.00	0.43
31:L:315:PHE:H	31:L:316:ASP:HB2	1.84	0.43
10:3:154:TYR:CZ	10:3:156:PRO:HA	2.54	0.43
20:Z:510:LEU:HB3	20:Z:511:PRO:HD3	2.01	0.42
33:J:232:GLU:HB3	33:J:236:MET:HE3	2.01	0.42
1:a:10:ALA:HB3	1:a:12:TYR:CE2	2.54	0.42
12:l:82:ARG:HD3	12:l:200:ASP:HA	2.01	0.42
7:G:109:ILE:N	7:G:110:PRO:HD2	2.34	0.42
20:Z:231:ASP:HB3	20:Z:236:PHE:CZ	2.53	0.42
1:A:83:VAL:HG11	1:A:90:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:784:SER:HB3	20:Z:792:VAL:HG11	2.01	0.42
21:N:176:GLN:HA	21:N:182:ASN:HD21	1.83	0.42
21:N:314:LEU:HD21	21:N:340:HIS:HE1	1.83	0.42
27:O:228:TYR:HA	27:O:230:PHE:CZ	2.54	0.42
28:H:97:LEU:HD23	28:H:97:LEU:HA	1.89	0.42
31:L:221:TYR:CD2	31:L:330:PRO:HG3	2.54	0.42
4:d:24:LEU:HD13	4:d:24:LEU:O	2.19	0.42
10:j:18:LYS:HB3	10:j:158:LEU:O	2.19	0.42
23:P:429:ILE:HG23	26:U:225:ILE:HG23	2.01	0.42
29:I:290:LYS:HG2	33:J:262:GLY:H	1.84	0.42
3:c:208:TYR:HA	3:c:211:LEU:HB2	2.02	0.42
4:d:33:ALA:HB1	4:d:134:LEU:HD12	2.01	0.42
11:4:5:LEU:HB2	11:4:16:ALA:HB3	2.01	0.42
21:N:314:LEU:HD21	21:N:340:HIS:CE1	2.54	0.42
23:P:235:LEU:HD23	23:P:235:LEU:H	1.84	0.42
11:k:15:LEU:HD12	11:k:43:LEU:HD23	2.00	0.42
14:n:122:PRO:HB2	14:n:159:PHE:CD1	2.54	0.42
18:X:11:ARG:HH21	18:X:104:LYS:N	2.16	0.42
27:O:385:GLU:HG2	27:O:389:GLN:HE22	1.85	0.42
33:J:210:PHE:O	33:J:211:ILE:HG12	2.20	0.42
3:C:112:VAL:HG13	3:C:137:TYR:CE1	2.55	0.42
3:C:201:THR:HG22	3:C:203:SER:H	1.85	0.42
12:5:253:TYR:CZ	12:5:262:TYR:CD1	3.08	0.42
28:H:292:ARG:O	28:H:296:GLU:HB2	2.20	0.42
5:e:88:MET:HE3	5:e:116:VAL:HG13	2.01	0.42
4:D:170:THR:O	4:D:173:GLU:HG2	2.20	0.42
7:G:242:PHE:O	7:G:246:GLU:HG2	2.19	0.42
29:I:401:LEU:HB2	33:J:312:ARG:HH21	1.85	0.42
31:L:113:SER:HB2	31:L:116:LYS:H	1.85	0.42
4:d:134:LEU:HG	4:d:164:ILE:HD11	2.02	0.42
9:i:33:VAL:HG22	9:i:188:ILE:HD11	2.02	0.42
16:V:159:ILE:HD11	16:V:197:TYR:HB2	2.01	0.41
21:N:31:VAL:HB	21:N:35:LEU:HD12	2.02	0.41
28:H:114:GLU:OE1	28:H:114:GLU:HA	2.20	0.41
30:K:352:ILE:HD12	34:K:501:ATP:C2	2.54	0.41
3:c:11:THR:HG22	3:c:11:THR:O	2.20	0.41
20:Z:269:TYR:CZ	20:Z:273:LEU:HD22	2.54	0.41
20:Z:734:ASP:O	20:Z:737:ALA:HB3	2.20	0.41
22:S:46:LEU:HD23	22:S:46:LEU:HA	1.91	0.41
28:H:70:LYS:H	33:J:80:SER:HB3	1.85	0.41
29:I:171:MET:HG2	29:I:245:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:148:GLN:HB3	6:F:149:PRO:HD2	2.02	0.41
1:a:31:ALA:C	1:a:33:LYS:H	2.28	0.41
5:e:85:ALA:HA	5:e:140:VAL:HG11	2.02	0.41
31:L:315:PHE:N	31:L:316:ASP:HB2	2.35	0.41
12:5:229:LEU:HD11	12:5:263:HIS:CD2	2.56	0.41
20:Z:308:LYS:HD2	20:Z:341:TYR:CE2	2.55	0.41
21:N:835:LYS:HD3	21:N:835:LYS:HA	1.86	0.41
27:O:137:TYR:CE1	27:O:149:LEU:HD11	2.54	0.41
28:H:188:PRO:HA	28:H:189:PRO:HD3	1.92	0.41
29:I:340:ARG:H	29:I:344:ILE:HD13	1.86	0.41
30:K:334:LEU:HD22	30:K:334:LEU:HA	1.83	0.41
8:h:141:THR:O	8:1:142:PHE:HA	2.21	0.41
20:Z:473:LEU:H	20:Z:473:LEU:HD22	1.84	0.41
21:N:608:LEU:H	21:N:608:LEU:HD12	1.85	0.41
28:H:221:LEU:HD13	28:H:246:ILE:HD13	2.02	0.41
30:K:235:ILE:HA	30:K:236:ARG:C	2.45	0.41
30:K:294:ARG:HH21	33:J:268:VAL:CG1	2.34	0.41
32:M:264:ARG:HA	32:M:267:PHE:CD1	2.55	0.41
11:k:29:LYS:HD2	11:k:29:LYS:HA	1.97	0.41
20:Z:440:LEU:HA	20:Z:448:LYS:HA	2.03	0.41
10:j:158:LEU:HB3	10:j:162:ASP:HB2	2.03	0.41
20:Z:502:ASN:HD22	20:Z:505:VAL:HG23	1.85	0.41
26:U:21:HIS:CE1	26:U:52:PHE:HA	2.56	0.41
27:O:329:MET:HE3	27:O:329:MET:HB3	1.82	0.41
3:c:185:LYS:HG3	3:c:187:ASP:H	1.85	0.41
10:j:23:ILE:HG12	10:j:43:ILE:HD12	2.03	0.41
21:N:375:HIS:HB3	21:N:385:VAL:HG11	2.02	0.41
23:P:66:LEU:N	23:P:67:ALA:HA	2.35	0.41
25:R:258:LEU:HD23	25:R:333:MET:HE2	2.03	0.41
13:m:213:LEU:CD2	13:m:222:LYS:HG2	2.51	0.40
16:V:210:THR:HG22	16:V:214:MET:HE2	2.02	0.40
20:Z:223:LEU:H	20:Z:223:LEU:HG	1.79	0.40
20:Z:239:GLU:HA	20:Z:242:PHE:CD2	2.56	0.40
27:O:165:LEU:H	27:O:165:LEU:HD23	1.86	0.40
29:I:171:MET:HG3	29:I:247:ILE:HB	2.02	0.40
1:a:214:LEU:HD23	1:a:214:LEU:HA	1.87	0.40
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.56	0.40
5:E:159:GLU:HG2	5:E:162:GLY:H	1.86	0.40
9:2:112:LEU:HD21	9:2:127:LEU:HD13	2.03	0.40
20:Z:309:GLN:HG2	20:Z:310:LEU:H	1.86	0.40
22:S:366:LYS:HE2	22:S:367:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:364:LEU:HG	25:R:368:LEU:HD11	2.04	0.40
27:O:227:ILE:HD13	27:O:227:ILE:HG21	1.90	0.40
1:a:81:MET:HE3	1:a:83:VAL:CG2	2.51	0.40
4:d:138:PHE:CZ	4:d:145:PRO:HB3	2.56	0.40
13:m:60:MET:HE3	13:m:117:THR:HG21	2.03	0.40
1:A:205:PHE:CZ	1:A:209:HIS:CE1	3.09	0.40
31:L:101:ILE:HD13	31:L:101:ILE:HA	1.93	0.40
21:N:89:PHE:C	21:N:139:ARG:HH22	2.29	0.40
3:c:50:ARG:HH12	3:c:63:THR:HA	1.87	0.40
8:h:184:MET:HE3	8:h:197:PHE:CE2	2.56	0.40
10:j:56:LEU:HD11	11:k:122:LEU:HD13	2.04	0.40
5:E:73:HIS:CD2	5:E:74:ILE:HG12	2.56	0.40
20:Z:620:LEU:O	20:Z:624:LEU:HG	2.21	0.40
23:P:234:TYR:HB2	23:P:271:SER:HA	2.03	0.40
26:U:54:LEU:HA	26:U:55:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	16 54
1	a	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	7 36
2	B	246/248 (99%)	226 (92%)	19 (8%)	1 (0%)	30 67
2	b	246/248 (99%)	231 (94%)	12 (5%)	3 (1%)	10 43
3	C	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	16 54
3	c	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	16 54
4	D	236/252 (94%)	221 (94%)	14 (6%)	1 (0%)	30 67
4	d	250/252 (99%)	237 (95%)	10 (4%)	3 (1%)	10 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	243/245 (99%)	228 (94%)	13 (5%)	2 (1%)	16 54
5	e	243/245 (99%)	225 (93%)	17 (7%)	1 (0%)	30 67
6	F	230/232 (99%)	214 (93%)	16 (7%)	0	100 100
6	f	230/232 (99%)	217 (94%)	13 (6%)	0	100 100
7	G	243/245 (99%)	226 (93%)	15 (6%)	2 (1%)	16 54
7	g	243/245 (99%)	228 (94%)	10 (4%)	5 (2%)	5 29
8	1	194/196 (99%)	183 (94%)	9 (5%)	2 (1%)	12 48
8	h	194/196 (99%)	187 (96%)	5 (3%)	2 (1%)	12 48
9	2	224/226 (99%)	213 (95%)	10 (4%)	1 (0%)	30 67
9	i	224/226 (99%)	209 (93%)	13 (6%)	2 (1%)	14 50
10	3	202/204 (99%)	192 (95%)	7 (4%)	3 (2%)	8 39
10	j	202/204 (99%)	186 (92%)	15 (7%)	1 (0%)	24 63
11	4	193/195 (99%)	180 (93%)	9 (5%)	4 (2%)	5 29
11	k	193/195 (99%)	177 (92%)	12 (6%)	4 (2%)	5 29
12	5	210/212 (99%)	199 (95%)	8 (4%)	3 (1%)	9 40
12	l	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	24 63
13	6	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	9 40
13	m	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	14 50
14	7	227/232 (98%)	211 (93%)	14 (6%)	2 (1%)	14 50
14	n	230/232 (99%)	213 (93%)	15 (6%)	2 (1%)	14 50
15	W	195/197 (99%)	180 (92%)	11 (6%)	4 (2%)	5 29
16	V	287/289 (99%)	261 (91%)	16 (6%)	10 (4%)	3 20
17	T	264/266 (99%)	247 (94%)	11 (4%)	6 (2%)	5 28
18	X	125/127 (98%)	101 (81%)	19 (15%)	5 (4%)	2 18
19	Y	87/89 (98%)	73 (84%)	11 (13%)	3 (3%)	3 21
20	Z	902/970 (93%)	805 (89%)	72 (8%)	25 (3%)	4 24
21	N	920/922 (100%)	853 (93%)	52 (6%)	15 (2%)	7 37
22	S	473/475 (100%)	441 (93%)	21 (4%)	11 (2%)	5 28
23	P	438/440 (100%)	418 (95%)	13 (3%)	7 (2%)	7 37
24	Q	432/434 (100%)	398 (92%)	21 (5%)	13 (3%)	3 22
25	R	403/405 (100%)	378 (94%)	20 (5%)	5 (1%)	10 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	U	302/304 (99%)	282 (93%)	16 (5%)	4 (1%)	9 42
27	O	386/388 (100%)	368 (95%)	15 (4%)	3 (1%)	16 54
28	H	424/426 (100%)	376 (89%)	36 (8%)	12 (3%)	4 24
29	I	383/385 (100%)	344 (90%)	25 (6%)	14 (4%)	2 19
30	K	392/394 (100%)	344 (88%)	36 (9%)	12 (3%)	3 22
31	L	386/388 (100%)	352 (91%)	25 (6%)	9 (2%)	5 28
32	M	419/421 (100%)	384 (92%)	24 (6%)	11 (3%)	4 25
33	J	403/405 (100%)	360 (89%)	27 (7%)	16 (4%)	2 18
All	All	13936/14113 (99%)	12887 (92%)	804 (6%)	245 (2%)	9 34

All (245) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
2	b	6	SER
2	b	53	SER
7	g	209	GLU
8	h	127	SER
13	m	138	SER
1	A	13	ASP
10	3	40	PHE
15	W	149	GLN
16	V	47	MET
16	V	171	ARG
16	V	185	ILE
17	T	173	GLU
18	X	29	VAL
20	Z	85	VAL
20	Z	802	ASP
21	N	17	GLN
22	S	84	ASP
23	P	46	THR
23	P	86	HIS
24	Q	384	LYS
25	R	72	VAL
25	R	146	ASP
25	R	245	SER
26	U	5	HIS
26	U	42	ASN

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Mol	Chain	Res	Type
27	O	243	VAL
28	H	112	SER
28	H	136	ALA
29	I	317	ASP
29	I	340	ARG
29	I	371	LEU
30	K	37	ASN
30	K	334	LEU
30	K	425	ASP
31	L	290	ARG
31	L	316	ASP
32	M	318	ASP
33	J	211	ILE
1	a	60	PRO
4	d	204	GLN
9	i	200	SER
7	G	9	ASP
7	G	209	GLU
8	1	40	THR
11	4	152	MET
12	5	286	ILE
13	6	138	SER
14	7	110	ASP
16	V	175	SER
16	V	271	VAL
17	T	97	SER
18	X	106	SER
20	Z	57	LYS
20	Z	82	MET
20	Z	205	LEU
20	Z	825	ALA
20	Z	899	GLN
21	N	123	PHE
21	N	175	ASP
21	N	473	ASP
21	N	634	LEU
21	N	832	HIS
21	N	855	GLU
22	S	47	THR
22	S	150	LYS
22	S	433	GLU
23	P	130	ILE

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Mol	Chain	Res	Type
24	Q	44	ALA
24	Q	68	MET
24	Q	170	ASP
24	Q	189	ARG
24	Q	286	TYR
24	Q	386	PHE
24	Q	387	TYR
25	R	280	ILE
26	U	160	THR
28	H	128	ASN
29	I	344	ILE
31	L	340	PRO
33	J	72	VAL
33	J	212	ARG
33	J	249	GLU
33	J	312	ARG
33	J	335	MET
1	a	11	GLY
5	e	73	HIS
7	g	9	ASP
12	l	183	GLU
14	n	262	GLY
3	C	183	ASP
4	D	204	GLN
8	1	41	ASP
10	3	182	GLY
10	3	184	GLY
12	5	98	GLY
16	V	262	THR
16	V	272	GLY
17	T	137	GLU
18	X	105	ASN
20	Z	578	GLY
20	Z	920	GLY
20	Z	947	GLY
20	Z	957	LEU
21	N	395	ALA
21	N	757	THR
21	N	831	GLU
21	N	842	ASN
21	N	862	SER
22	S	100	HIS

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Mol	Chain	Res	Type
23	P	89	LEU
23	P	272	PRO
24	Q	126	LYS
24	Q	211	PRO
24	Q	230	LYS
24	Q	253	ASN
24	Q	353	PRO
25	R	182	ASN
27	O	70	TYR
28	H	381	ASP
28	H	401	GLY
29	I	115	ASP
29	I	216	PRO
29	I	298	GLY
29	I	339	ILE
30	K	231	LYS
30	K	236	ARG
30	K	308	GLN
30	K	417	THR
31	L	101	ILE
31	L	177	GLU
31	L	282	GLU
32	M	17	GLU
32	M	109	ASP
32	M	114	GLY
33	J	119	SER
33	J	263	GLY
3	c	7	ASP
7	g	73	HIS
10	j	116	SER
11	k	72	ASP
11	k	73	TYR
13	m	208	ASP
1	A	11	GLY
5	E	130	GLU
11	4	2	ASP
12	5	183	GLU
13	6	27	ASP
13	6	173	ASN
16	V	61	TYR
17	T	251	HIS
20	Z	65	GLU

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Mol	Chain	Res	Type
20	Z	80	SER
20	Z	143	VAL
20	Z	233	LEU
20	Z	377	ALA
20	Z	770	GLU
20	Z	870	ALA
20	Z	932	ALA
20	Z	940	GLY
21	N	712	ASN
21	N	765	ASP
23	P	255	ALA
26	U	30	ASN
28	H	126	ASN
28	H	190	ARG
28	H	314	VAL
29	I	116	ASP
29	I	163	ASP
29	I	290	LYS
29	I	372	SER
29	I	426	ASN
30	K	49	PHE
30	K	284	ALA
31	L	317	ASN
31	L	343	LEU
32	M	240	ASN
32	M	352	PRO
33	J	275	LEU
33	J	284	THR
11	k	2	ASP
11	k	132	ALA
3	C	184	MET
11	4	73	TYR
14	7	111	ASN
15	W	144	PHE
16	V	72	PRO
16	V	184	ASN
18	X	21	SER
18	X	24	CYS
19	Y	43	TRP
20	Z	25	PRO
20	Z	309	GLN
20	Z	376	SER

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Mol	Chain	Res	Type
20	Z	513	ALA
21	N	88	ARG
22	S	83	PRO
22	S	97	THR
22	S	126	LYS
22	S	153	GLU
23	P	372	THR
28	H	303	ALA
29	I	427	LYS
30	K	330	ARG
31	L	178	ILE
32	M	91	ILE
32	M	173	ASP
32	M	287	GLY
32	M	384	ASP
32	M	433	TYR
33	J	218	LEU
33	J	261	SER
33	J	373	ARG
33	J	398	ILE
1	a	10	ALA
4	d	103	PRO
7	g	131	PRO
7	g	187	LEU
9	i	249	ILE
14	n	43	SER
5	E	73	HIS
9	2	120	GLN
15	W	180	LEU
15	W	190	ILE
17	T	117	ASN
17	T	257	THR
19	Y	44	ALA
19	Y	49	ILE
22	S	44	THR
27	O	225	ASP
28	H	145	TYR
33	J	341	ILE
28	H	152	ILE
28	H	345	PRO
3	c	129	ARG
20	Z	254	PRO

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Mol	Chain	Res	Type
22	S	115	PRO
2	b	129	PRO
4	d	185	PRO
8	h	123	PRO
2	B	53	SER
30	K	314	VAL
11	4	173	PRO
33	J	10	ILE
30	K	274	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/207 (100%)	197 (95%)	10 (5%)	23	44
1	a	207/207 (100%)	203 (98%)	4 (2%)	50	67
2	B	207/207 (100%)	195 (94%)	12 (6%)	18	40
2	b	207/207 (100%)	200 (97%)	7 (3%)	32	54
3	C	201/201 (100%)	189 (94%)	12 (6%)	17	39
3	c	201/201 (100%)	190 (94%)	11 (6%)	19	41
4	D	210/224 (94%)	206 (98%)	4 (2%)	50	67
4	d	224/224 (100%)	212 (95%)	12 (5%)	20	41
5	E	201/201 (100%)	197 (98%)	4 (2%)	48	66
5	e	201/201 (100%)	196 (98%)	5 (2%)	42	62
6	F	191/191 (100%)	186 (97%)	5 (3%)	40	61
6	f	191/191 (100%)	183 (96%)	8 (4%)	26	48
7	G	202/202 (100%)	199 (98%)	3 (2%)	57	72
7	g	202/202 (100%)	193 (96%)	9 (4%)	24	46
8	1	162/162 (100%)	158 (98%)	4 (2%)	42	62
8	h	162/162 (100%)	157 (97%)	5 (3%)	35	56
9	2	185/185 (100%)	176 (95%)	9 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	185/185 (100%)	177 (96%)	8 (4%)	26	47
10	3	172/172 (100%)	167 (97%)	5 (3%)	37	58
10	j	172/172 (100%)	168 (98%)	4 (2%)	44	64
11	4	173/173 (100%)	165 (95%)	8 (5%)	24	45
11	k	173/173 (100%)	169 (98%)	4 (2%)	44	64
12	5	169/169 (100%)	160 (95%)	9 (5%)	20	41
12	l	169/169 (100%)	166 (98%)	3 (2%)	51	67
13	6	185/185 (100%)	180 (97%)	5 (3%)	39	60
13	m	185/185 (100%)	180 (97%)	5 (3%)	39	60
14	7	195/198 (98%)	193 (99%)	2 (1%)	68	78
14	n	198/198 (100%)	193 (98%)	5 (2%)	42	62
15	W	171/171 (100%)	167 (98%)	4 (2%)	44	64
16	V	253/253 (100%)	241 (95%)	12 (5%)	23	44
17	T	249/249 (100%)	241 (97%)	8 (3%)	34	56
18	X	116/116 (100%)	113 (97%)	3 (3%)	40	61
19	Y	81/81 (100%)	79 (98%)	2 (2%)	42	62
20	Z	773/828 (93%)	741 (96%)	32 (4%)	27	48
21	N	776/776 (100%)	756 (97%)	20 (3%)	40	61
22	S	447/447 (100%)	432 (97%)	15 (3%)	32	54
23	P	412/412 (100%)	404 (98%)	8 (2%)	50	67
24	Q	391/391 (100%)	384 (98%)	7 (2%)	51	67
25	R	356/356 (100%)	347 (98%)	9 (2%)	42	62
26	U	277/277 (100%)	271 (98%)	6 (2%)	45	64
27	O	363/363 (100%)	351 (97%)	12 (3%)	33	55
28	H	361/361 (100%)	351 (97%)	10 (3%)	38	59
29	I	342/342 (100%)	332 (97%)	10 (3%)	37	58
30	K	346/346 (100%)	334 (96%)	12 (4%)	32	53
31	L	332/332 (100%)	321 (97%)	11 (3%)	33	55
32	M	364/364 (100%)	343 (94%)	21 (6%)	18	40
33	J	352/352 (100%)	339 (96%)	13 (4%)	30	51
All	All	12099/12171 (99%)	11702 (97%)	397 (3%)	34	55

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	16	ILE
1	a	38	THR
1	a	195	ASN
1	a	232	LYS
2	b	97	TYR
2	b	127	VAL
2	b	164	ILE
2	b	168	SER
2	b	178	ARG
2	b	194	LEU
2	b	209	ILE
3	c	12	ILE
3	c	21	GLN
3	c	41	SER
3	c	66	LEU
3	c	96	GLN
3	c	108	VAL
3	c	133	VAL
3	c	158	THR
3	c	202	ASP
3	c	213	PHE
3	c	221	ASN
4	d	10	ILE
4	d	24	LEU
4	d	40	ASN
4	d	46	CYS
4	d	54	LEU
4	d	71	VAL
4	d	106	VAL
4	d	139	ASP
4	d	164	ILE
4	d	171	VAL
4	d	180	ASP
4	d	248	LYS
5	e	9	ASP
5	e	43	LYS
5	e	104	ASP
5	e	113	THR
5	e	222	ILE
6	f	52	ASN
6	f	58	SER
6	f	72	LEU

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Mol	Chain	Res	Type
6	f	130	VAL
6	f	150	SER
6	f	153	VAL
6	f	197	ILE
6	f	219	ASP
7	g	9	ASP
7	g	29	LYS
7	g	36	THR
7	g	52	LYS
7	g	107	ILE
7	g	109	ILE
7	g	212	PHE
7	g	224	THR
7	g	245	LYS
8	h	13	MET
8	h	49	LYS
8	h	130	LYS
8	h	153	GLU
8	h	158	GLU
9	i	54	ILE
9	i	105	VAL
9	i	109	LEU
9	i	113	LYS
9	i	196	LEU
9	i	206	VAL
9	i	227	GLU
9	i	228	LYS
10	j	13	VAL
10	j	82	ILE
10	j	156	PRO
10	j	193	ASP
11	k	66	LEU
11	k	77	PRO
11	k	120	ASP
11	k	186	LYS
12	l	79	LEU
12	l	106	VAL
12	l	233	LYS
13	m	15	ASP
13	m	115	VAL
13	m	122	LEU
13	m	136	VAL

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Mol	Chain	Res	Type
13	m	217	LYS
14	n	106	GLU
14	n	112	PRO
14	n	197	ASP
14	n	216	VAL
14	n	245	LEU
1	A	13	ASP
1	A	16	ILE
1	A	65	ASP
1	A	86	PRO
1	A	87	ILE
1	A	130	GLN
1	A	139	VAL
1	A	220	LYS
1	A	227	VAL
1	A	232	LYS
2	B	33	THR
2	B	35	LEU
2	B	43	VAL
2	B	60	THR
2	B	74	VAL
2	B	109	LEU
2	B	164	ILE
2	B	194	LEU
2	B	205	ASN
2	B	209	ILE
2	B	225	THR
2	B	233	PRO
3	C	45	VAL
3	C	52	VAL
3	C	66	LEU
3	C	87	LEU
3	C	96	GLN
3	C	112	VAL
3	C	123	THR
3	C	128	LEU
3	C	165	VAL
3	C	168	ASN
3	C	186	VAL
3	C	213	PHE
4	D	24	LEU
4	D	61	PRO

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Mol	Chain	Res	Type
4	D	106	VAL
4	D	222	VAL
5	E	9	ASP
5	E	43	LYS
5	E	71	ASP
5	E	116	VAL
6	F	72	LEU
6	F	79	PRO
6	F	120	THR
6	F	134	ILE
6	F	159	THR
7	G	77	VAL
7	G	82	ILE
7	G	224	THR
8	1	85	GLU
8	1	92	LYS
8	1	128	VAL
8	1	135	ILE
9	2	54	ILE
9	2	67	SER
9	2	68	PRO
9	2	105	VAL
9	2	132	VAL
9	2	161	LEU
9	2	173	GLN
9	2	200	SER
9	2	236	ARG
10	3	13	VAL
10	3	26	ASP
10	3	141	THR
10	3	147	PHE
10	3	196	VAL
11	4	22	THR
11	4	30	ASP
11	4	58	GLU
11	4	101	ASN
11	4	126	VAL
11	4	141	PHE
11	4	145	ASP
11	4	168	LEU
12	5	79	LEU
12	5	109	VAL

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Mol	Chain	Res	Type
12	5	133	TRP
12	5	161	LEU
12	5	179	TYR
12	5	212	TYR
12	5	222	ASP
12	5	250	VAL
12	5	285	VAL
13	6	31	LEU
13	6	165	LYS
13	6	185	VAL
13	6	216	THR
13	6	217	LYS
14	7	39	VAL
14	7	205	VAL
15	W	14	GLU
15	W	59	PRO
15	W	140	ASP
15	W	173	THR
16	V	29	ILE
16	V	32	ILE
16	V	47	MET
16	V	58	VAL
16	V	76	THR
16	V	78	VAL
16	V	140	VAL
16	V	223	SER
16	V	238	LEU
16	V	253	LYS
16	V	262	THR
16	V	283	THR
17	T	44	LEU
17	T	90	PHE
17	T	94	HIS
17	T	96	LEU
17	T	107	SER
17	T	147	LYS
17	T	150	ARG
17	T	228	ILE
18	X	67	ILE
18	X	68	LEU
18	X	76	VAL
19	Y	29	LEU

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Mol	Chain	Res	Type
19	Y	62	GLU
20	Z	61	SER
20	Z	71	LEU
20	Z	104	ASP
20	Z	146	PHE
20	Z	191	SER
20	Z	221	VAL
20	Z	245	VAL
20	Z	297	VAL
20	Z	323	TYR
20	Z	386	VAL
20	Z	473	LEU
20	Z	490	ILE
20	Z	517	ASP
20	Z	534	PHE
20	Z	546	ILE
20	Z	557	GLU
20	Z	560	THR
20	Z	566	LEU
20	Z	609	THR
20	Z	617	ILE
20	Z	630	LYS
20	Z	735	GLU
20	Z	748	LEU
20	Z	764	LEU
20	Z	776	VAL
20	Z	809	MET
20	Z	817	LEU
20	Z	834	LEU
20	Z	842	GLN
20	Z	850	LEU
20	Z	913	ILE
20	Z	945	ILE
21	N	72	LEU
21	N	143	LYS
21	N	175	ASP
21	N	185	ILE
21	N	228	VAL
21	N	245	LEU
21	N	282	TYR
21	N	297	ASP
21	N	301	THR

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Mol	Chain	Res	Type
21	N	316	LYS
21	N	326	SER
21	N	328	PHE
21	N	366	THR
21	N	546	LEU
21	N	562	THR
21	N	774	ASN
21	N	784	TYR
21	N	829	LYS
21	N	891	VAL
21	N	920	VAL
22	S	49	ASP
22	S	72	GLU
22	S	101	LYS
22	S	165	PRO
22	S	180	ASN
22	S	216	LYS
22	S	219	LYS
22	S	264	VAL
22	S	290	ASN
22	S	291	GLU
22	S	330	LEU
22	S	388	ILE
22	S	419	VAL
22	S	455	GLU
22	S	490	ASN
23	P	48	GLN
23	P	176	LYS
23	P	228	SER
23	P	235	LEU
23	P	321	VAL
23	P	376	THR
23	P	396	PRO
23	P	419	VAL
24	Q	73	LYS
24	Q	131	VAL
24	Q	147	GLN
24	Q	198	LEU
24	Q	211	PRO
24	Q	221	MET
24	Q	241	GLU
25	R	199	GLU

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Mol	Chain	Res	Type
25	R	212	THR
25	R	229	LYS
25	R	239	THR
25	R	274	PRO
25	R	282	THR
25	R	333	MET
25	R	348	LEU
25	R	359	VAL
26	U	5	HIS
26	U	34	VAL
26	U	116	ASN
26	U	142	GLN
26	U	236	LEU
26	U	239	LEU
27	O	25	LEU
27	O	34	GLU
27	O	58	ARG
27	O	70	TYR
27	O	128	LEU
27	O	144	VAL
27	O	241	THR
27	O	272	VAL
27	O	289	GLN
27	O	291	ILE
27	O	348	VAL
27	O	367	LYS
28	H	52	THR
28	H	74	THR
28	H	163	VAL
28	H	186	PRO
28	H	274	VAL
28	H	333	MET
28	H	375	VAL
28	H	395	SER
28	H	399	GLU
28	H	409	ARG
29	I	216	PRO
29	I	225	PRO
29	I	243	THR
29	I	287	ILE
29	I	333	THR
29	I	346	ARG

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Mol	Chain	Res	Type
29	I	401	LEU
29	I	408	ARG
29	I	423	VAL
29	I	435	LEU
30	K	67	TYR
30	K	103	ILE
30	K	121	ARG
30	K	137	VAL
30	K	169	VAL
30	K	237	VAL
30	K	251	PRO
30	K	274	VAL
30	K	330	ARG
30	K	334	LEU
30	K	358	SER
30	K	400	TYR
31	L	86	LYS
31	L	109	MET
31	L	128	ILE
31	L	131	VAL
31	L	148	LEU
31	L	155	ILE
31	L	187	THR
31	L	333	LEU
31	L	365	THR
31	L	410	ILE
31	L	415	LEU
32	M	18	LEU
32	M	66	LYS
32	M	119	VAL
32	M	134	LEU
32	M	158	THR
32	M	167	VAL
32	M	172	VAL
32	M	179	THR
32	M	200	PRO
32	M	202	LYS
32	M	205	ASP
32	M	244	LEU
32	M	263	VAL
32	M	277	ILE
32	M	284	ASP

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Mol	Chain	Res	Type
32	M	289	LYS
32	M	305	MET
32	M	331	ASP
32	M	352	PRO
32	M	421	GLU
32	M	433	TYR
33	J	54	LYS
33	J	68	PRO
33	J	81	ASP
33	J	105	LYS
33	J	186	ILE
33	J	218	LEU
33	J	233	LEU
33	J	249	GLU
33	J	251	ASP
33	J	257	ARG
33	J	288	ILE
33	J	299	ILE
33	J	373	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (344) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	84	ASN
1	a	92	ASN
1	a	126	GLN
1	a	130	GLN
1	a	175	GLN
1	a	176	GLN
1	a	184	ASN
1	a	195	ASN
1	a	251	GLN
2	b	30	GLN
2	b	180	ASN
2	b	205	ASN
2	b	244	ASN
3	c	21	GLN
3	c	89	ASN
3	c	120	GLN
3	c	125	HIS
3	c	177	GLN
4	d	122	GLN

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Mol	Chain	Res	Type
4	d	149	GLN
4	d	178	ASN
4	d	230	ASN
4	d	253	ASN
5	e	114	GLN
5	e	154	GLN
5	e	215	ASN
5	e	216	ASN
5	e	218	GLN
6	f	93	ASN
6	f	119	ASN
7	g	43	ASN
7	g	64	ASN
7	g	73	HIS
7	g	147	HIS
7	g	207	ASN
7	g	244	GLN
7	g	248	ASN
8	h	47	HIS
8	h	69	GLN
8	h	170	GLN
9	i	59	ASN
9	i	110	GLN
9	i	189	GLN
10	j	8	ASN
10	j	38	ASN
10	j	48	HIS
10	j	72	ASN
10	j	145	GLN
11	k	63	ASN
11	k	99	GLN
11	k	147	HIS
11	k	166	GLN
12	l	104	GLN
12	l	160	ASN
12	l	251	ASN
12	l	254	HIS
12	l	266	HIS
12	l	283	ASN
13	m	9	GLN
13	m	57	ASN
13	m	63	ASN

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Mol	Chain	Res	Type
13	m	103	HIS
13	m	160	ASN
13	m	161	GLN
13	m	163	ASN
13	m	167	GLN
13	m	203	HIS
14	n	35	GLN
14	n	51	ASN
14	n	94	GLN
14	n	111	ASN
14	n	153	GLN
14	n	158	GLN
14	n	185	ASN
14	n	227	ASN
14	n	249	ASN
14	n	264	GLN
1	A	126	GLN
1	A	175	GLN
1	A	184	ASN
1	A	185	HIS
1	A	193	HIS
1	A	209	HIS
1	A	240	ASN
2	B	20	GLN
2	B	143	ASN
2	B	180	ASN
2	B	205	ASN
3	C	103	ASN
3	C	120	GLN
3	C	147	GLN
3	C	168	ASN
3	C	173	GLN
4	D	16	HIS
4	D	178	ASN
4	D	204	GLN
4	D	209	ASN
5	E	147	HIS
5	E	157	HIS
5	E	233	ASN
6	F	21	GLN
6	F	31	GLN
6	F	43	HIS

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Mol	Chain	Res	Type
6	F	60	GLN
6	F	90	GLN
6	F	93	ASN
6	F	166	GLN
6	F	199	GLN
7	G	43	ASN
7	G	68	GLN
7	G	73	HIS
7	G	87	HIS
7	G	127	ASN
7	G	144	ASN
8	1	98	ASN
8	1	129	HIS
8	1	150	ASN
8	1	166	HIS
8	1	170	GLN
9	2	95	HIS
9	2	115	HIS
9	2	138	HIS
9	2	143	HIS
9	2	201	ASN
9	2	218	ASN
10	3	8	ASN
10	3	48	HIS
10	3	72	ASN
10	3	89	GLN
10	3	169	GLN
11	4	55	GLN
11	4	61	GLN
11	4	65	GLN
11	4	133	HIS
12	5	128	GLN
12	5	218	ASN
12	5	251	ASN
12	5	254	HIS
12	5	263	HIS
12	5	265	ASN
12	5	266	HIS
12	5	283	ASN
13	6	87	HIS
13	6	163	ASN
13	6	205	GLN

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Mol	Chain	Res	Type
14	7	59	ASN
14	7	81	ASN
14	7	95	HIS
14	7	145	ASN
14	7	153	GLN
14	7	182	HIS
15	W	29	GLN
15	W	44	ASN
15	W	77	HIS
15	W	92	GLN
15	W	106	GLN
15	W	108	GLN
15	W	143	ASN
15	W	149	GLN
15	W	165	GLN
16	V	102	GLN
16	V	181	ASN
16	V	193	ASN
16	V	195	HIS
16	V	200	ASN
16	V	215	ASN
17	T	112	ASN
17	T	118	ASN
17	T	123	HIS
17	T	236	ASN
18	X	18	ASN
18	X	38	ASN
18	X	105	ASN
18	X	130	ASN
19	Y	25	ASN
19	Y	63	ASN
19	Y	89	GLN
20	Z	9	GLN
20	Z	132	HIS
20	Z	151	HIS
20	Z	215	ASN
20	Z	275	GLN
20	Z	307	HIS
20	Z	338	HIS
20	Z	379	GLN
20	Z	391	ASN
20	Z	403	ASN

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Mol	Chain	Res	Type
20	Z	405	ASN
20	Z	427	GLN
20	Z	475	GLN
20	Z	502	ASN
20	Z	628	ASN
20	Z	763	HIS
20	Z	769	ASN
20	Z	771	HIS
20	Z	789	GLN
20	Z	829	GLN
20	Z	871	HIS
20	Z	897	HIS
20	Z	905	ASN
20	Z	926	ASN
20	Z	938	GLN
21	N	111	GLN
21	N	116	GLN
21	N	187	ASN
21	N	199	ASN
21	N	231	ASN
21	N	256	GLN
21	N	280	GLN
21	N	375	HIS
21	N	378	ASN
21	N	506	GLN
21	N	509	GLN
21	N	510	HIS
21	N	613	HIS
21	N	614	ASN
21	N	654	GLN
21	N	666	GLN
21	N	674	GLN
21	N	690	HIS
21	N	703	GLN
21	N	747	HIS
21	N	859	ASN
21	N	900	ASN
22	S	19	HIS
22	S	32	GLN
22	S	91	ASN
22	S	100	HIS
22	S	122	ASN

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Mol	Chain	Res	Type
22	S	135	ASN
22	S	280	ASN
22	S	283	GLN
22	S	312	GLN
22	S	335	GLN
22	S	412	ASN
22	S	488	GLN
22	S	490	ASN
23	P	30	ASN
23	P	88	GLN
23	P	164	GLN
23	P	296	GLN
23	P	334	ASN
23	P	337	HIS
23	P	348	HIS
23	P	401	ASN
23	P	410	GLN
23	P	440	HIS
24	Q	16	ASN
24	Q	21	ASN
24	Q	54	GLN
24	Q	106	GLN
24	Q	114	GLN
24	Q	145	HIS
24	Q	147	GLN
24	Q	178	HIS
24	Q	186	HIS
24	Q	206	ASN
24	Q	315	ASN
24	Q	346	ASN
24	Q	392	GLN
24	Q	420	ASN
25	R	23	ASN
25	R	35	GLN
25	R	76	GLN
25	R	136	ASN
25	R	143	GLN
25	R	184	GLN
25	R	208	ASN
25	R	314	ASN
25	R	323	ASN
25	R	325	HIS

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Mol	Chain	Res	Type
25	R	340	GLN
25	R	378	ASN
25	R	395	ASN
25	R	401	HIS
25	R	406	GLN
26	U	4	GLN
26	U	21	HIS
26	U	26	GLN
26	U	30	ASN
26	U	50	ASN
26	U	70	HIS
26	U	75	ASN
26	U	84	ASN
26	U	201	GLN
26	U	222	ASN
26	U	230	GLN
26	U	234	ASN
27	O	75	GLN
27	O	105	GLN
27	O	107	GLN
27	O	114	GLN
27	O	141	ASN
27	O	183	ASN
27	O	236	HIS
27	O	282	GLN
27	O	362	GLN
27	O	376	GLN
27	O	389	GLN
28	H	109	ASN
28	H	120	ASN
28	H	121	ASN
28	H	128	ASN
28	H	148	ASN
28	H	217	GLN
28	H	348	ASN
28	H	356	ASN
28	H	387	ASN
28	H	392	HIS
29	I	117	HIS
29	I	151	HIS
29	I	266	GLN
29	I	329	ASN

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Mol	Chain	Res	Type
29	I	365	HIS
30	K	74	HIS
30	K	98	GLN
30	K	200	GLN
31	L	58	ASN
31	L	242	ASN
31	L	273	HIS
31	L	317	ASN
31	L	328	ASN
31	L	364	HIS
31	L	387	ASN
31	L	409	HIS
31	L	411	ASN
32	M	71	ASN
32	M	72	ASN
32	M	74	GLN
32	M	107	ASN
32	M	125	GLN
32	M	143	ASN
32	M	149	ASN
32	M	189	GLN
32	M	240	ASN
33	J	28	GLN
33	J	52	ASN
33	J	220	GLN
33	J	240	HIS
33	J	269	GLN
33	J	336	ASN
33	J	351	ASN
33	J	376	HIS
33	J	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	ATP	J	501	35	32,33,33	4.11	6 (18%)	48,52,52	1.53	3 (6%)
36	ADP	M	501	35	28,29,29	1.56	4 (14%)	43,45,45	1.45	3 (6%)
36	ADP	L	501	35	28,29,29	2.74	5 (17%)	43,45,45	1.47	8 (18%)
34	ATP	K	501	35	32,33,33	4.16	8 (25%)	48,52,52	1.85	12 (25%)
34	ATP	I	501	35	32,33,33	4.03	8 (25%)	48,52,52	1.91	13 (27%)
34	ATP	H	501	35	32,33,33	5.08	10 (31%)	48,52,52	1.41	6 (12%)

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

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

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	501	ATP	PB-O3A	19.67	1.80	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	501	ATP	PB-O3B	16.37	1.77	1.59
34	I	501	ATP	PB-O3B	15.49	1.76	1.59
34	K	501	ATP	PB-O3B	14.20	1.74	1.59
34	J	501	ATP	PB-O3B	14.04	1.74	1.59
34	J	501	ATP	PB-O3A	13.77	1.74	1.59
34	K	501	ATP	PB-O3A	13.60	1.74	1.59
34	I	501	ATP	PB-O3A	13.56	1.74	1.59
36	L	501	ADP	PA-O3A	12.98	1.73	1.59
34	K	501	ATP	PA-O3A	10.95	1.71	1.59
34	J	501	ATP	PA-O3A	9.88	1.70	1.59
34	H	501	ATP	PA-O3A	8.96	1.69	1.59
34	I	501	ATP	PA-O3A	6.60	1.66	1.59
36	M	501	ADP	PA-O3A	4.82	1.64	1.59
34	J	501	ATP	C3'-C4'	-4.34	1.42	1.53
36	M	501	ADP	C5-C4	4.33	1.46	1.39
34	H	501	ATP	O4'-C4'	4.33	1.54	1.45
34	H	501	ATP	C8-N9	3.66	1.43	1.37
34	I	501	ATP	O4'-C4'	-3.18	1.37	1.45
34	I	501	ATP	C3'-C4'	2.78	1.60	1.53
36	L	501	ADP	C3'-C4'	-2.74	1.46	1.53
36	L	501	ADP	C2-N1	2.66	1.38	1.33
34	H	501	ATP	C5-N7	2.66	1.43	1.39
34	K	501	ATP	C8-N9	2.61	1.42	1.37
34	H	501	ATP	PG-O1G	2.55	1.58	1.50
34	I	501	ATP	C8-N7	-2.42	1.27	1.31
34	I	501	ATP	C5-N7	-2.34	1.34	1.39
34	K	501	ATP	C2-N1	-2.32	1.29	1.33
34	K	501	ATP	O2'-C2'	-2.31	1.37	1.43
36	L	501	ADP	C6-N1	2.29	1.42	1.35
34	J	501	ATP	C5-C4	-2.27	1.35	1.39
34	K	501	ATP	O3'-C3'	2.23	1.48	1.43
36	M	501	ADP	C5-N7	2.19	1.43	1.39
34	J	501	ATP	C2-N3	2.13	1.37	1.33
34	H	501	ATP	C5-C4	2.10	1.42	1.39
36	M	501	ADP	PA-O5'	2.08	1.67	1.59
36	L	501	ADP	C8-N9	2.06	1.41	1.37
34	I	501	ATP	PA-O2A	-2.04	1.45	1.55
34	H	501	ATP	C5'-C4'	2.04	1.57	1.51
34	H	501	ATP	C5-C6	-2.03	1.35	1.41
34	K	501	ATP	PA-O2A	-2.02	1.46	1.55

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	J	501	ATP	N6-C6-N1	6.07	131.89	118.38
34	I	501	ATP	N6-C6-N1	5.49	130.60	118.38
34	I	501	ATP	C4-N9-C1'	5.33	139.09	126.63
34	K	501	ATP	N6-C6-N1	4.79	129.06	118.38
34	J	501	ATP	C5-C6-N6	-4.70	111.65	123.29
34	H	501	ATP	N6-C6-N1	4.48	128.36	118.38
34	K	501	ATP	C5-C4-N3	-4.30	120.79	126.72
34	I	501	ATP	C1'-N9-C8	-4.16	117.86	127.09
34	K	501	ATP	C5-N7-C8	4.12	109.93	103.45
36	M	501	ADP	N6-C6-N1	4.00	127.30	118.38
34	K	501	ATP	N9-C8-N7	-3.82	108.52	113.94
34	H	501	ATP	C5-C6-N6	-3.82	113.83	123.29
36	L	501	ADP	N6-C6-N1	3.75	126.72	118.38
36	L	501	ADP	C5-C6-N6	-3.67	114.19	123.29
36	M	501	ADP	N9-C8-N7	3.49	118.88	113.94
34	K	501	ATP	C5-C6-N6	-3.43	114.79	123.29
34	I	501	ATP	O4'-C1'-N9	3.36	114.53	108.09
34	K	501	ATP	C4-C5-N7	-3.34	106.76	110.58
36	L	501	ADP	C2-N1-C6	-3.27	113.36	118.73
34	I	501	ATP	C4-N9-C8	-3.17	102.41	105.74
34	I	501	ATP	C2-N1-C6	2.86	123.43	118.73
36	L	501	ADP	C4-N9-C8	-2.86	102.74	105.74
34	I	501	ATP	C5-C6-N6	-2.71	116.58	123.29
34	J	501	ATP	O4'-C1'-N9	2.65	113.19	108.09
36	M	501	ADP	C4-C5-N7	-2.58	107.63	110.58
34	I	501	ATP	O2B-PB-O3A	2.55	114.15	107.27
34	H	501	ATP	O5'-C5'-C4'	2.53	117.62	108.99
34	I	501	ATP	C5-N7-C8	2.41	107.23	103.45
34	K	501	ATP	C6-C5-C4	2.34	120.37	117.18
34	I	501	ATP	O3B-PB-O1B	-2.31	103.75	110.70
34	I	501	ATP	O4'-C4'-C3'	-2.31	100.57	105.15
34	K	501	ATP	C2-N1-C6	-2.27	115.00	118.73
34	H	501	ATP	O3G-PG-O2G	2.24	116.19	107.80
34	H	501	ATP	O2A-PA-O3A	2.20	113.23	107.27
36	L	501	ADP	C4-N9-C1'	2.20	131.77	126.63
34	K	501	ATP	N3-C4-N9	2.16	130.84	127.17
34	H	501	ATP	O4'-C4'-C3'	-2.14	100.91	105.15
36	L	501	ADP	N3-C2-N1	2.12	131.79	128.58
36	L	501	ADP	C5-C4-N9	2.11	108.11	105.81
34	K	501	ATP	N3-C2-N1	2.09	131.74	128.58
34	K	501	ATP	C5-C4-N9	2.08	108.08	105.81
34	K	501	ATP	O3G-PG-O2G	2.07	115.56	107.80
36	L	501	ADP	C5-C4-N3	-2.06	123.89	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	501	ATP	O3A-PA-O1A	-2.04	104.58	110.70
34	I	501	ATP	O4'-C4'-C5'	2.03	115.83	109.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O2A
34	I	501	ATP	C5'-O5'-PA-O3A
34	K	501	ATP	C5'-O5'-PA-O1A
34	K	501	ATP	C5'-O5'-PA-O2A
34	K	501	ATP	C5'-O5'-PA-O3A
34	J	501	ATP	C5'-O5'-PA-O1A
34	J	501	ATP	C5'-O5'-PA-O2A
34	J	501	ATP	C5'-O5'-PA-O3A
36	L	501	ADP	C5'-O5'-PA-O2A
36	L	501	ADP	C5'-O5'-PA-O3A
36	M	501	ADP	PA-O3A-PB-O2B
36	M	501	ADP	PA-O3A-PB-O3B
36	M	501	ADP	C5'-O5'-PA-O2A
36	M	501	ADP	C5'-O5'-PA-O3A
34	H	501	ATP	C4'-C5'-O5'-PA
34	H	501	ATP	O4'-C4'-C5'-O5'
34	K	501	ATP	C2'-C1'-N9-C8
34	H	501	ATP	C5'-O5'-PA-O1A
34	I	501	ATP	C5'-O5'-PA-O1A
34	I	501	ATP	C2'-C1'-N9-C8
34	K	501	ATP	C2'-C1'-N9-C4
34	K	501	ATP	O4'-C1'-N9-C8
36	L	501	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

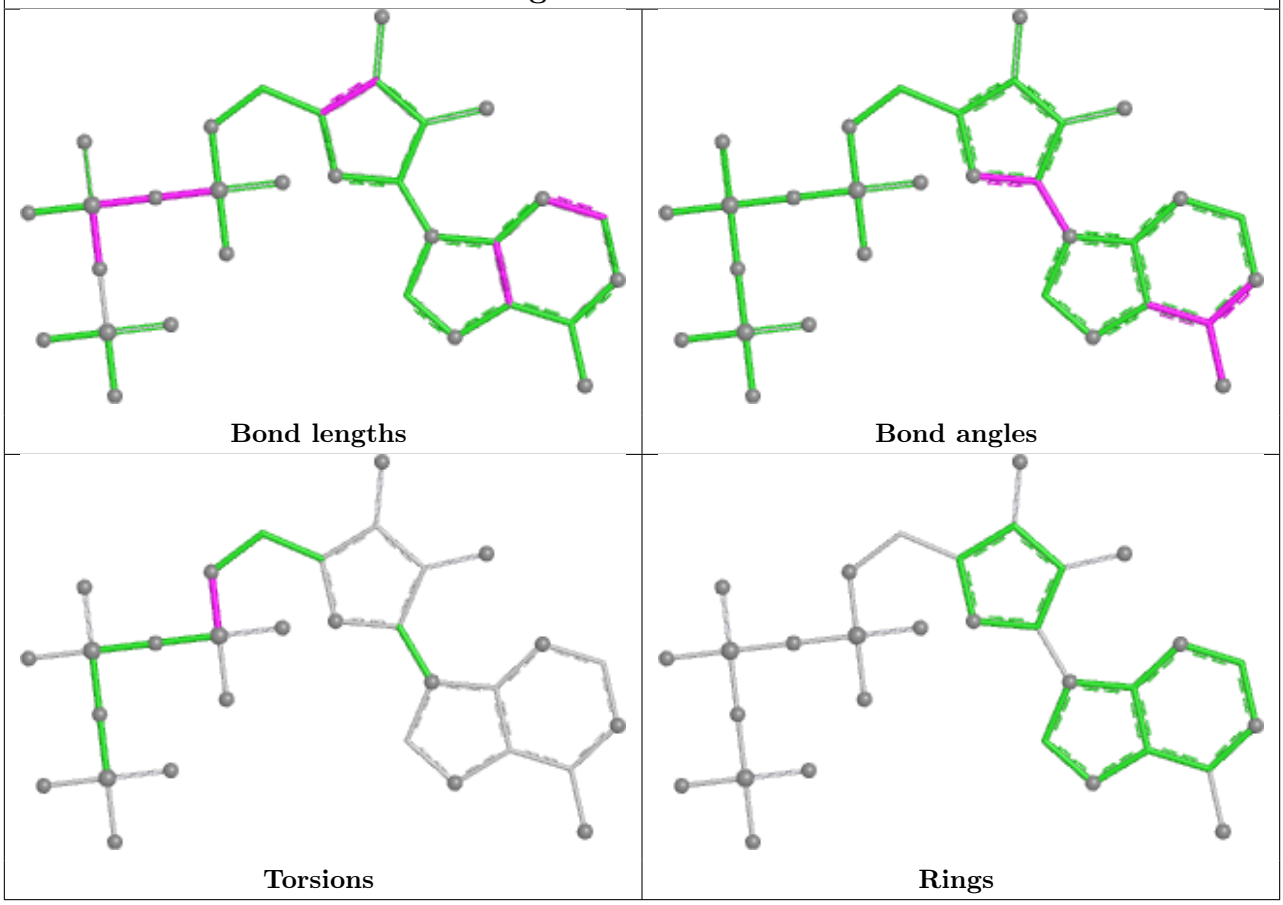
1 monomer is involved in 2 short contacts:

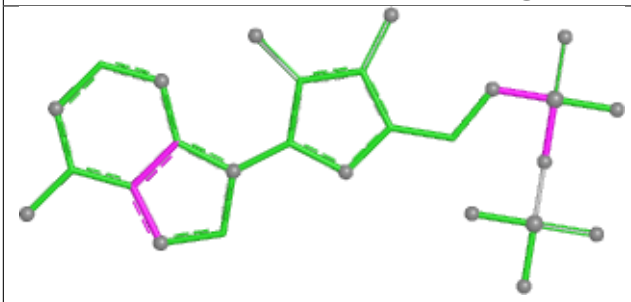
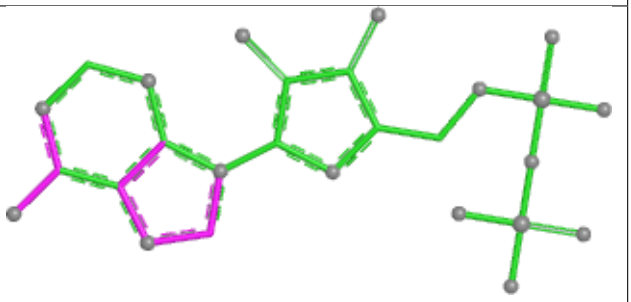
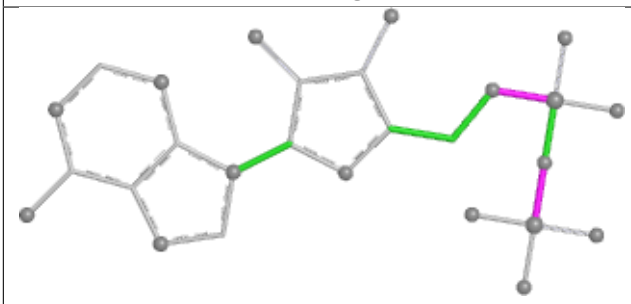
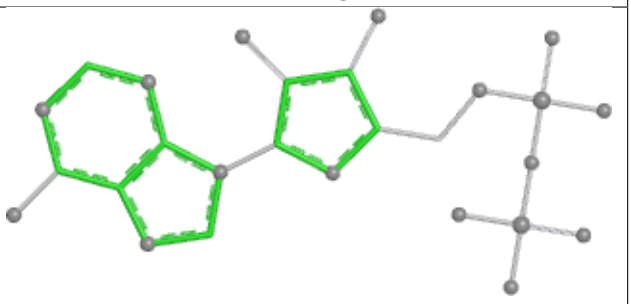
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	K	501	ATP	2	0

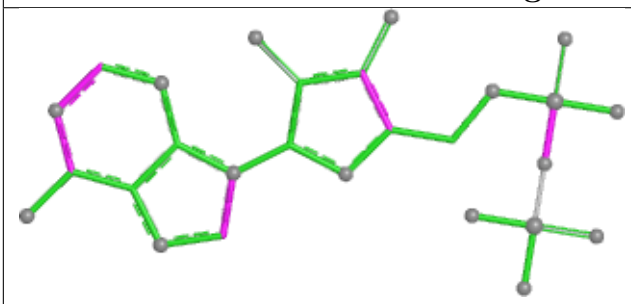
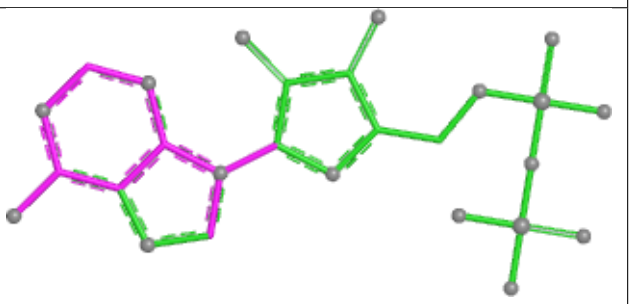
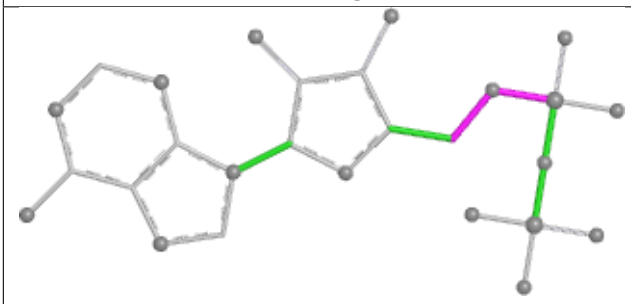
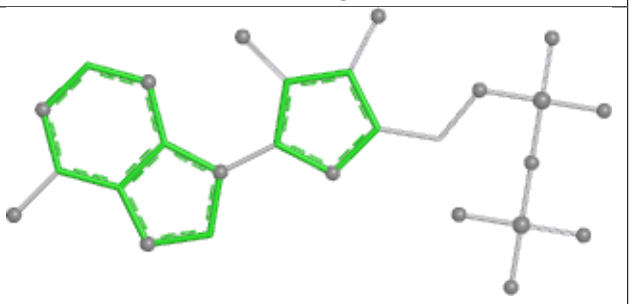
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

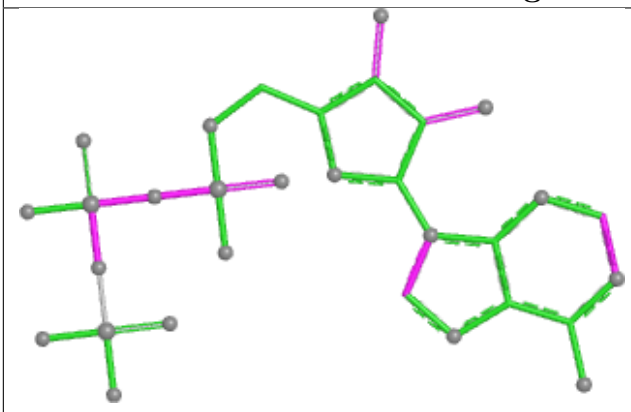
Ligand ATP J 501



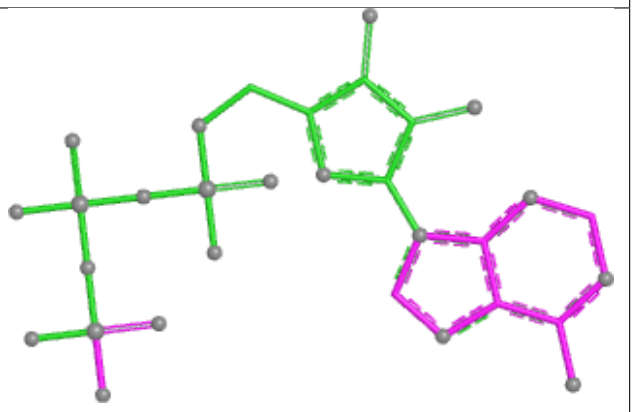
Ligand ADP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

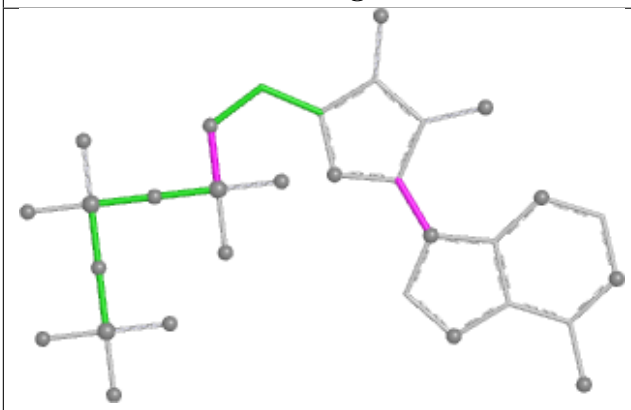
Ligand ATP K 501



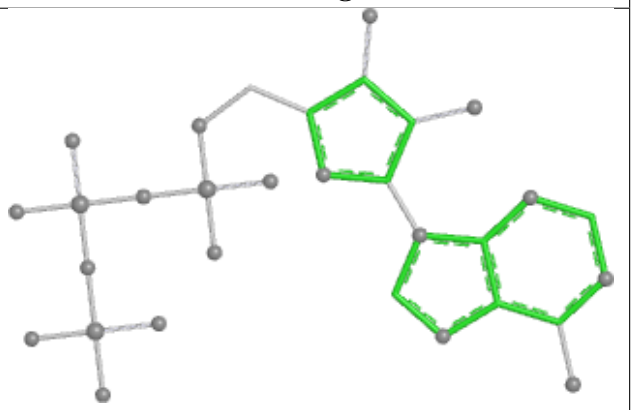
Bond lengths



Bond angles

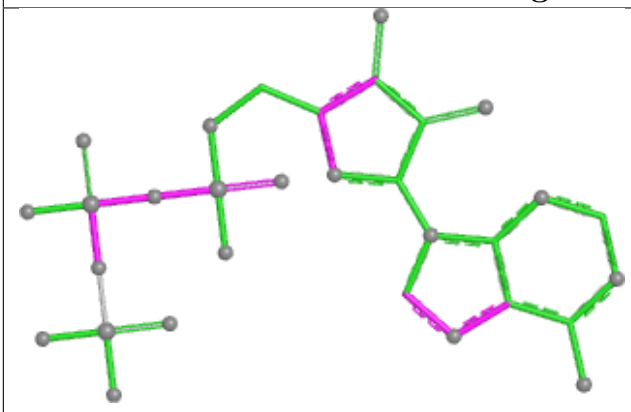


Torsions

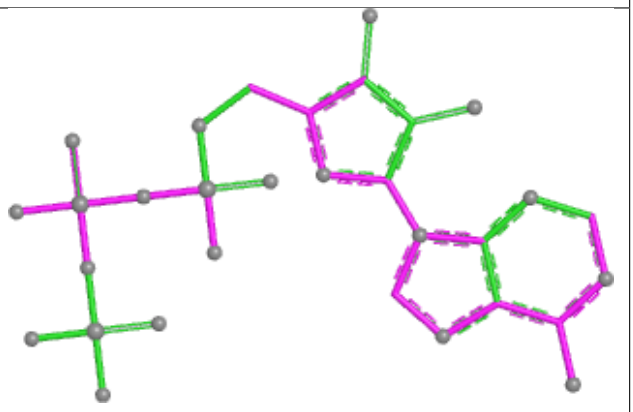


Rings

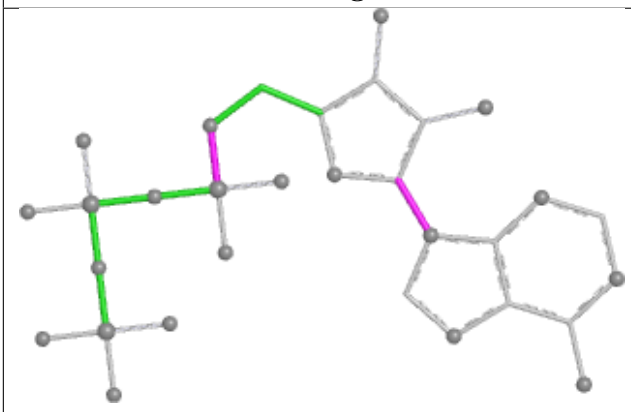
Ligand ATP I 501



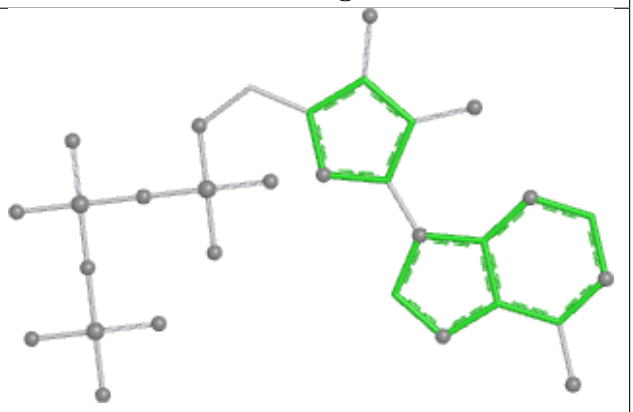
Bond lengths



Bond angles

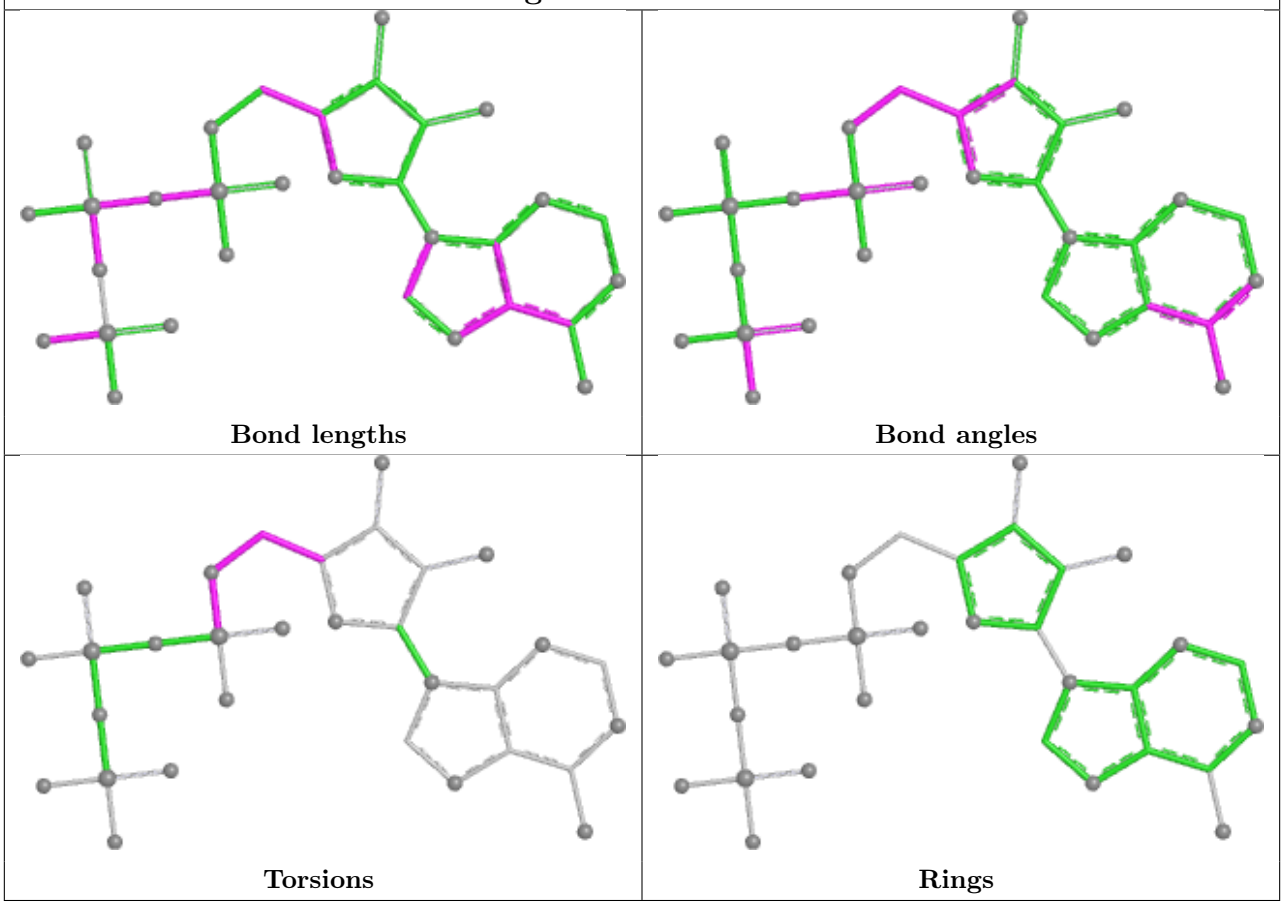


Torsions



Rings

Ligand ATP H 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

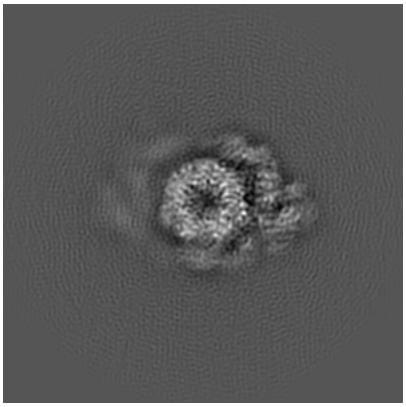
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4324. These allow visual inspection of the internal detail of the map and identification of artifacts.

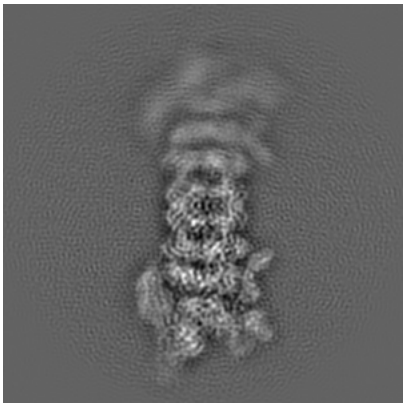
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

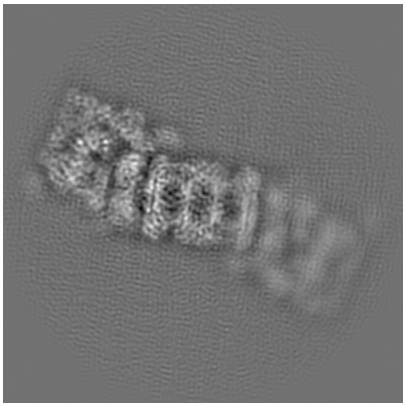
6.1.1 Primary map



X



Y

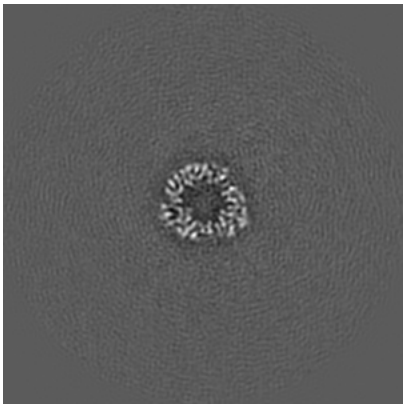


Z

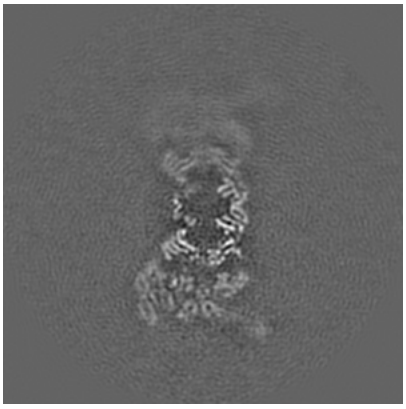
The images above show the map projected in three orthogonal directions.

6.2 Central slices

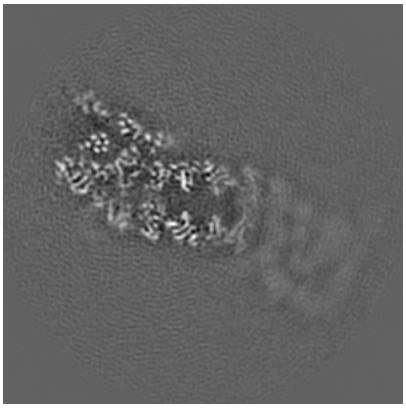
6.2.1 Primary map



X Index: 192



Y Index: 192

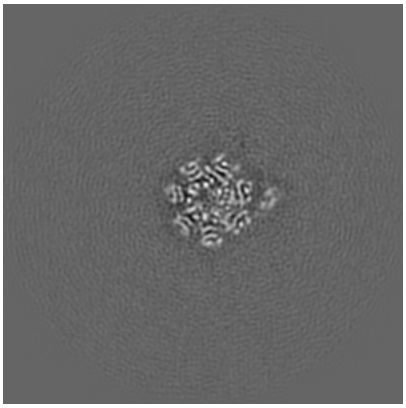


Z Index: 192

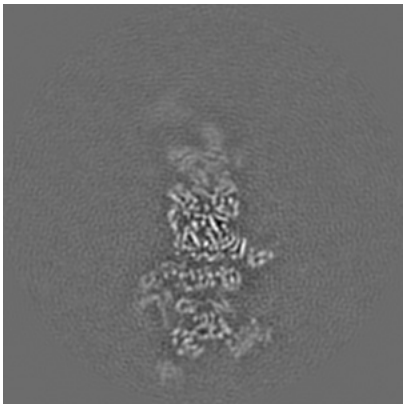
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

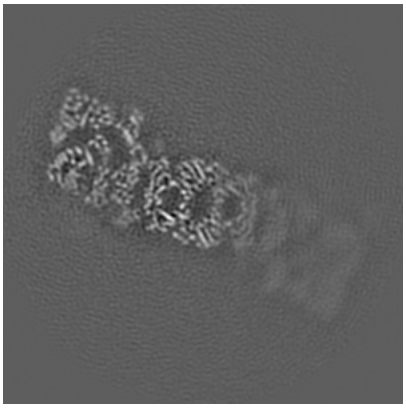
6.3.1 Primary map



X Index: 150



Y Index: 213

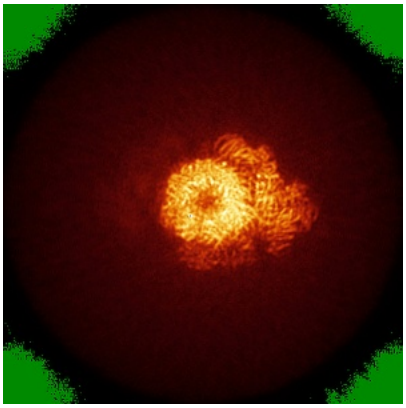


Z Index: 181

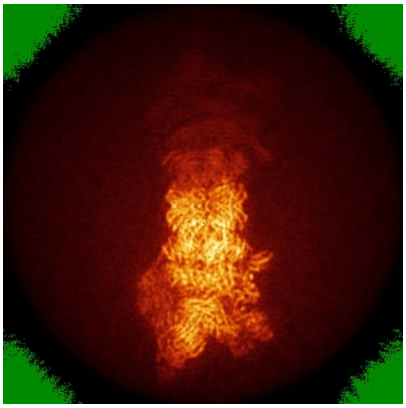
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

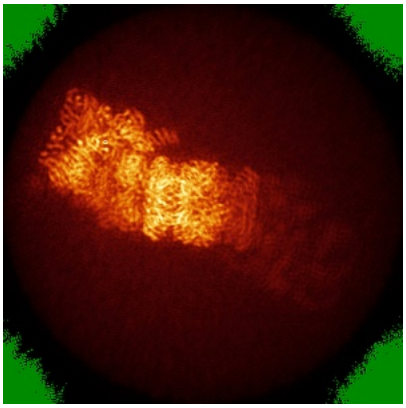
6.4.1 Primary map



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

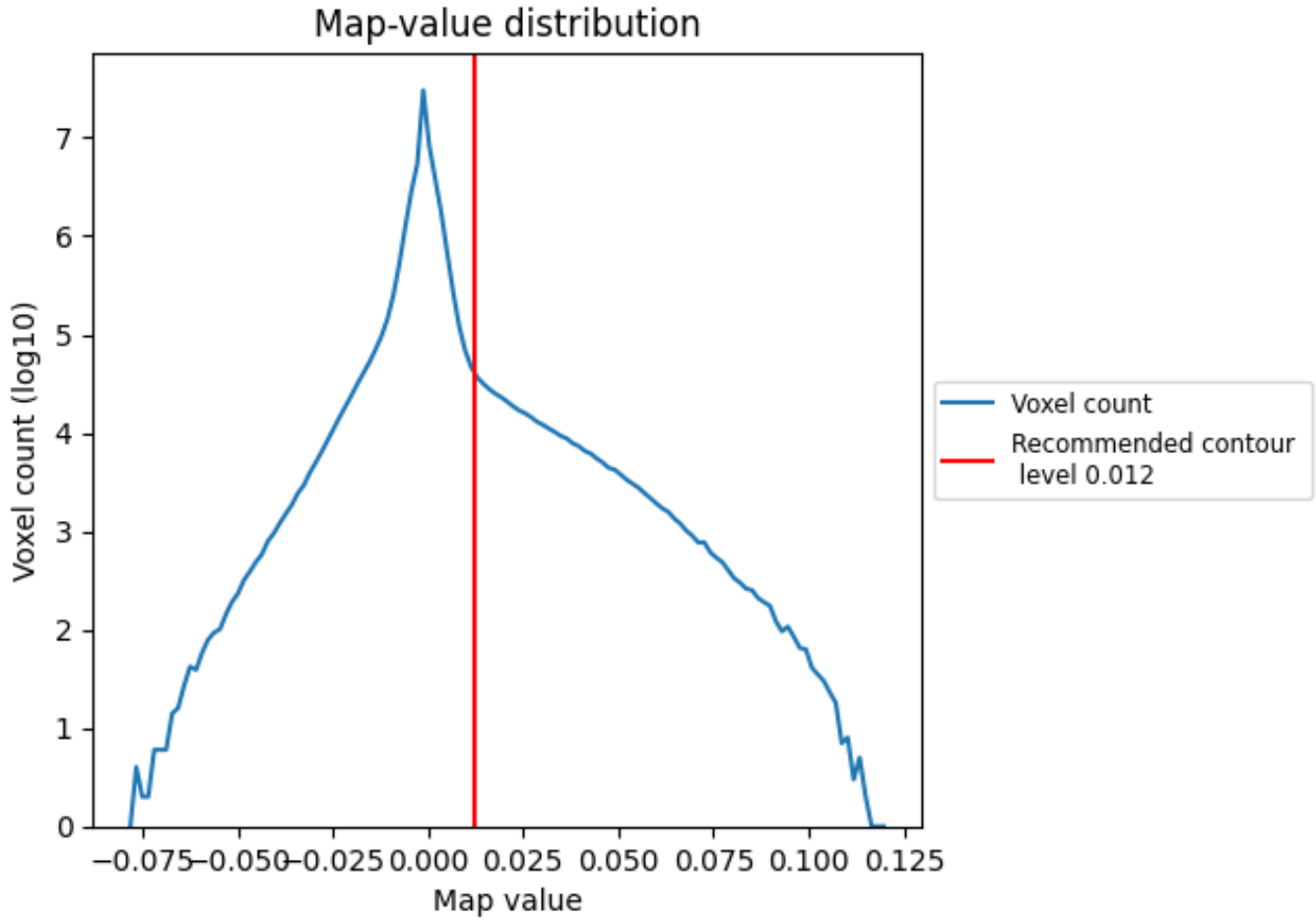
6.6 Mask visualisation (i)

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

7 Map analysis

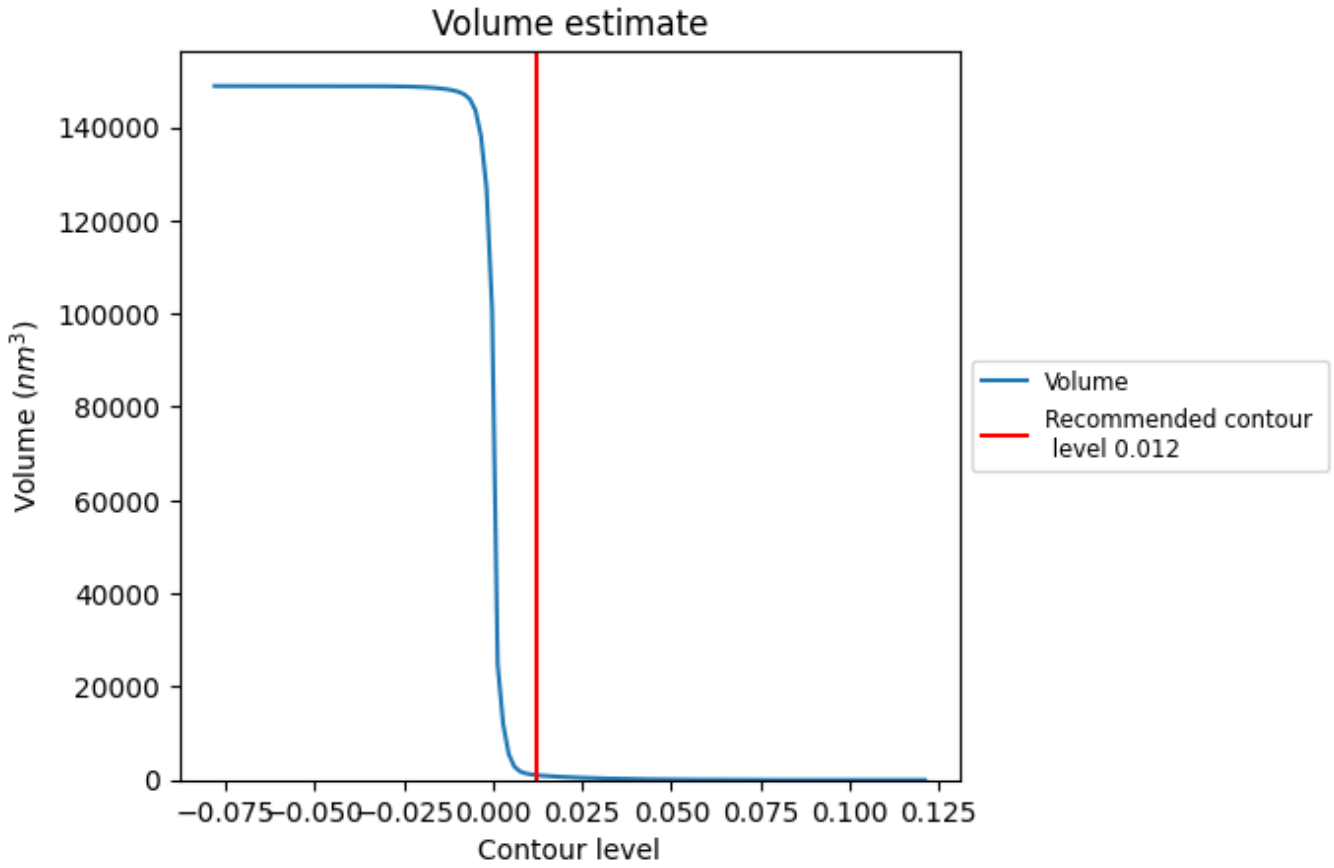
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

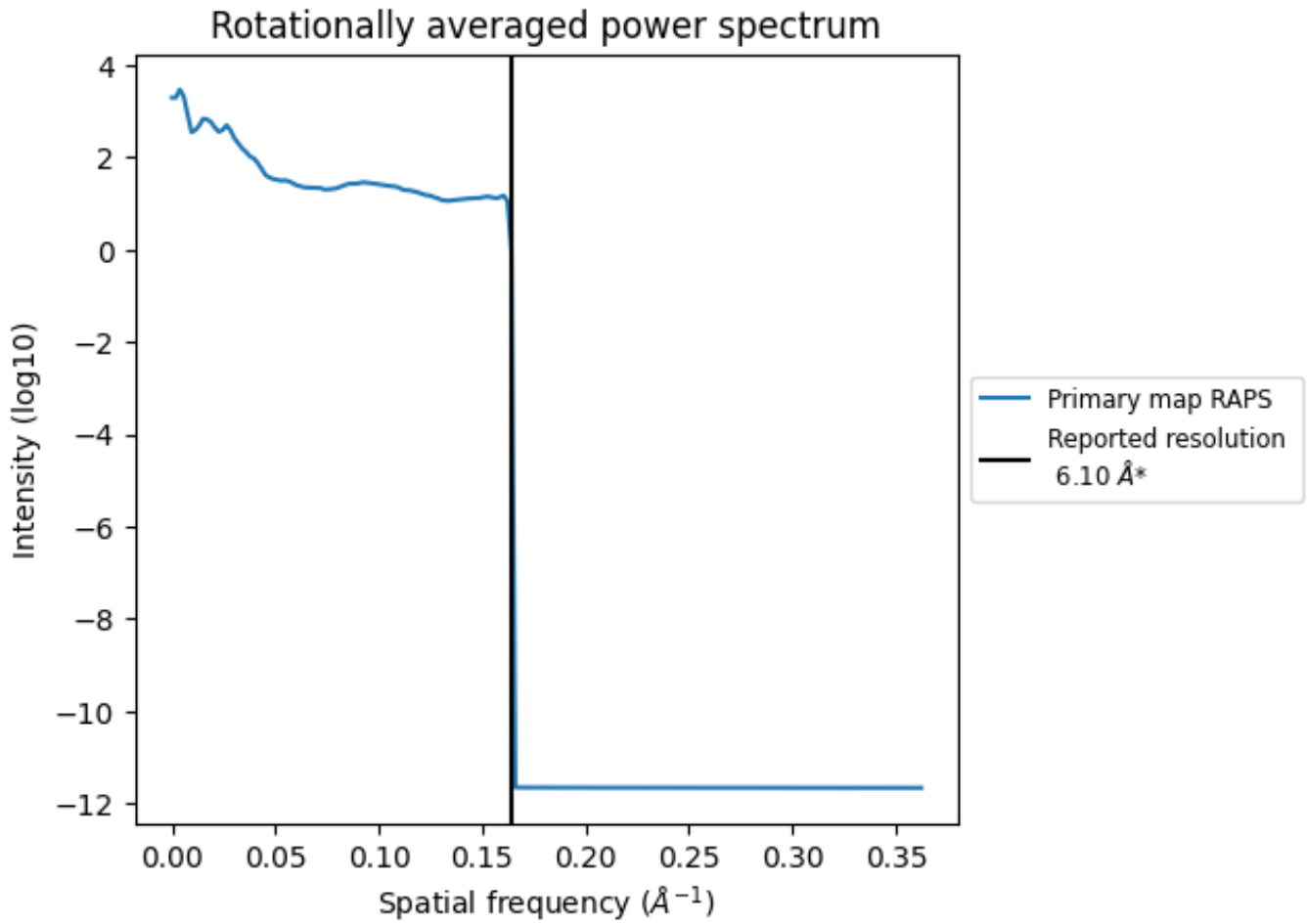
7.2 Volume estimate



The volume at the recommended contour level is 1059 nm^3; this corresponds to an approximate mass of 957 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 (i)



*Reported resolution corresponds to spatial frequency of 0.164 Å^{-1}

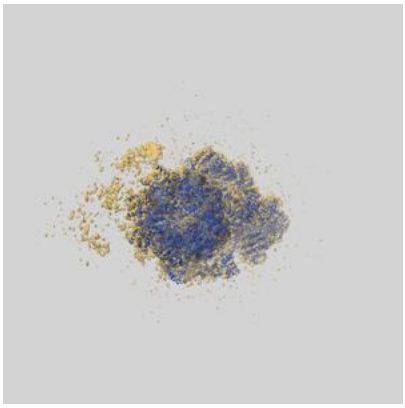
8 Fourier-Shell correlation

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

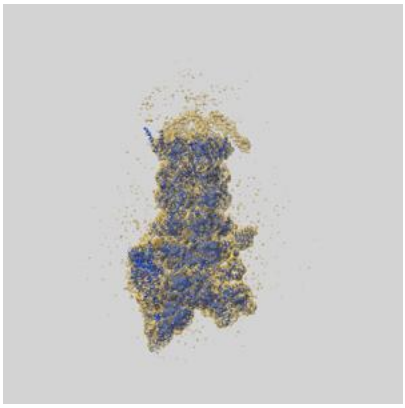
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4324 and PDB model 6FVY. Per-residue inclusion information can be found in section 3 on page 13.

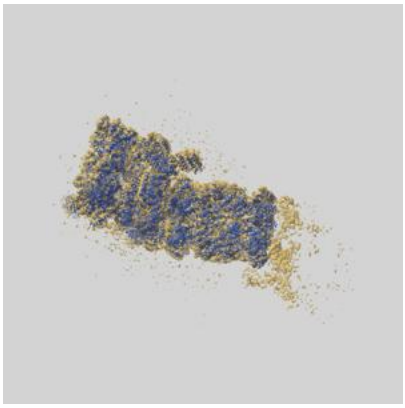
9.1 Map-model overlay



X



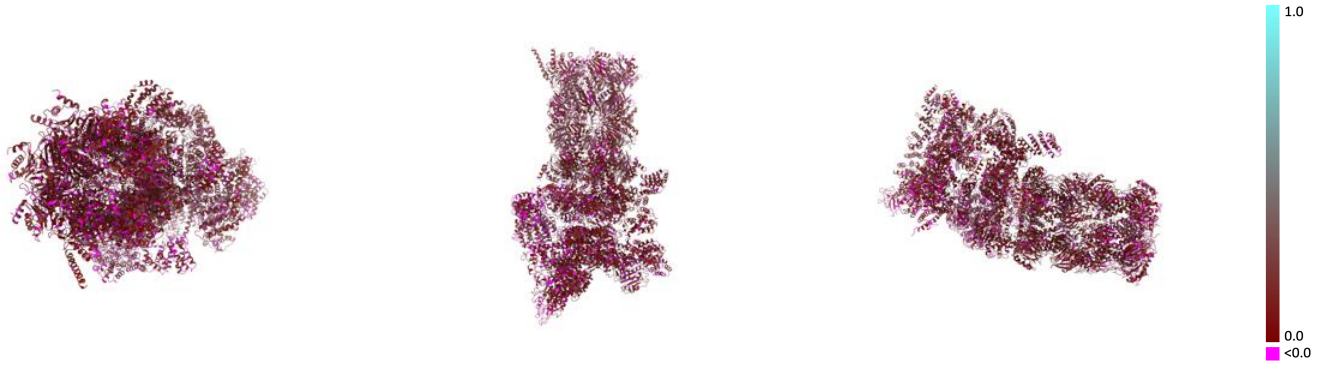
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

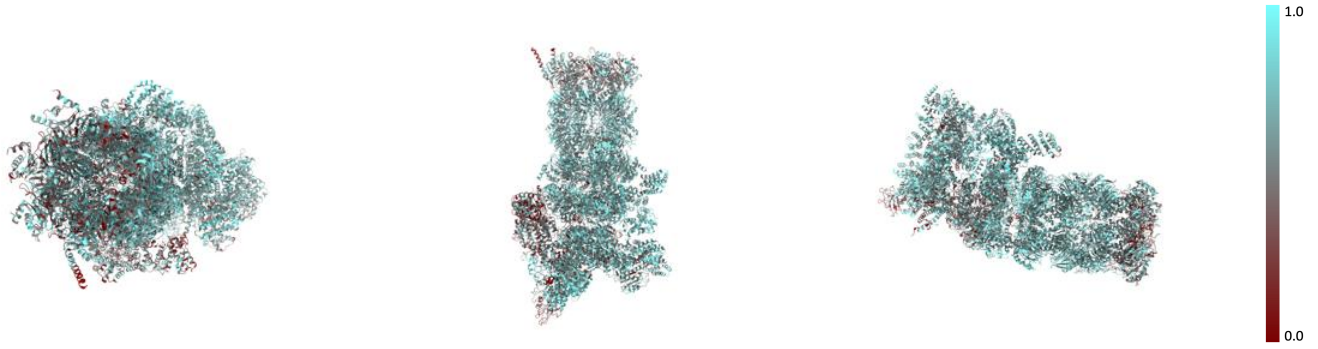
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

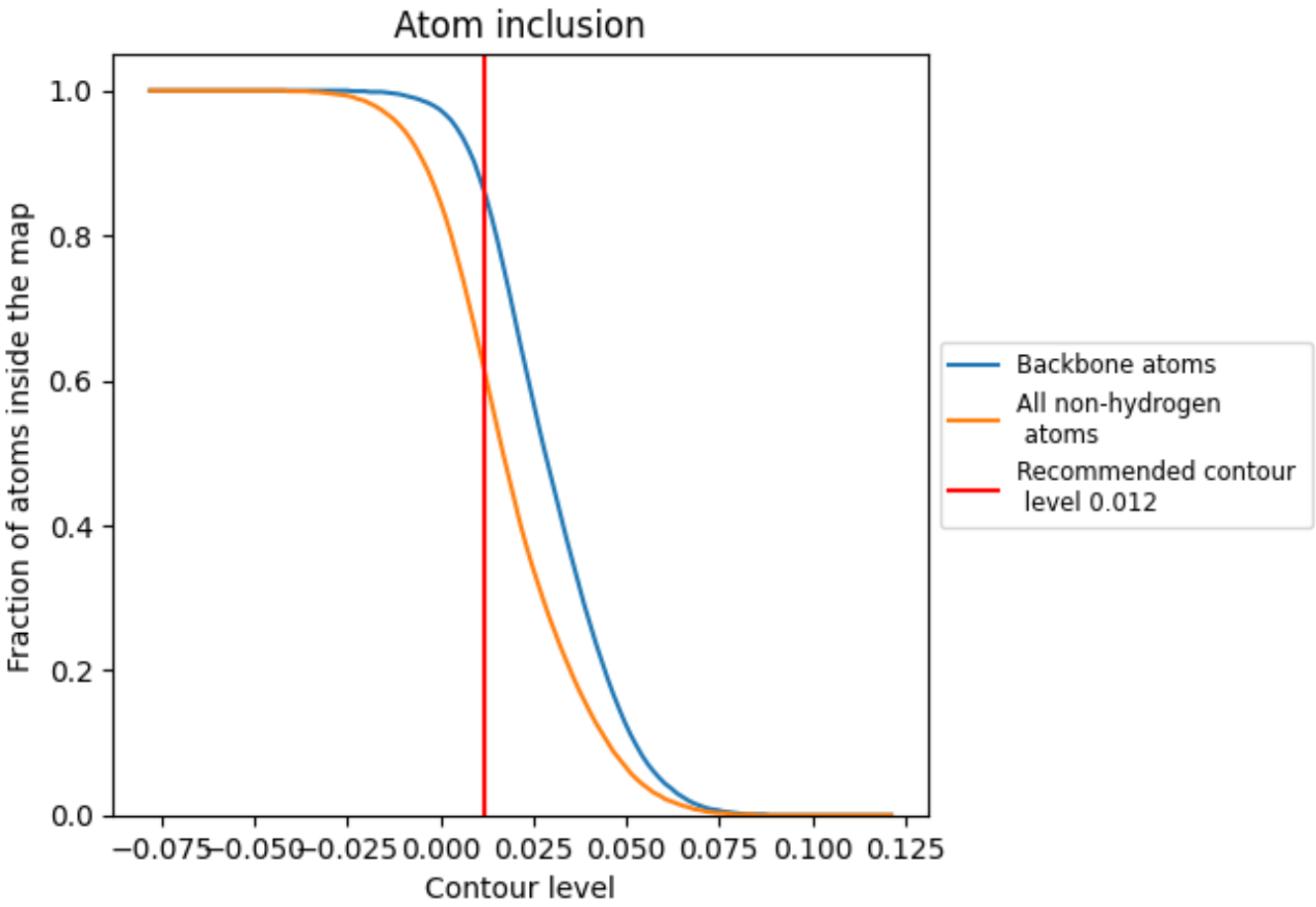
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.1360
1	0.7010	0.1640
2	0.6930	0.1730
3	0.6640	0.1570
4	0.6930	0.1590
5	0.7230	0.1650
6	0.7030	0.1680
7	0.7080	0.1630
A	0.6790	0.1610
B	0.6830	0.1720
C	0.6730	0.1650
D	0.6820	0.1620
E	0.6750	0.1630
F	0.7080	0.1770
G	0.7000	0.1750
H	0.5330	0.1100
I	0.5800	0.1360
J	0.5710	0.1200
K	0.6120	0.1380
L	0.6340	0.1470
M	0.5820	0.1220
N	0.6430	0.1420
O	0.6700	0.1350
P	0.7320	0.1450
Q	0.6910	0.1360
R	0.6860	0.1350
S	0.6050	0.1280
T	0.6300	0.1350
U	0.5990	0.1340
V	0.6320	0.1410
W	0.5700	0.1240
X	0.2030	0.0430
Y	0.4440	0.0820
Z	0.4330	0.0710
a	0.4870	0.1350

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Chain	Atom inclusion	Q-score
b	0.4730	0.1430
c	0.4800	0.1220
d	0.4360	0.1190
e	0.4650	0.1210
f	0.5030	0.1260
g	0.4960	0.1360
h	0.6720	0.1370
i	0.6480	0.1460
j	0.6520	0.1450
k	0.6340	0.1410
l	0.6740	0.1520
m	0.6580	0.1460
n	0.6590	0.1530