Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID	:	6FVX / pdb_00006fvx
EMDB ID	:	EMD-4323
Title	:	26S proteasome, s5 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	4.90 Å(reported)

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

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

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

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

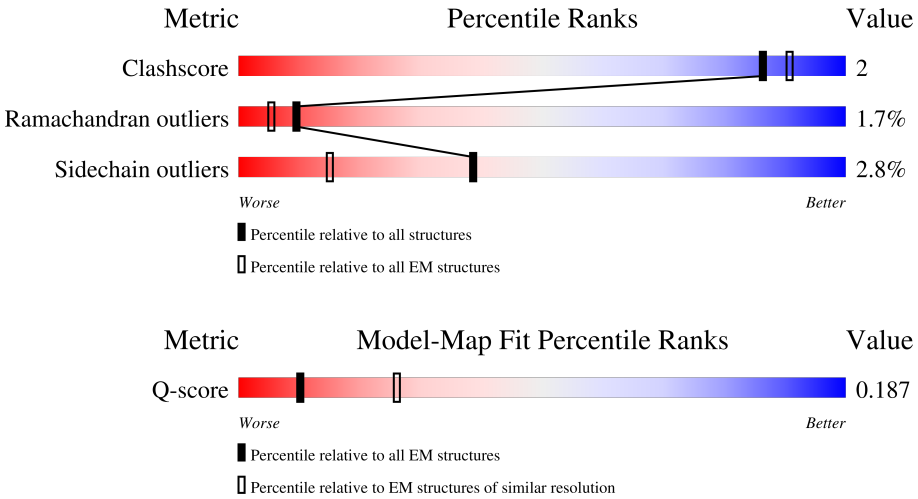
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 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	1274 (4.40 - 5.40)

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	242	44% 48% 7%
1	a	242	17% 49% 48%
2	B	246	45% 51%
2	b	246	22% 44% 52%

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Mol	Chain	Length	Quality of chain
3	C	241	49% 46% 5%
3	c	241	19% 49% 47%
4	D	252	42% 48% 6%
4	d	252	26% 45% 50%
5	E	244	5% 43% 52% 5%
5	e	244	21% 44% 50% 6%
6	F	232	46% 49%
6	f	232	20% 44% 48% 8%
7	G	244	48% 46% 5%
7	g	244	20% 51% 44% 5%
8	1	196	47% 48% 5%
8	h	196	47% 49%
9	2	226	43% 53%
9	i	226	8% 49% 47%
10	3	204	38% 57% 5%
10	j	204	54% 44%
11	4	195	45% 50% 5%
11	k	195	5% 41% 50% 9%
12	5	212	47% 49%
12	l	212	5% 45% 51%
13	6	222	45% 49% 6%
13	m	222	42% 54%
14	7	232	44% 51%
14	n	232	5% 43% 52% 5%
15	W	197	16% 50% 44% 5%

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Mol	Chain	Length	Quality of chain
16	V	289	10% 42% 52% 6%
17	T	266	24% 40% 55% 5%
18	X	127	87% 45% 46% 9%
19	Y	89	55% 37% 57% 6%
20	Z	970	61% 81% 10% 7%
21	N	922	14% 43% 52%
22	S	475	23% 43% 52% 5%
23	P	440	5% 46% 50%
24	Q	434	11% 42% 51% 7%
25	R	405	11% 42% 55%
26	U	304	12% 44% 53%
27	O	388	9% 44% 52%
28	H	426	26% 41% 52% 6%
29	I	385	19% 40% 52% 7%
30	K	394	18% 43% 53%
31	L	388	14% 48% 45% 6%
32	M	421	19% 44% 51% 5%
33	J	405	30% 44% 49% 6%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110471 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	246	Total	C	N	O	S	0	0
			1881	1200	308	370	3		
2	B	246	Total	C	N	O	S	0	0
			1881	1200	308	370	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	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		
5	E	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	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	244	Total	C	N	O	S	0	0
			1897	1205	330	358	4		
7	G	244	Total	C	N	O	S	0	0
			1897	1205	330	358	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		

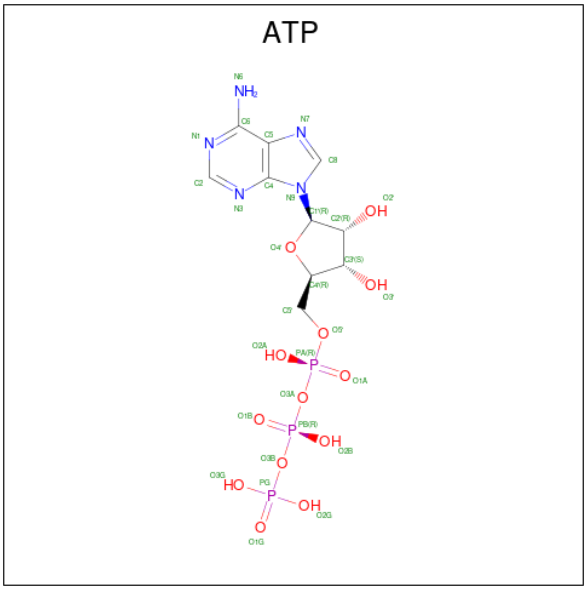
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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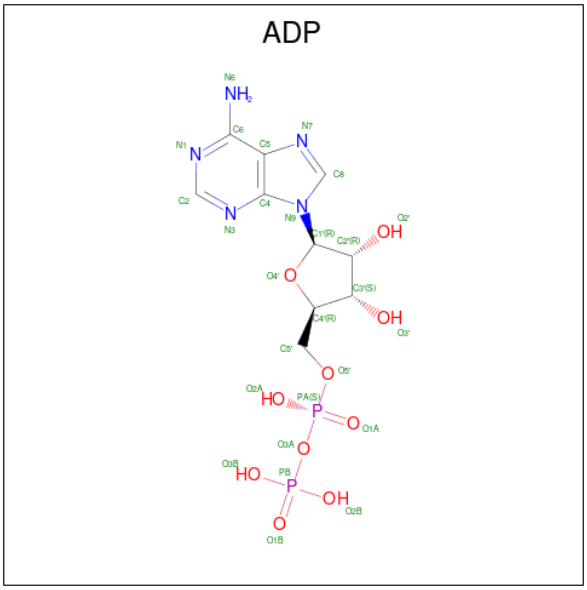
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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



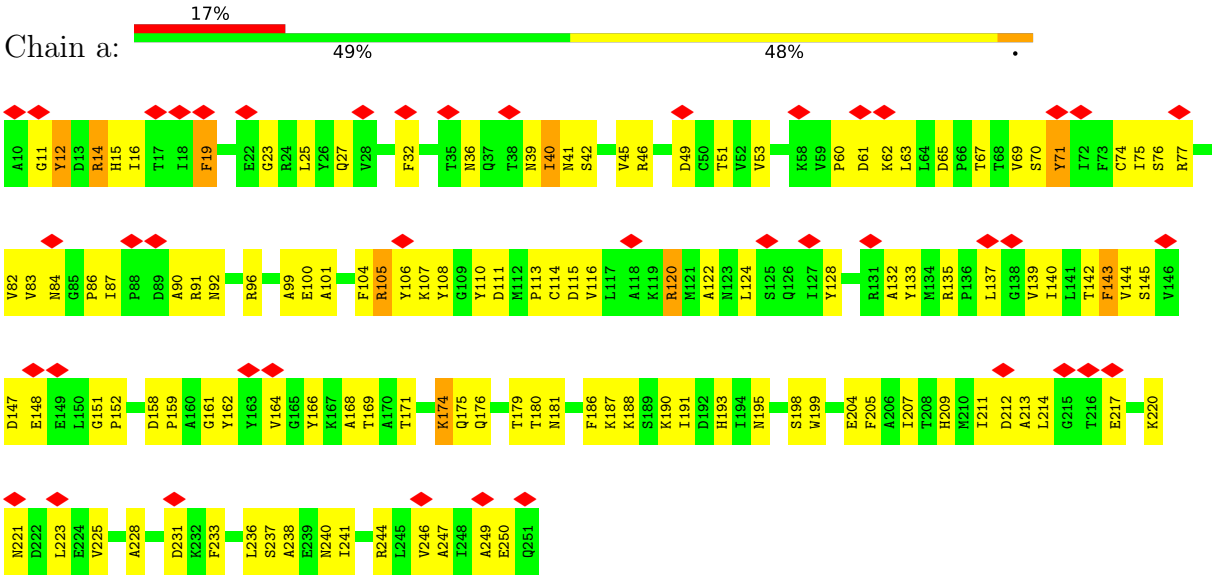
Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

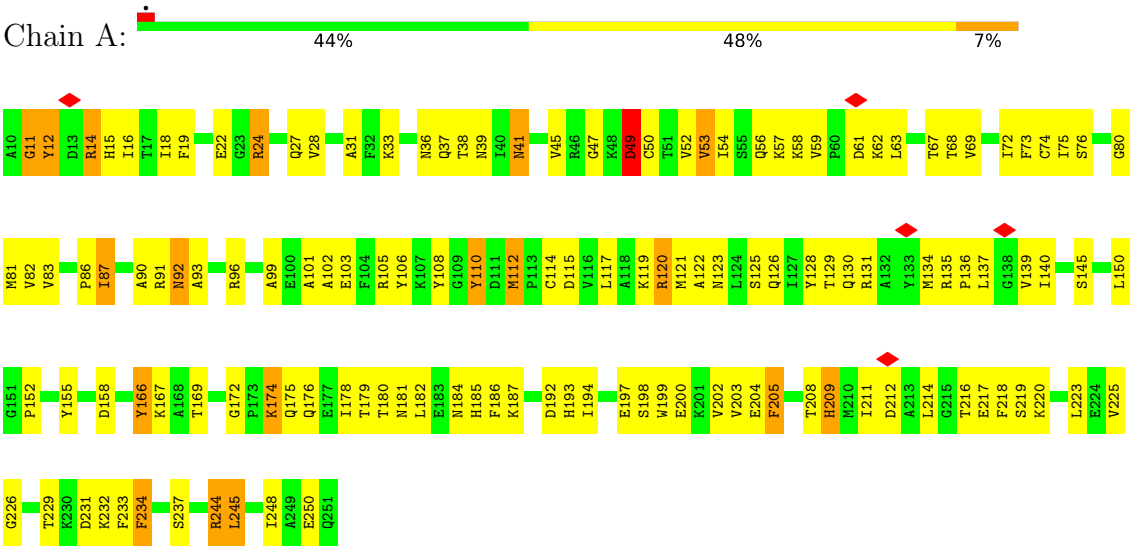
• Molecule 1: Proteasome subunit alpha type-1

Chain a:



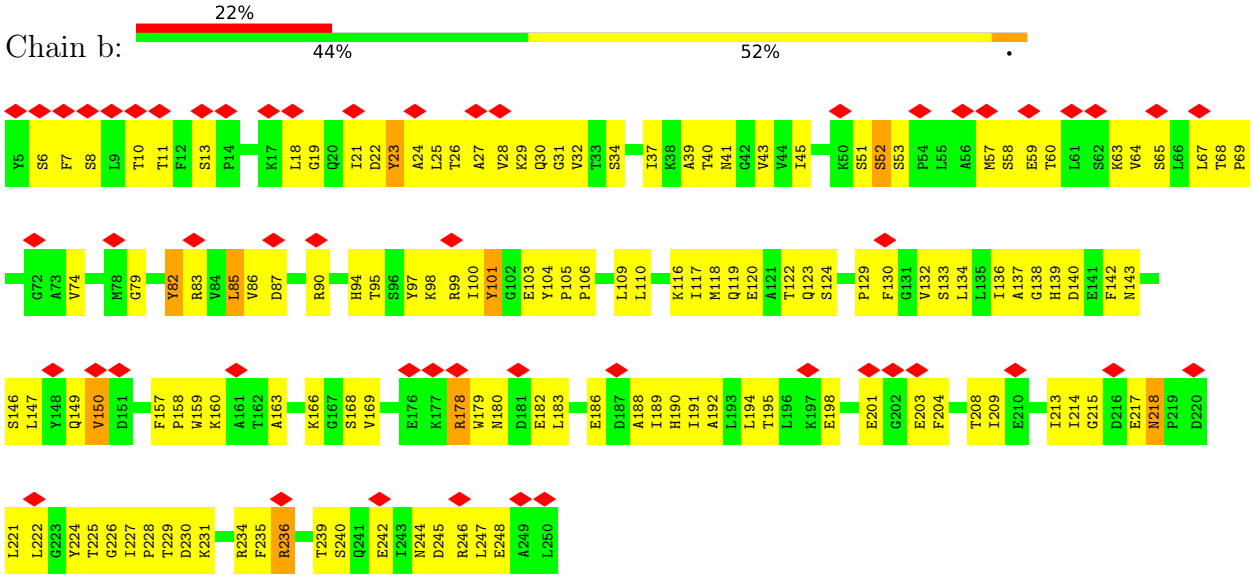
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



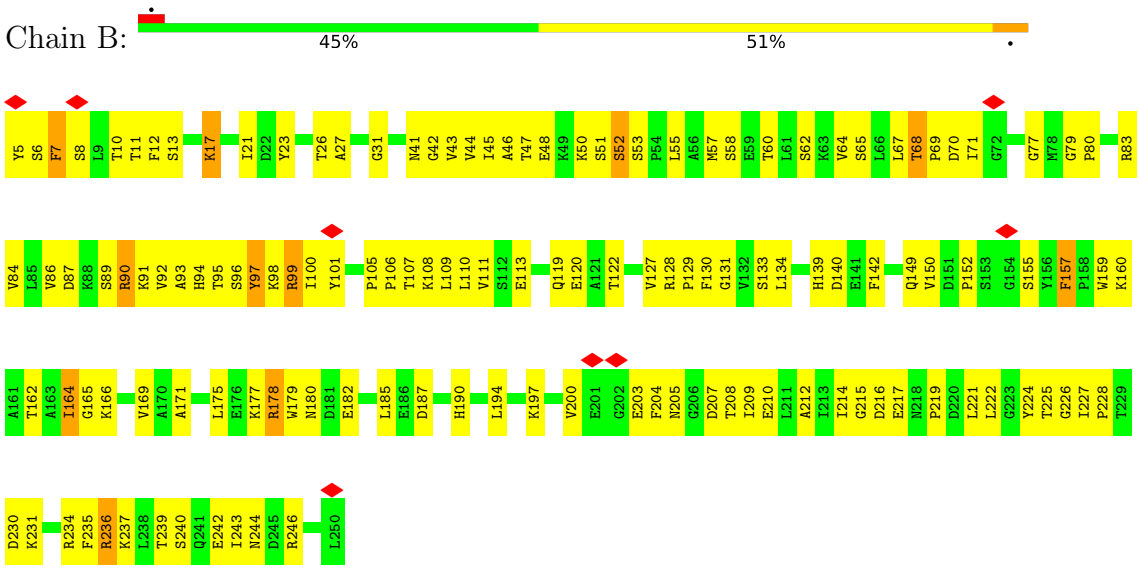
• Molecule 2: Proteasome subunit alpha type-2

Chain b:



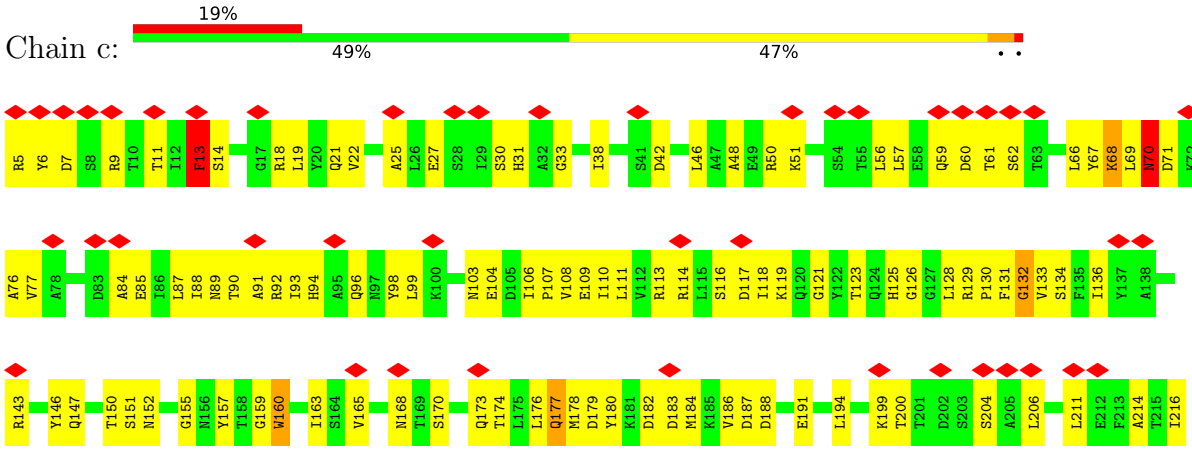
• Molecule 2: Proteasome subunit alpha type-2

Chain B:

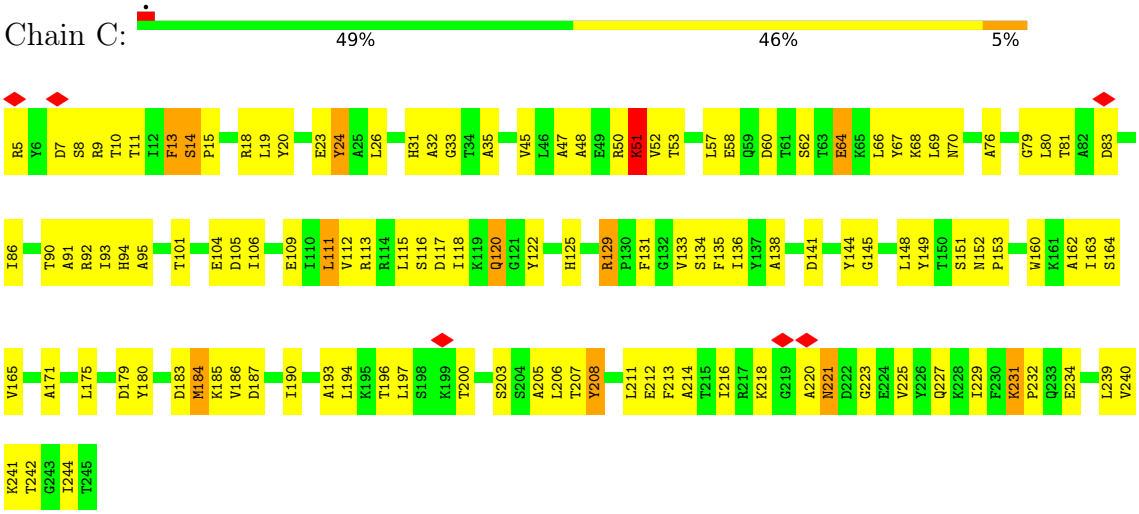


• Molecule 3: Proteasome subunit alpha type-3

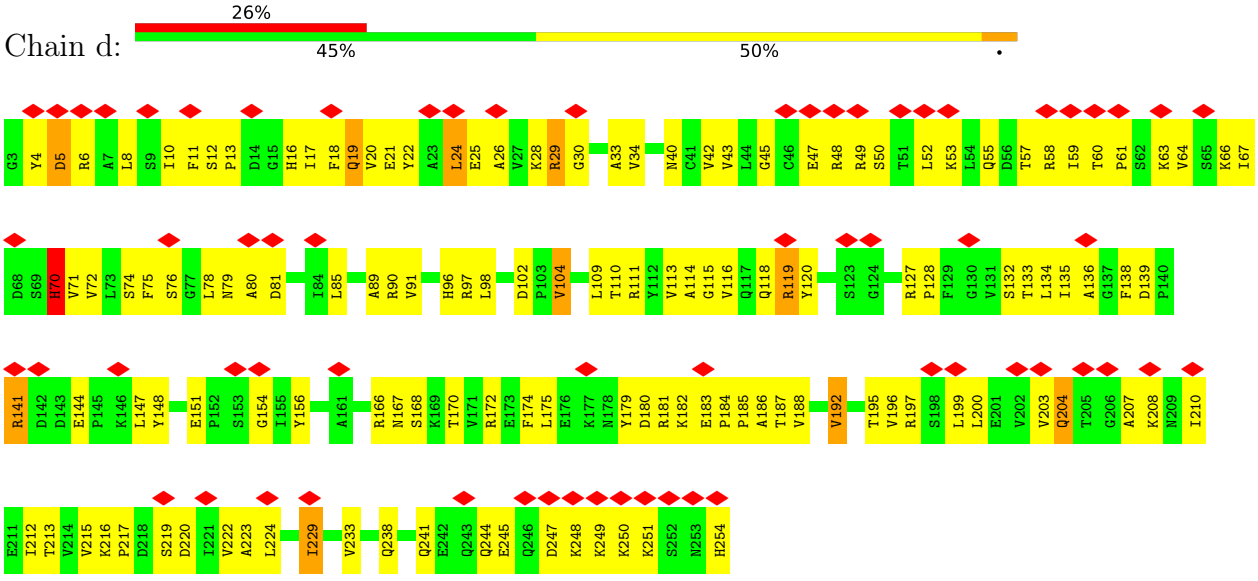
Chain c:



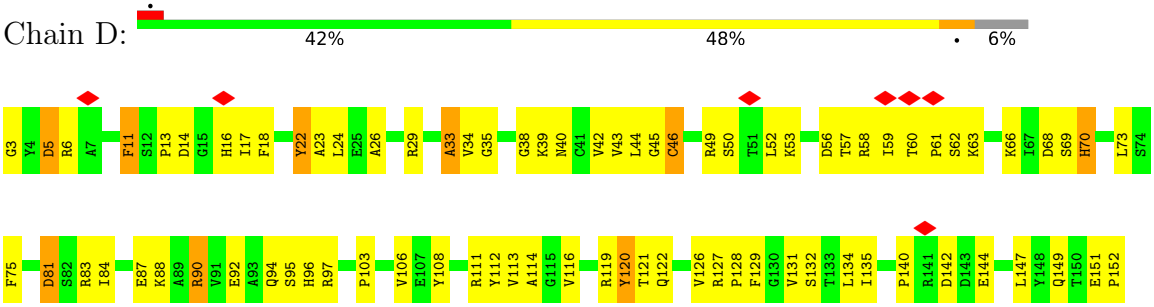
• Molecule 3: Proteasome subunit alpha type-3

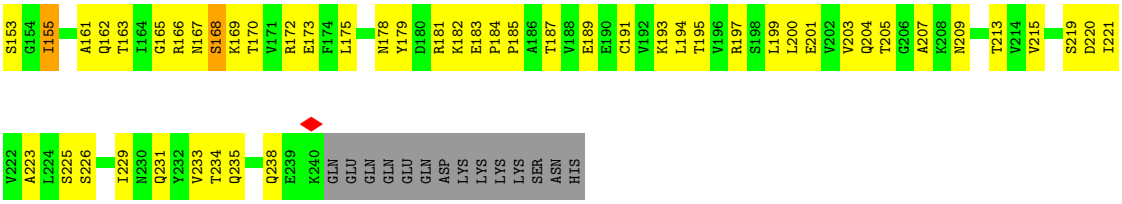


• Molecule 4: Proteasome subunit alpha type-4

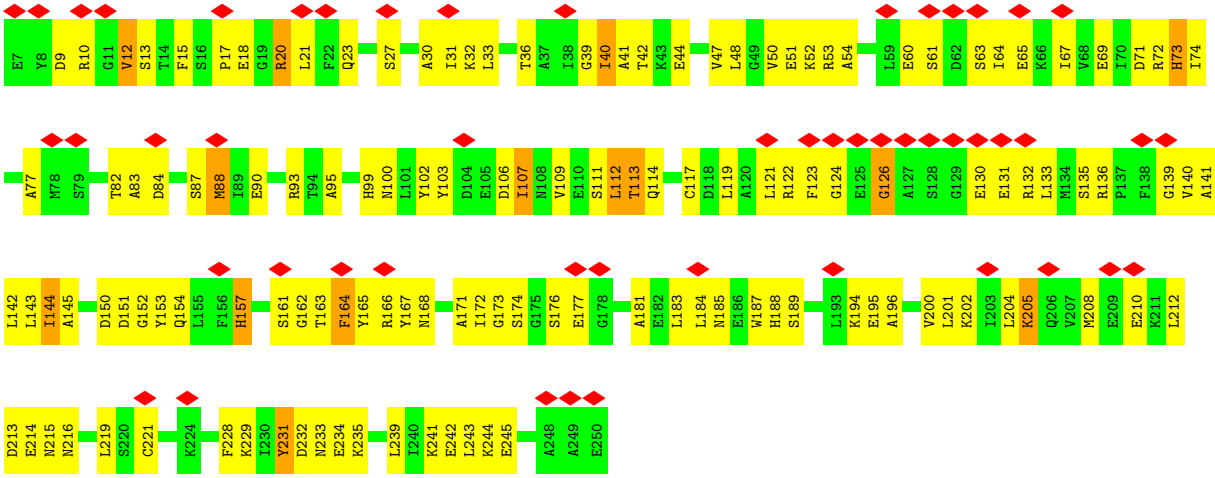


• Molecule 4: Proteasome subunit alpha type-4

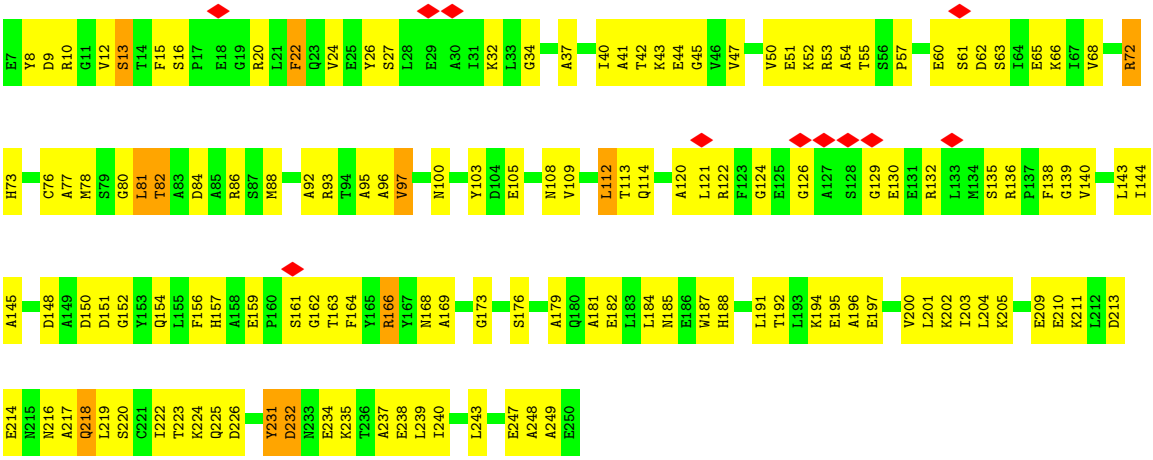




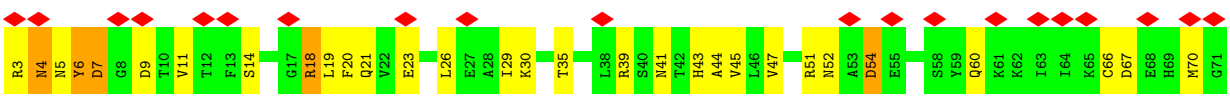
• Molecule 5: Proteasome subunit alpha type-5

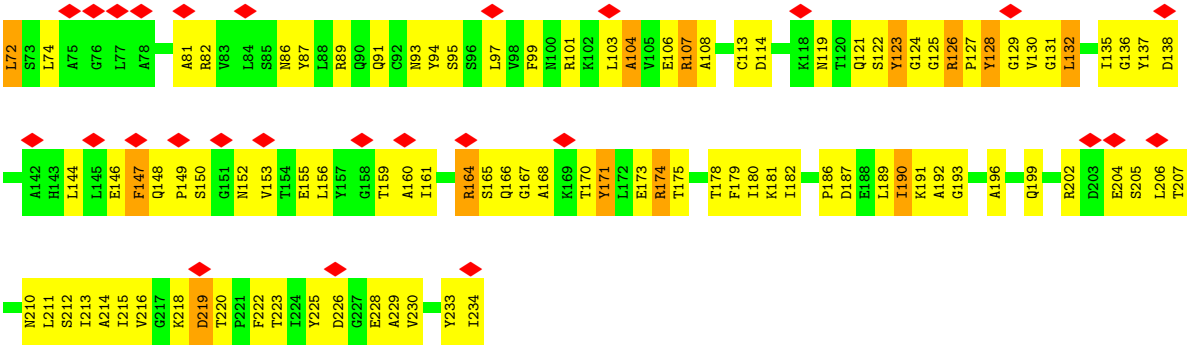


• Molecule 5: Proteasome subunit alpha type-5



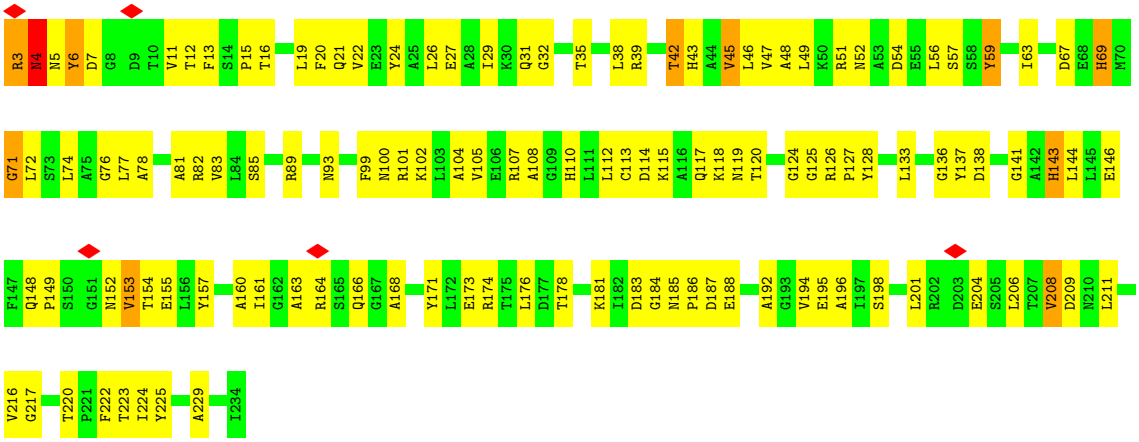
• Molecule 6: Proteasome subunit alpha type-6





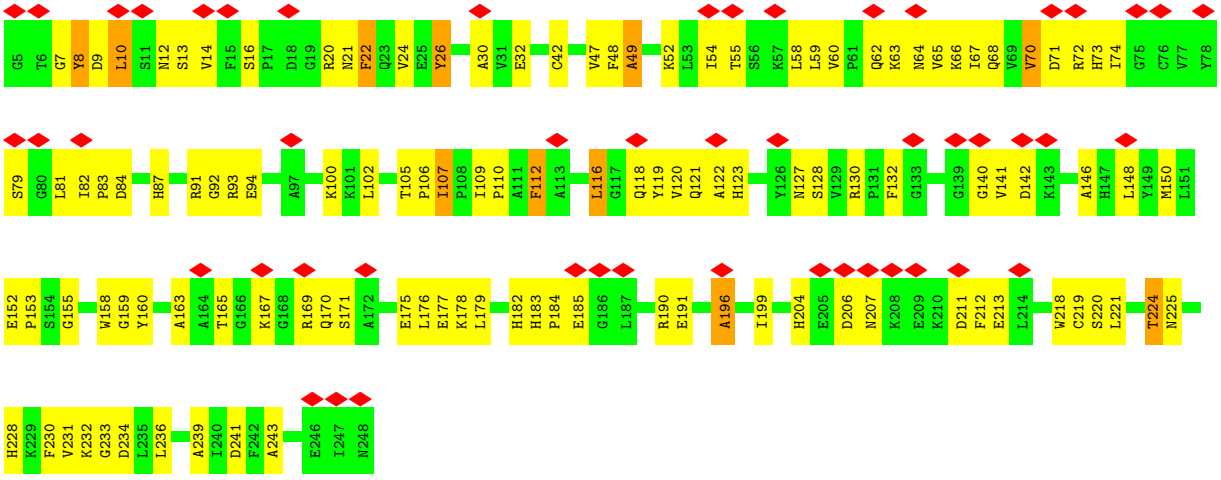
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



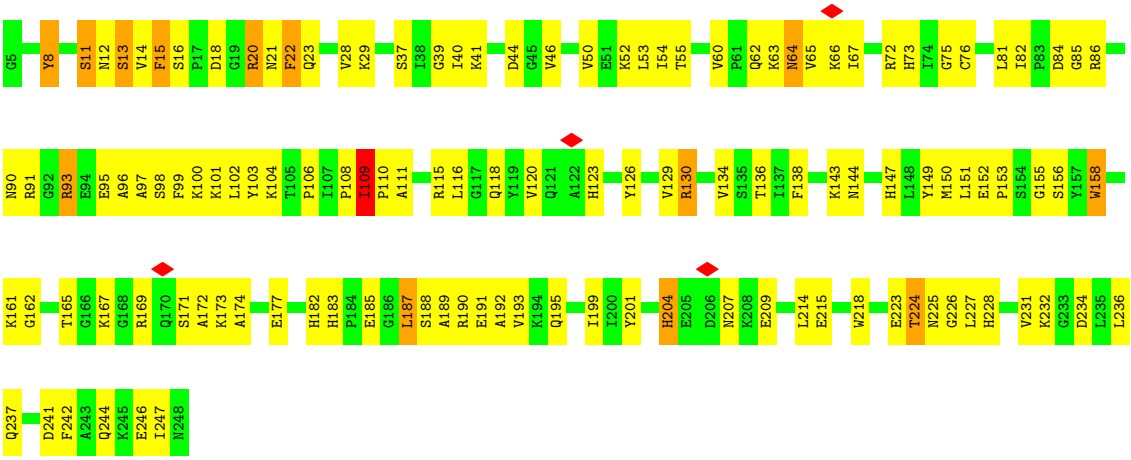
• Molecule 7: Probable proteasome subunit alpha type-7

Chain g:



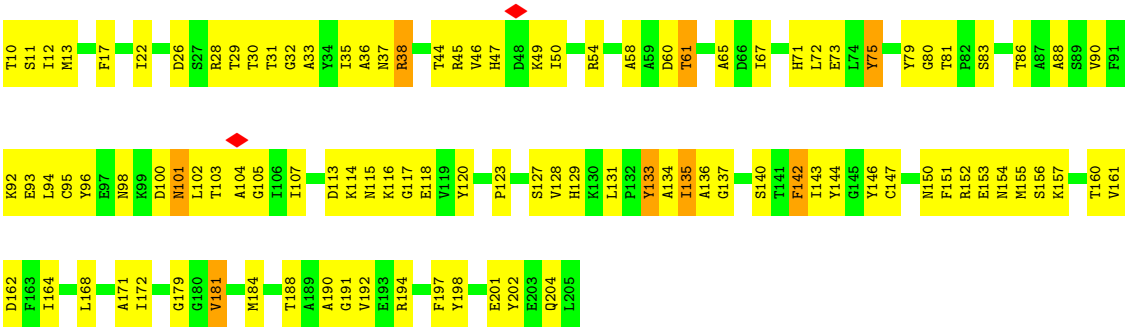
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



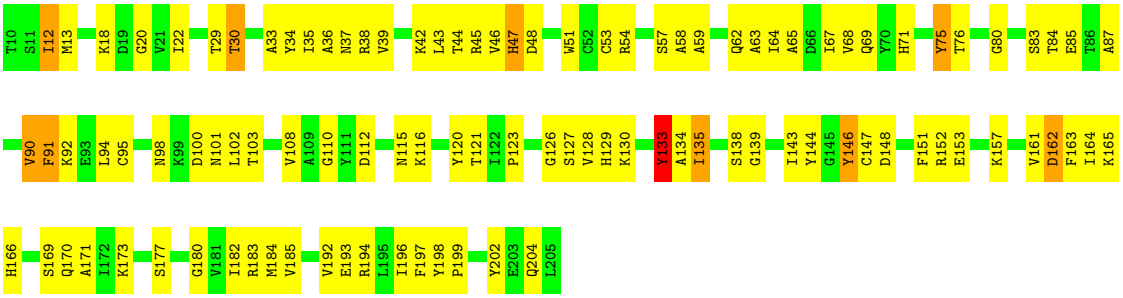
• Molecule 8: Proteasome subunit beta type-1

Chain h:



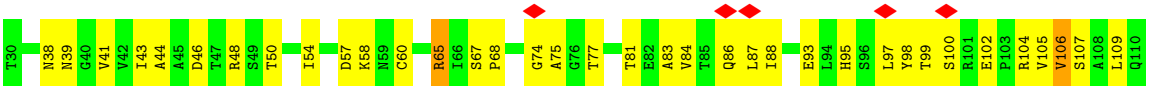
• Molecule 8: Proteasome subunit beta type-1

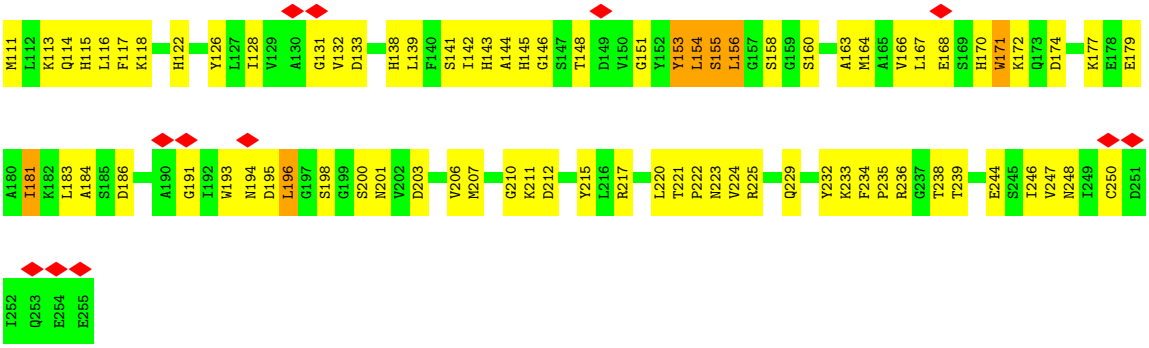
Chain 1:



• Molecule 9: Proteasome subunit beta type-2

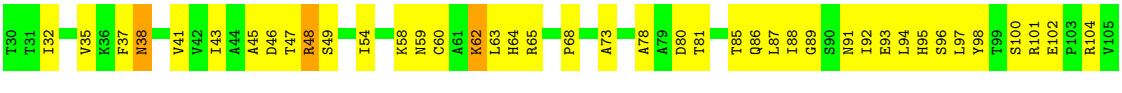
Chain i:

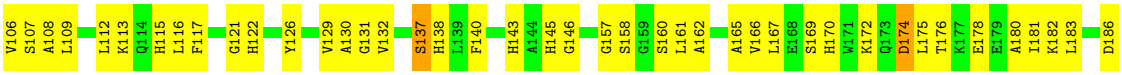


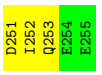


• Molecule 9: Proteasome subunit beta type-2

Chain 2:

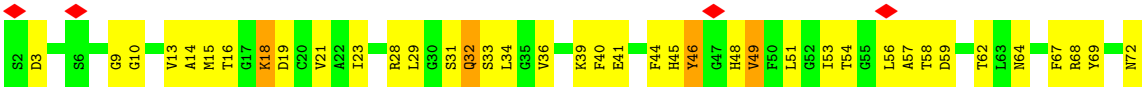


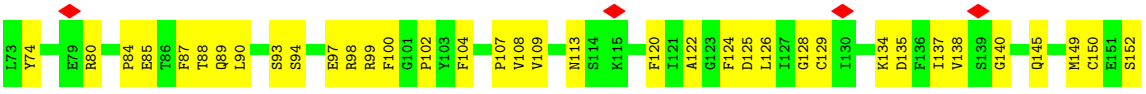




• Molecule 10: Proteasome subunit beta type-3

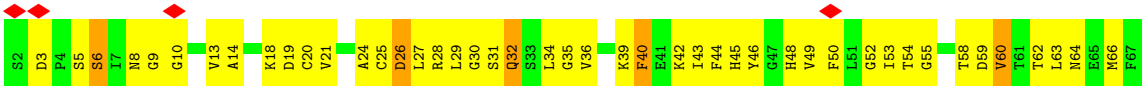
Chain j:

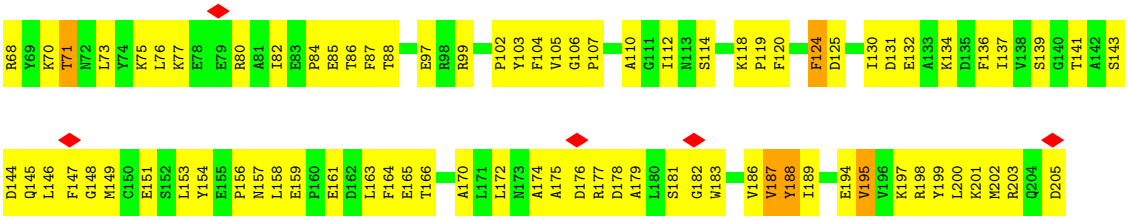




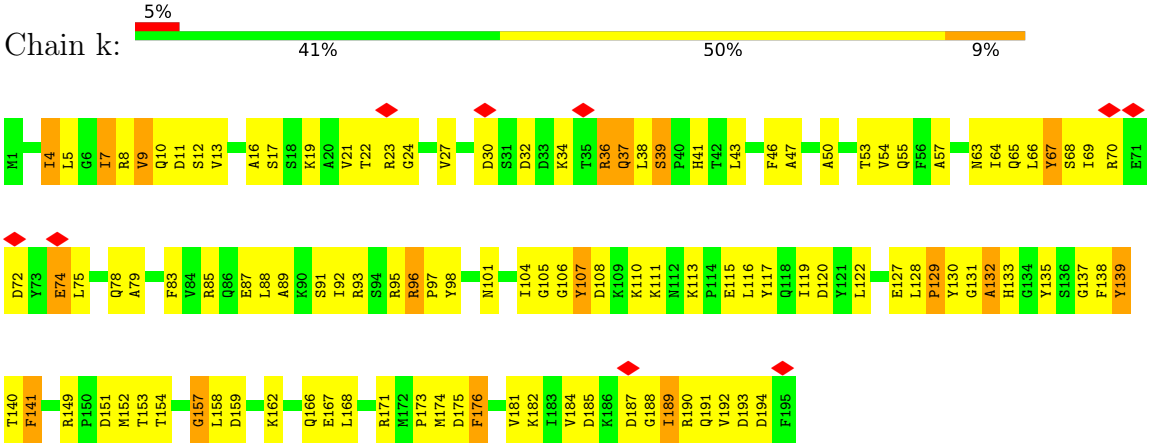
• Molecule 10: Proteasome subunit beta type-3

Chain 3:

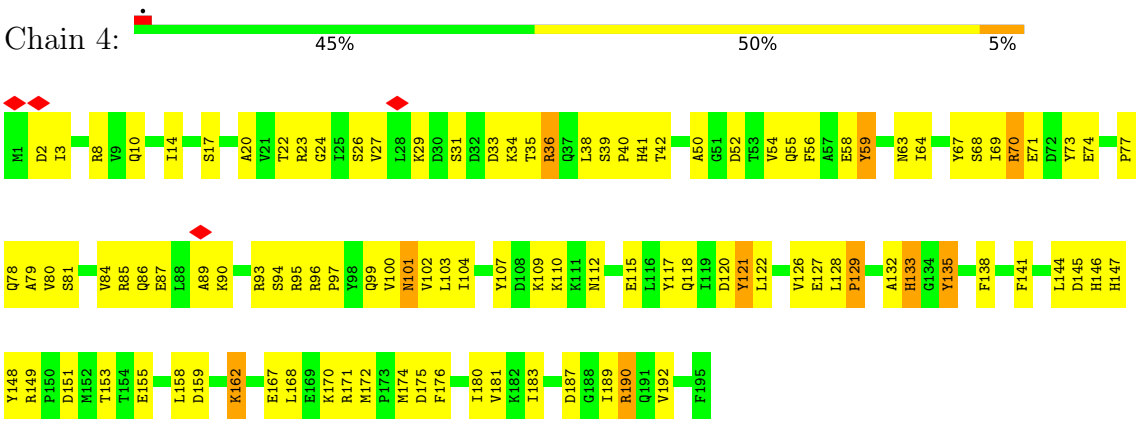




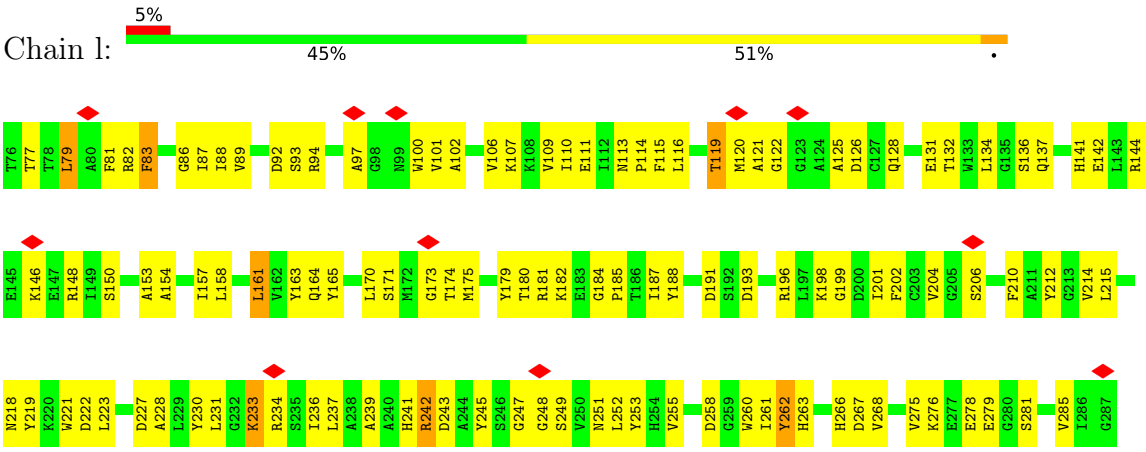
• Molecule 11: Proteasome subunit beta type-4



• Molecule 11: Proteasome subunit beta type-4

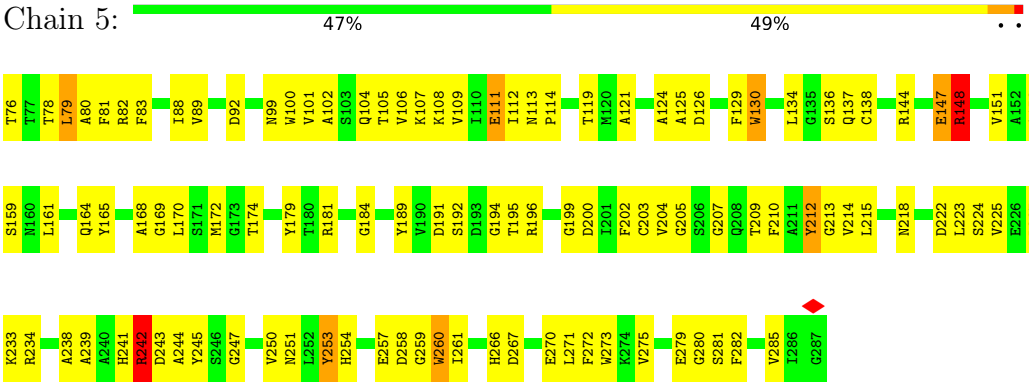


• Molecule 12: Proteasome subunit beta type-5



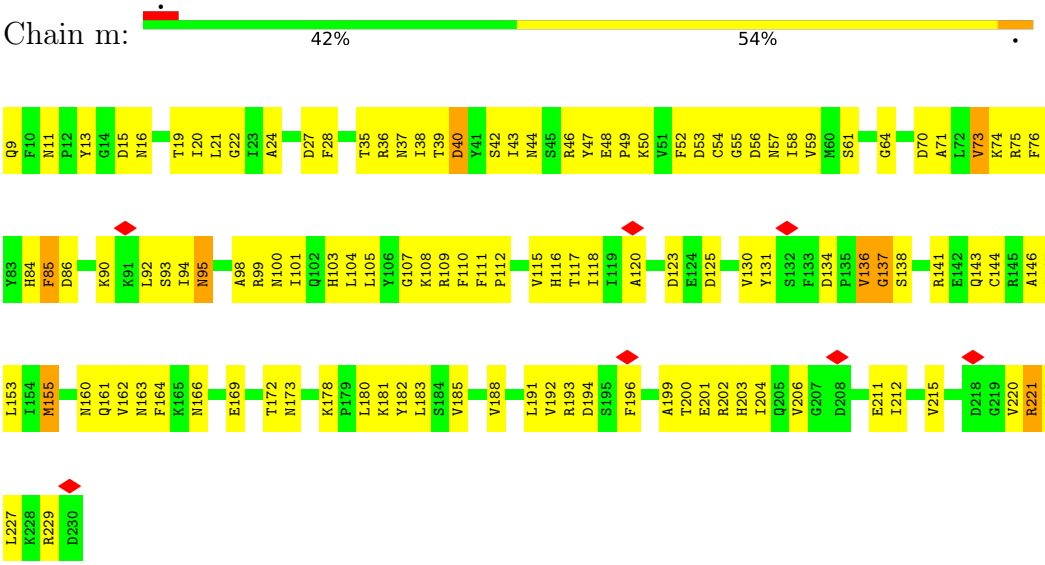
• Molecule 12: Proteasome subunit beta type-5

Chain 5:



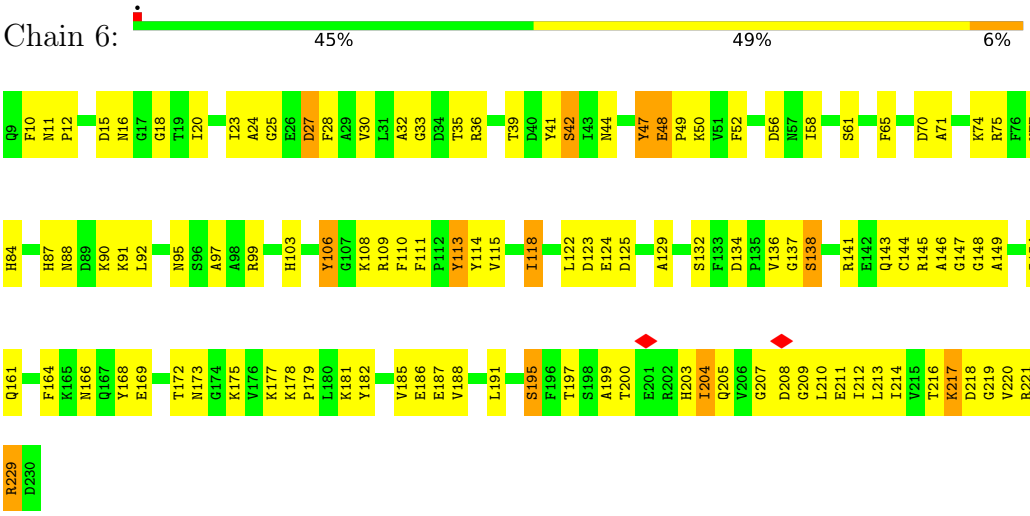
• Molecule 13: Proteasome subunit beta type-6

Chain m:



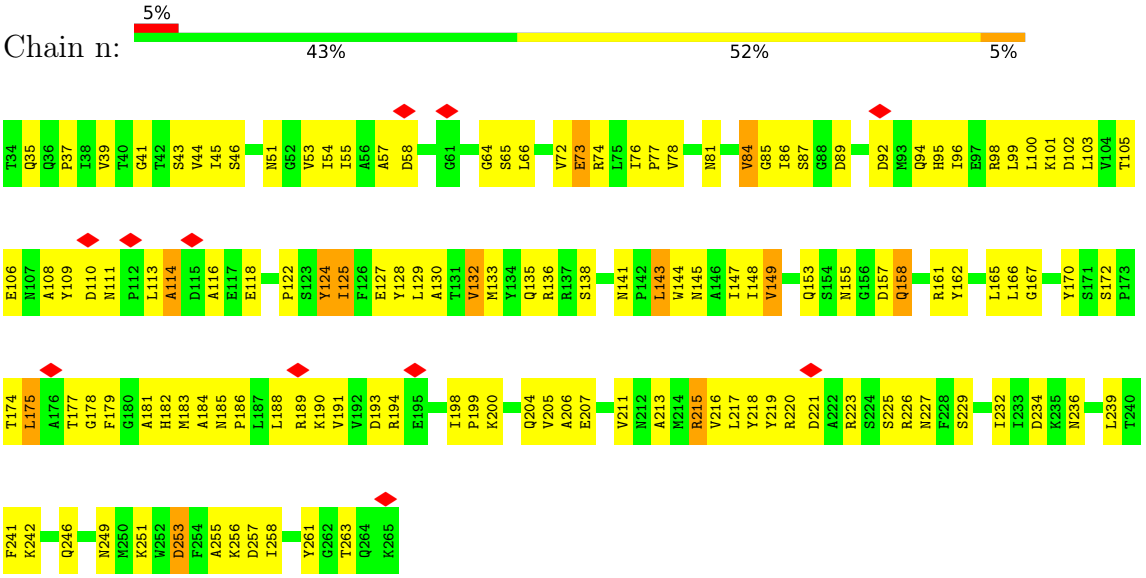
• Molecule 13: Proteasome subunit beta type-6

Chain 6:



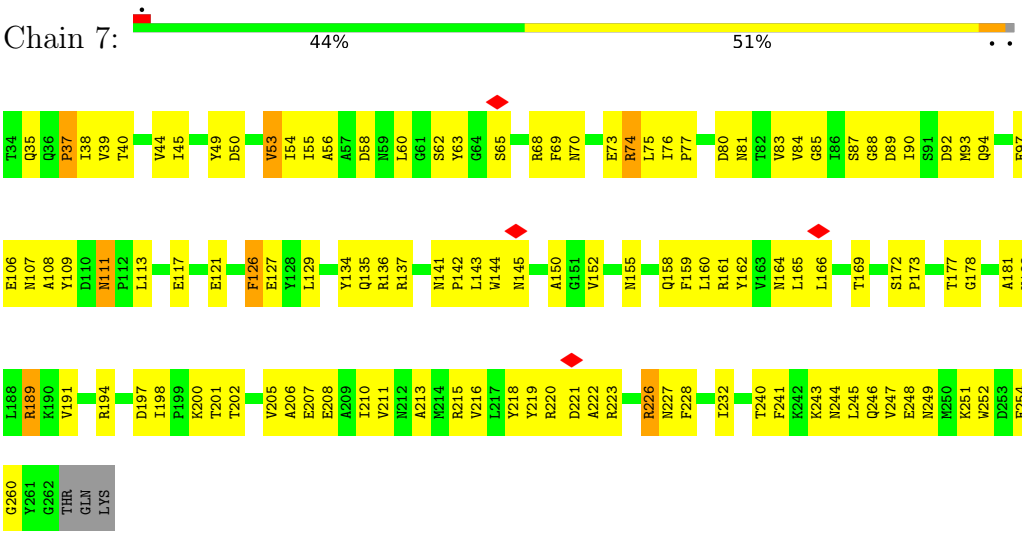
• Molecule 14: Proteasome subunit beta type-7

Chain n:

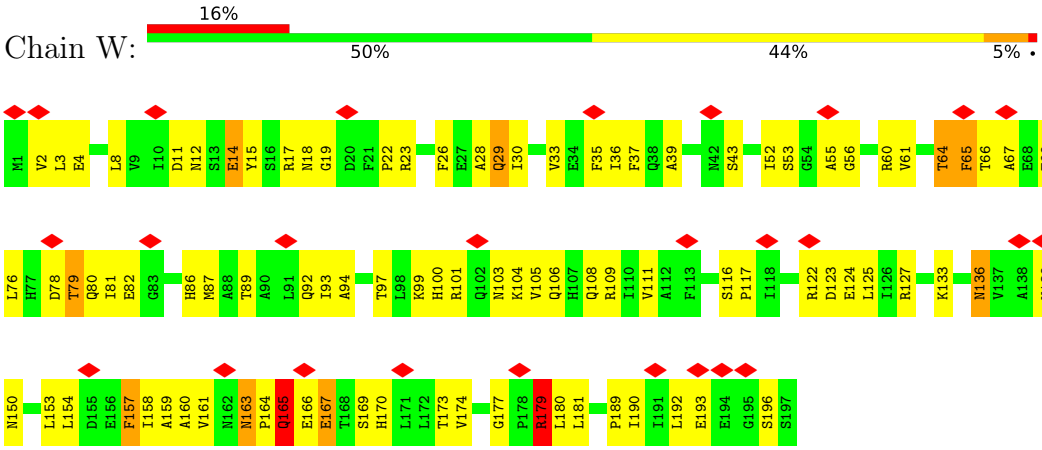


• Molecule 14: Proteasome subunit beta type-7

Chain 7:

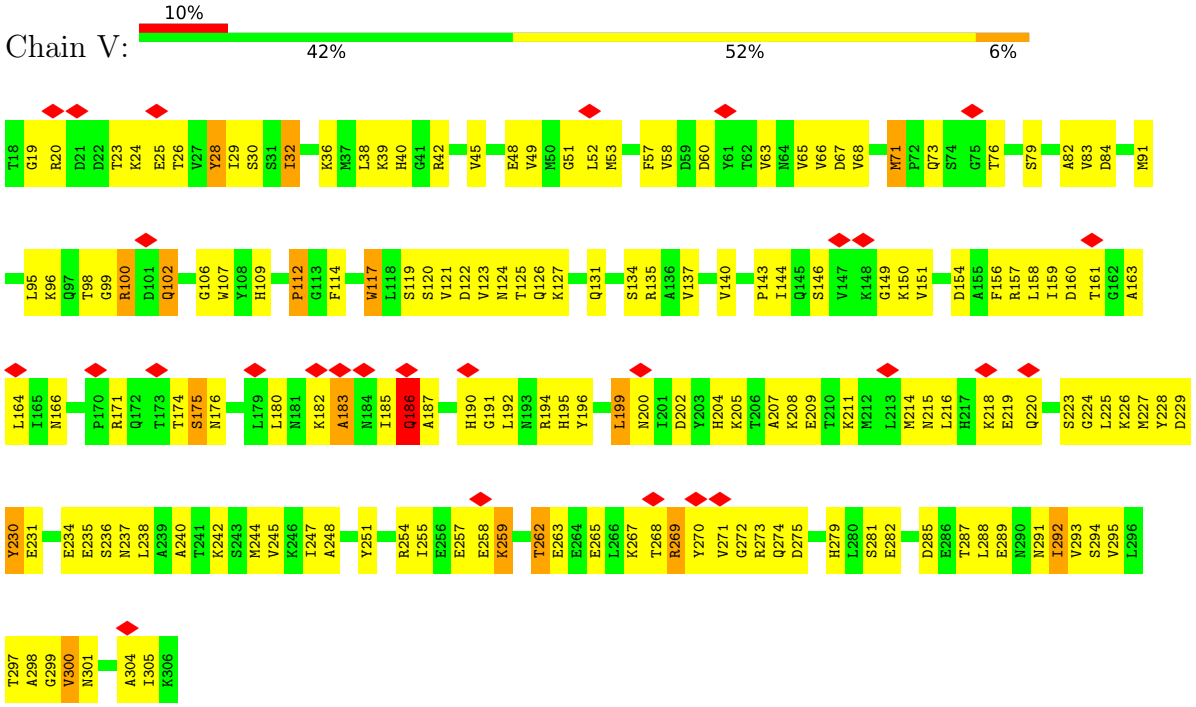


Chain W:



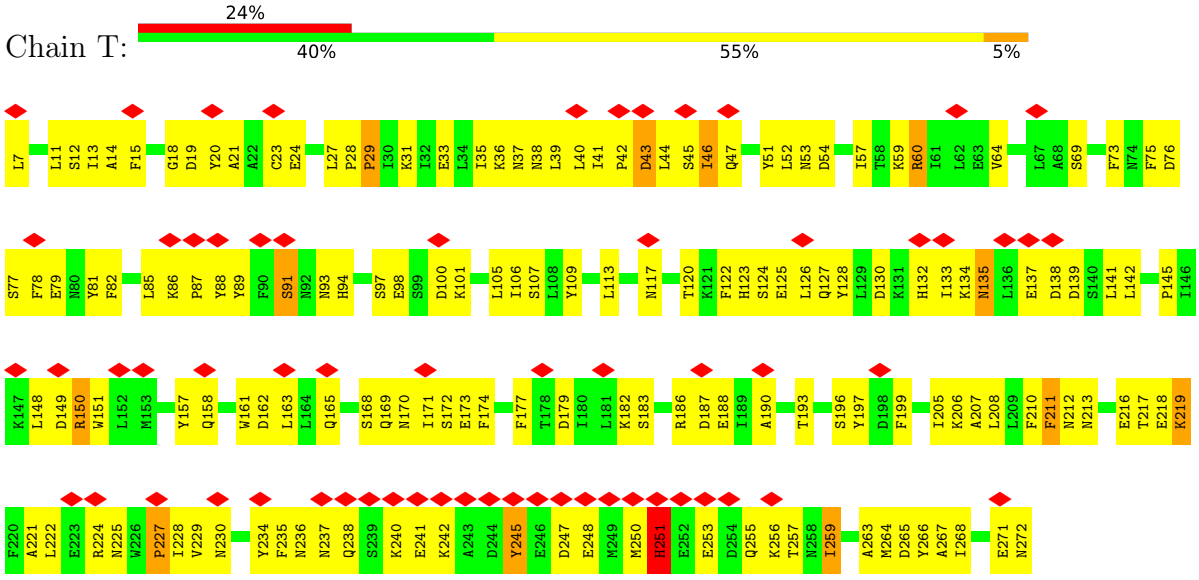
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



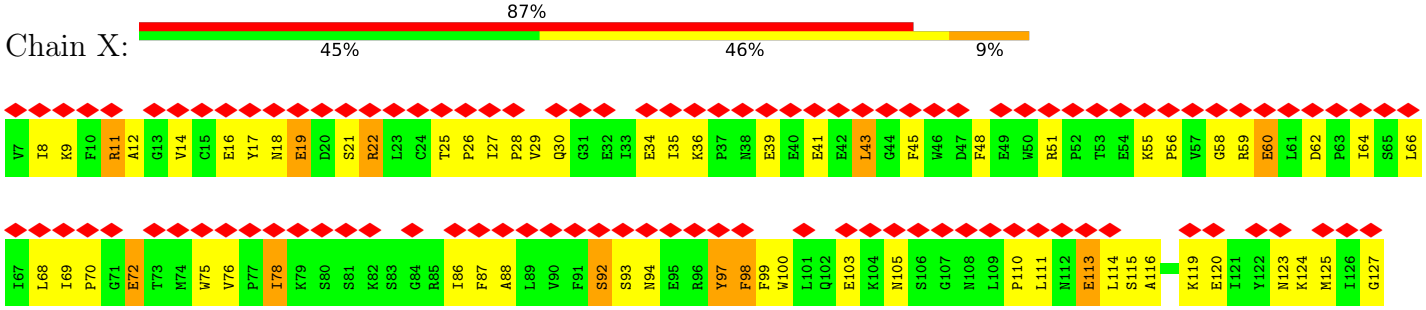
• Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:



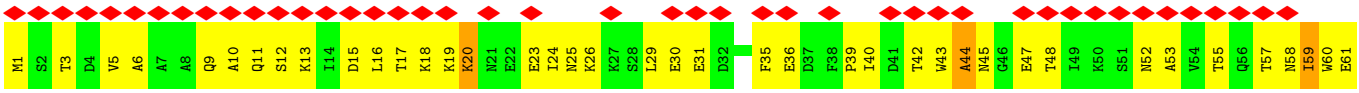
• Molecule 18: 26S proteasome regulatory subunit RPN13

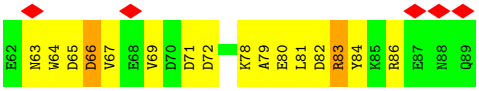
Chain X:



• Molecule 19: 26S proteasome complex subunit SEM1

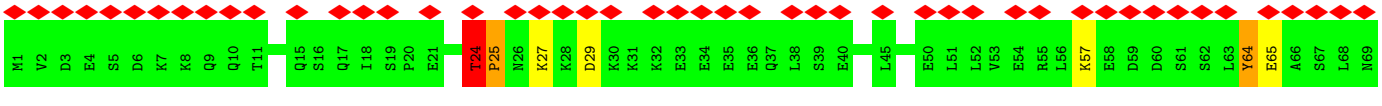
Chain Y:

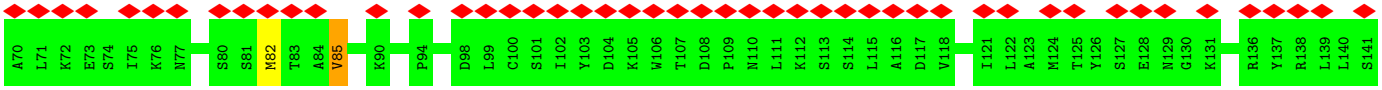


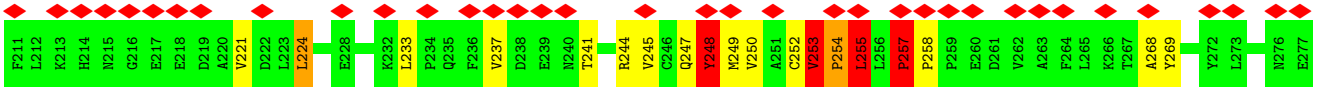


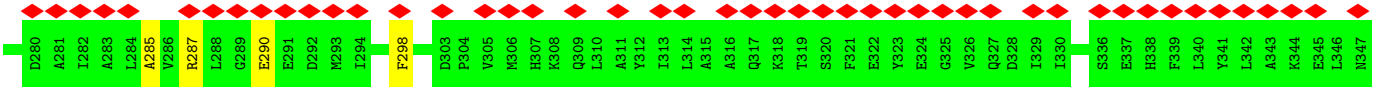
• Molecule 20: 26S proteasome regulatory subunit RPN1

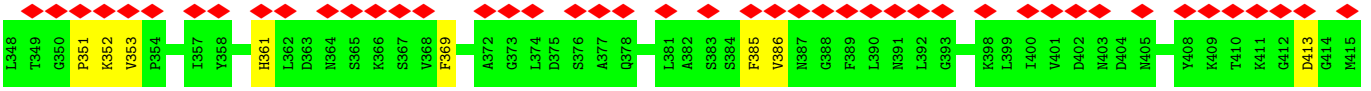
Chain Z:

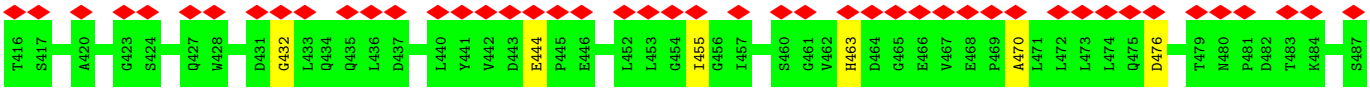


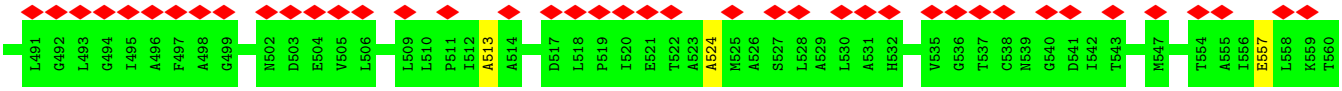


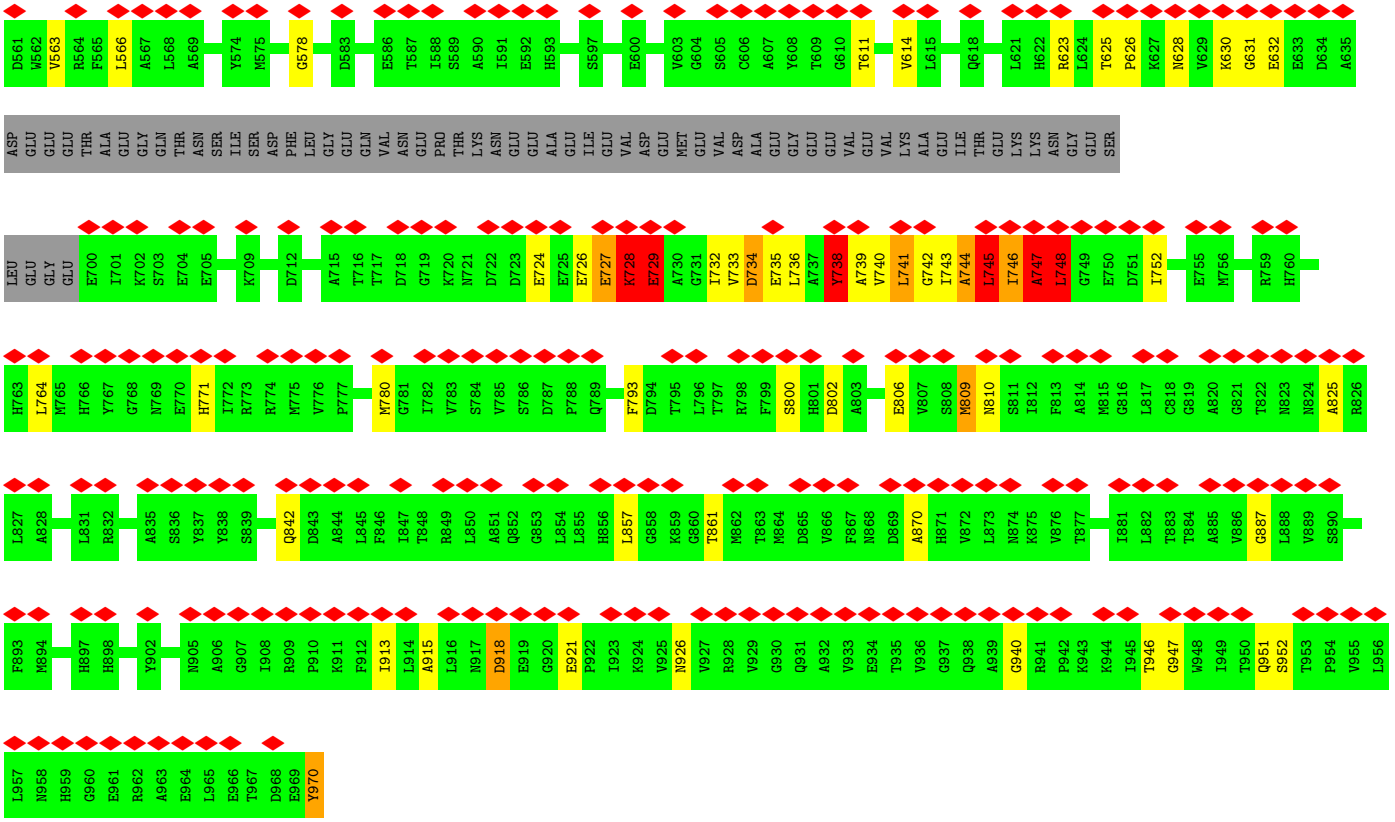




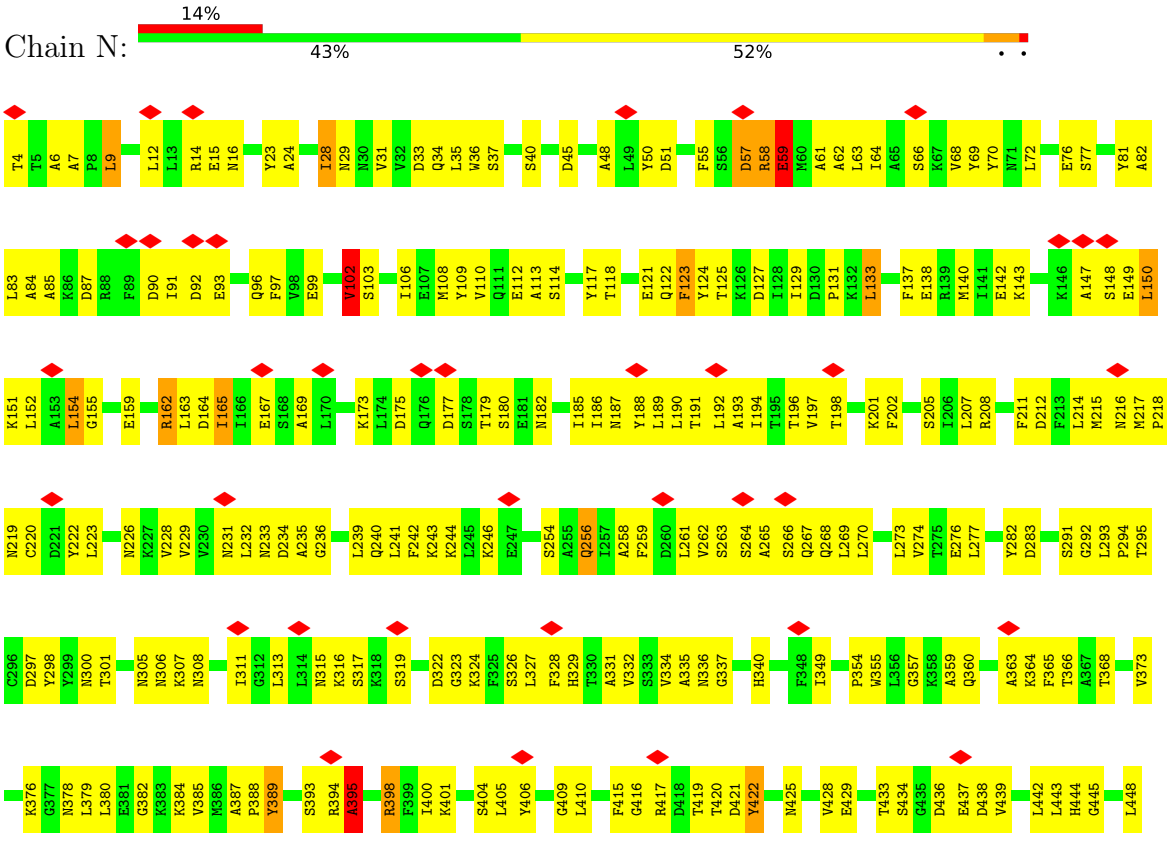


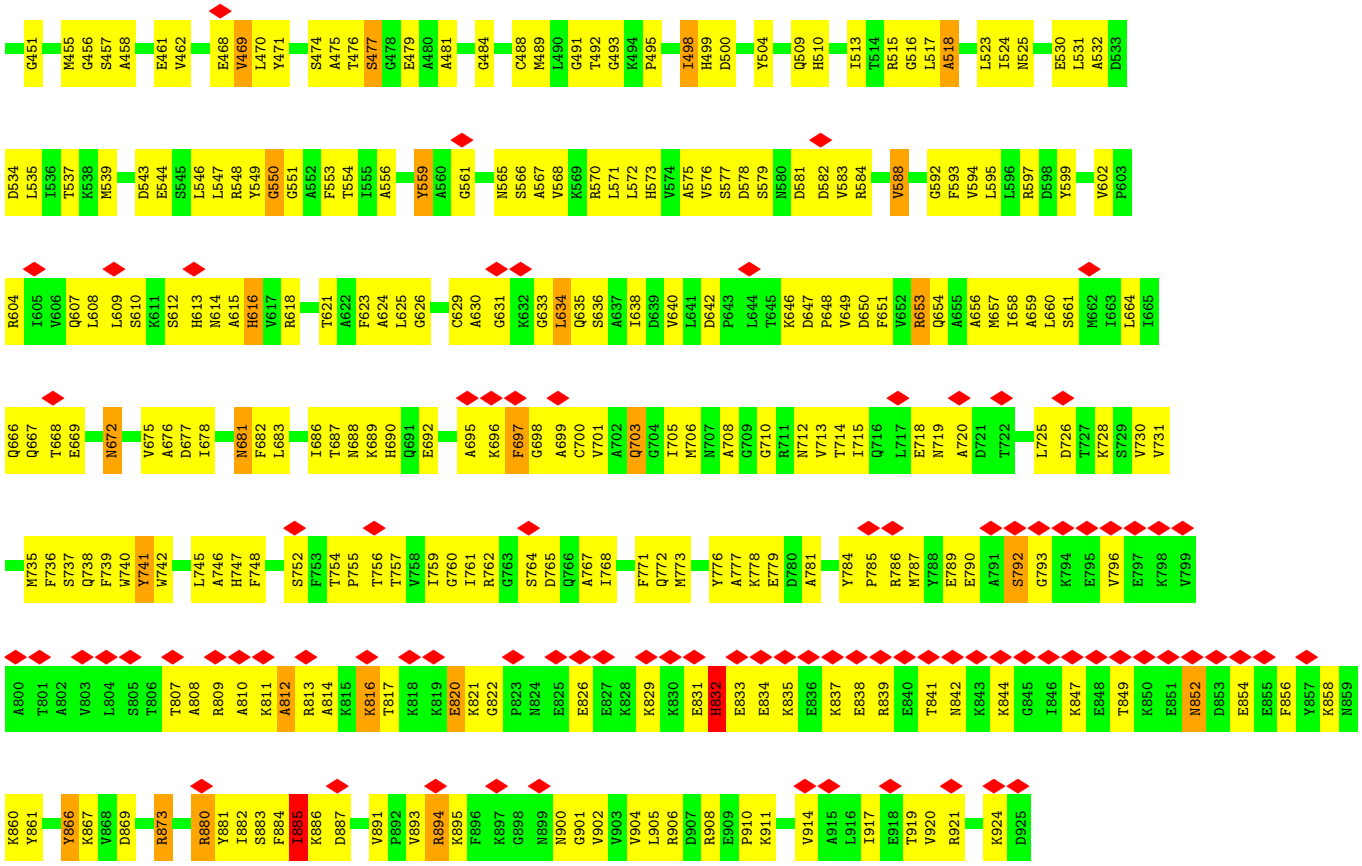






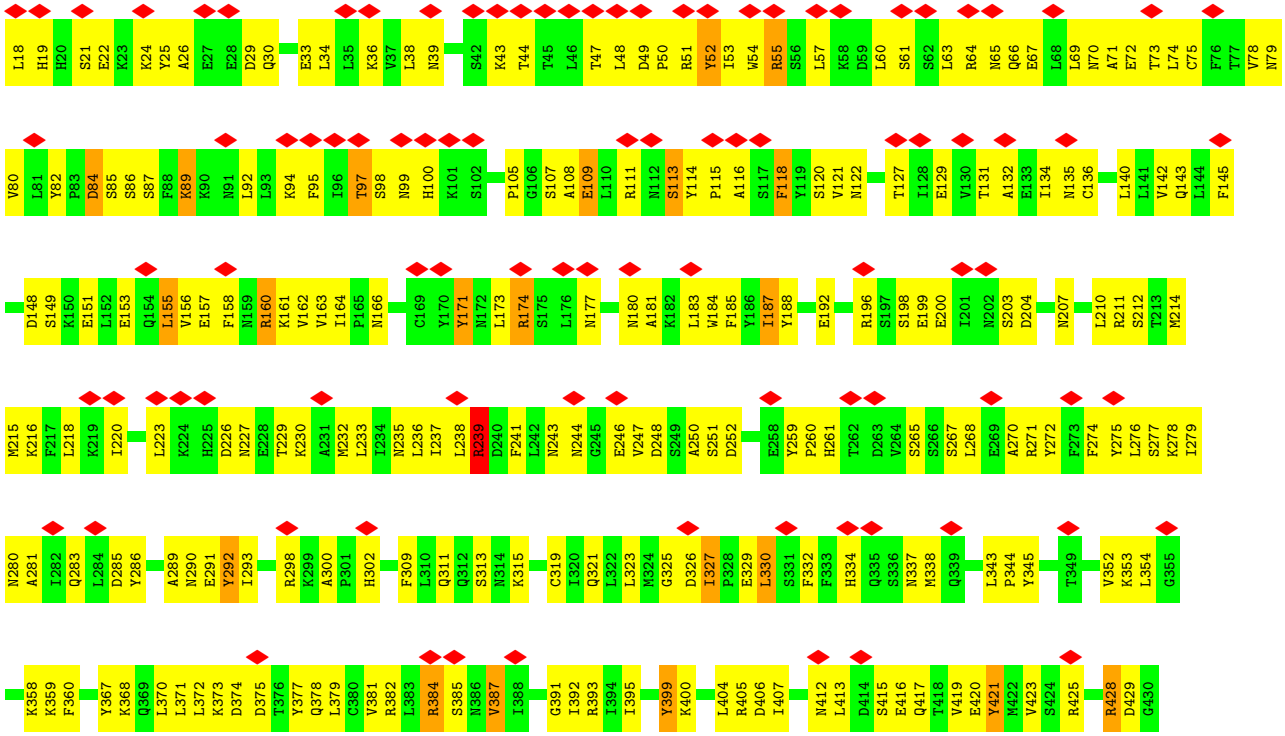
• Molecule 21: 26S proteasome regulatory subunit RPN2

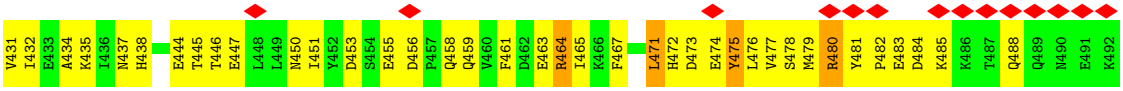




• Molecule 22: 26S proteasome regulatory subunit RPN3

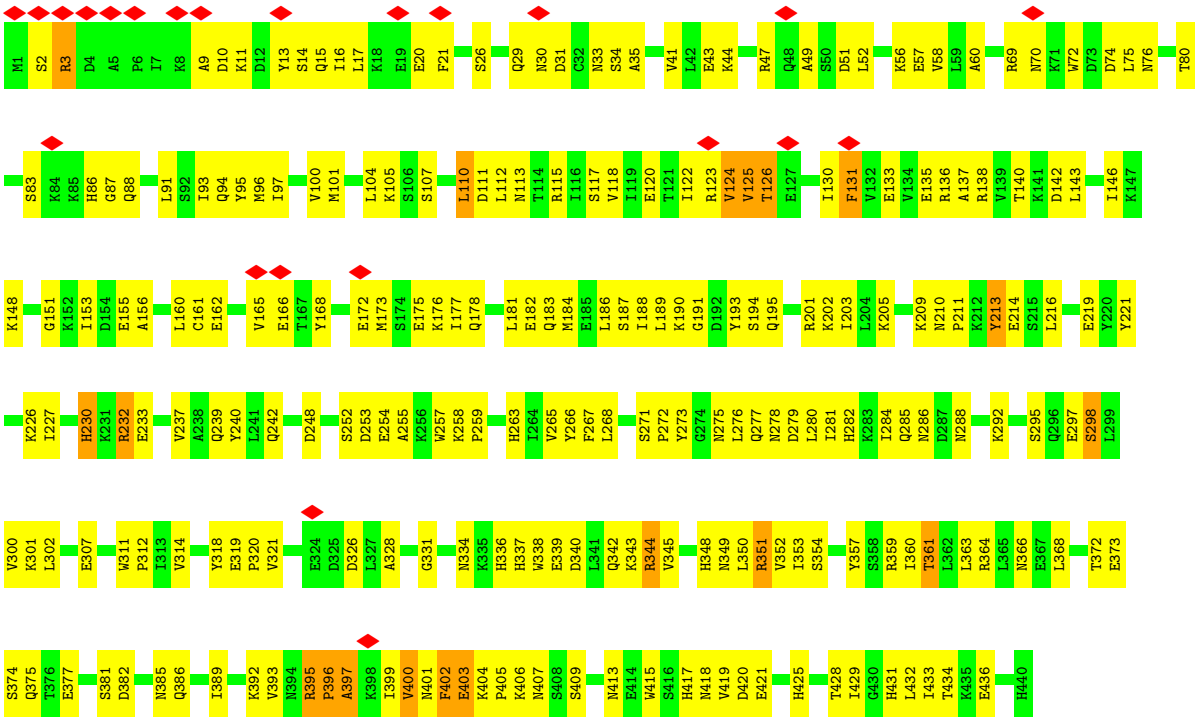
Chain S:





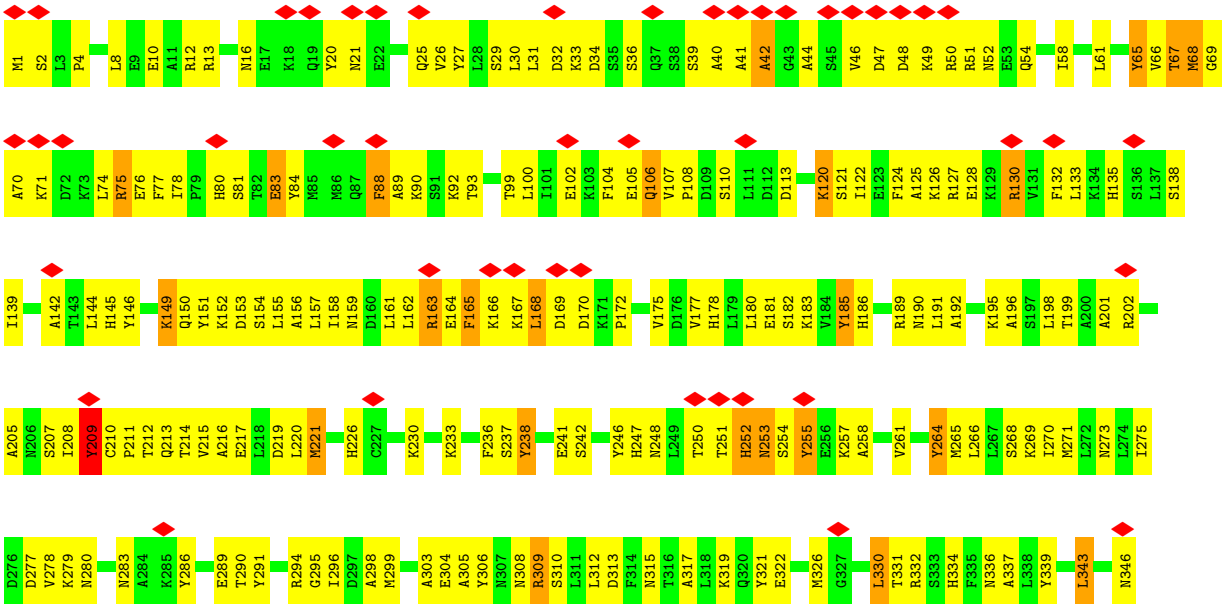
• Molecule 23: 26S proteasome regulatory subunit RPN5

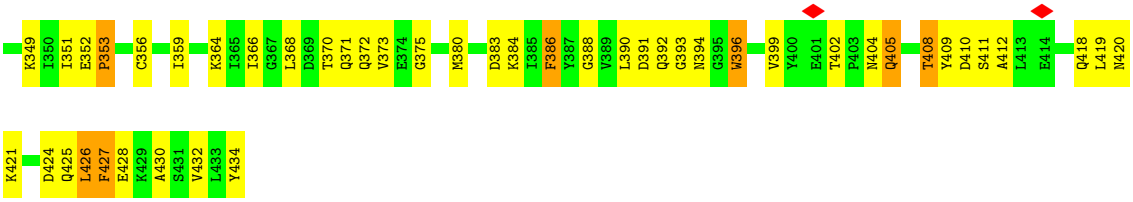
Chain P:



• Molecule 24: 26S proteasome regulatory subunit RPN6

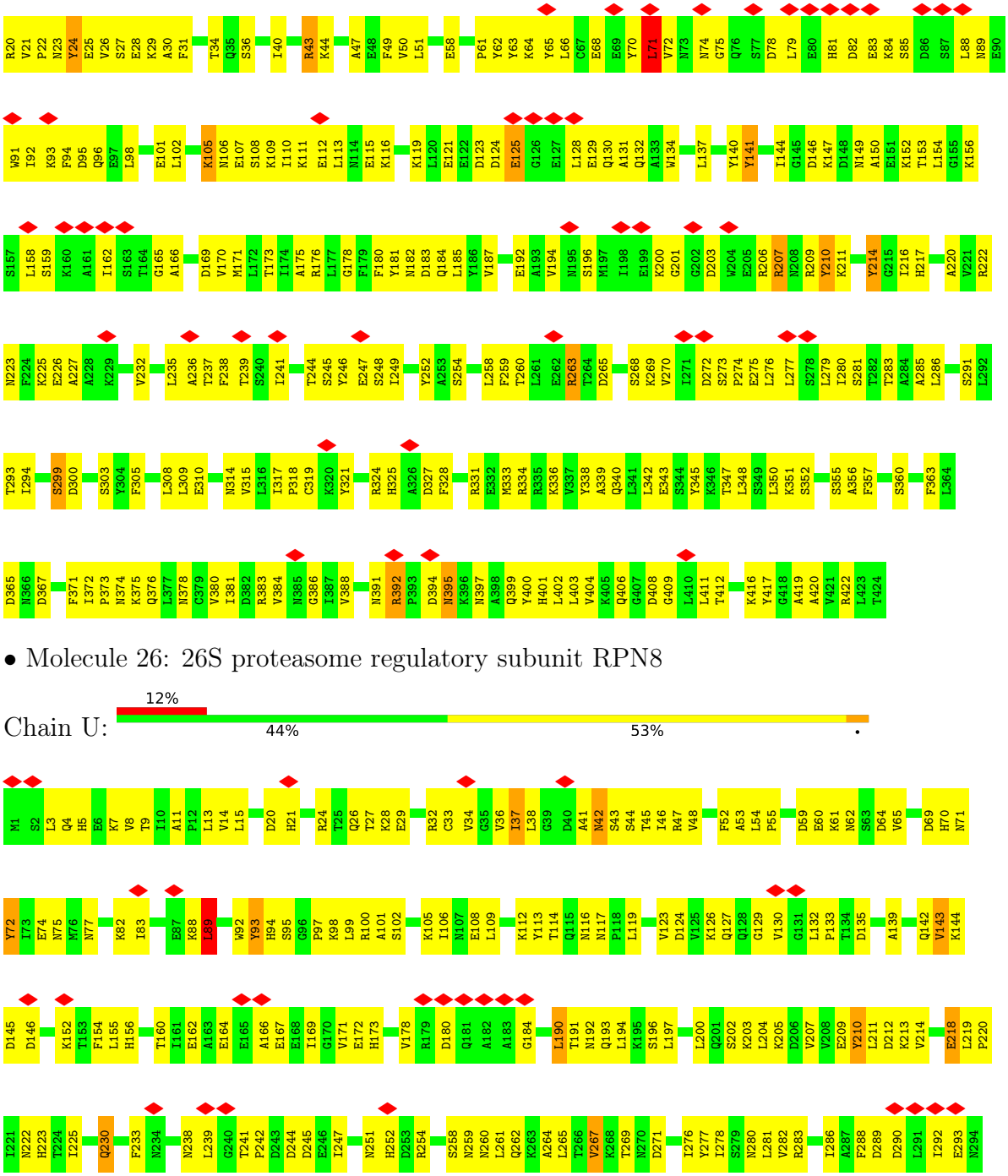
Chain Q:





• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:

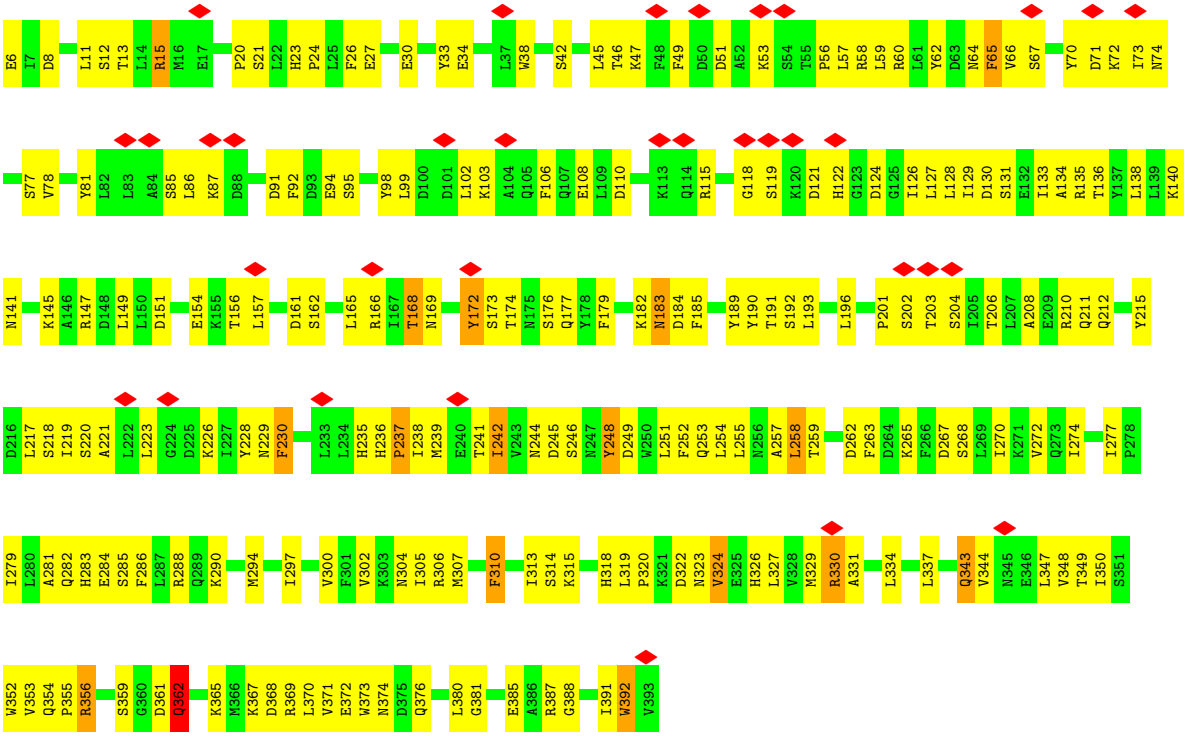


• Molecule 26: 26S proteasome regulatory subunit RPN8

Chain U:

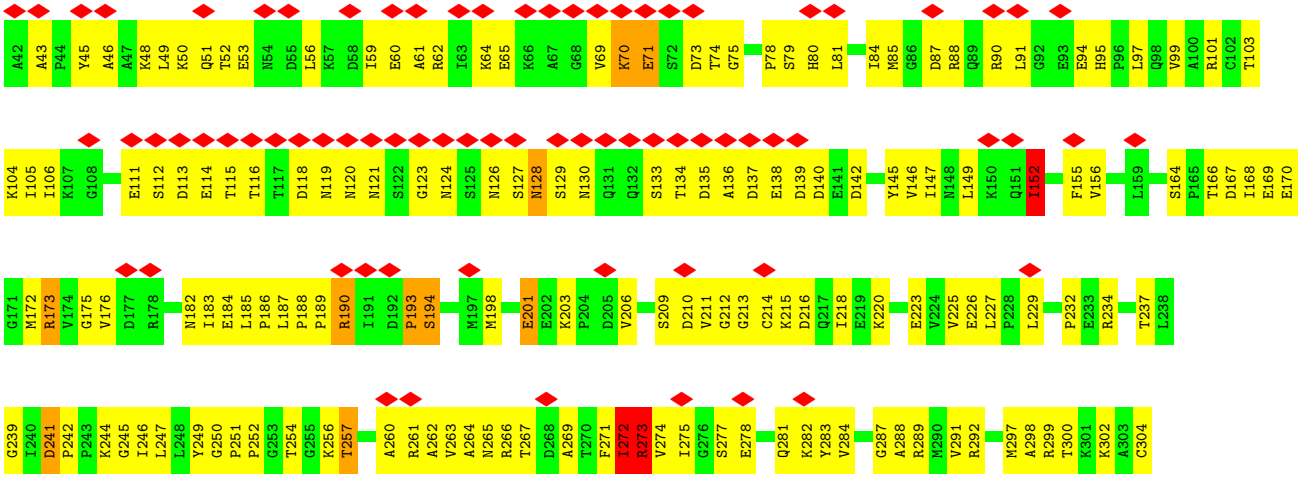
• Molecule 27: 26S proteasome regulatory subunit RPN9

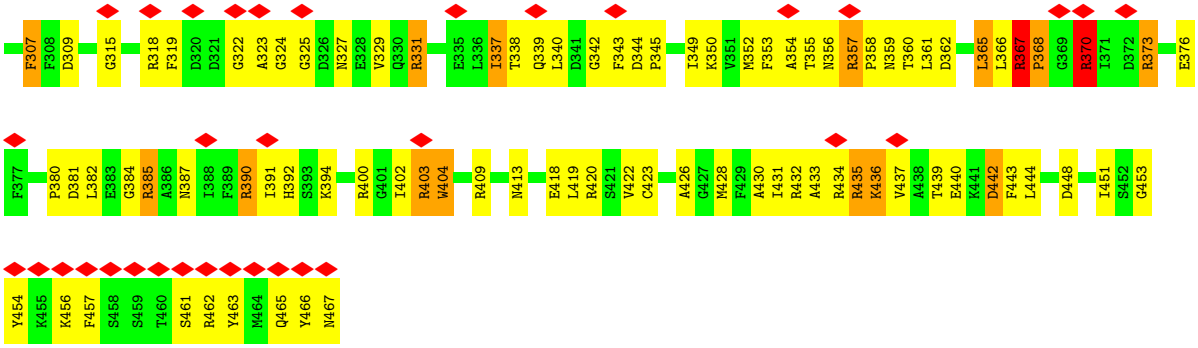
Chain O:



• Molecule 28: 26S proteasome regulatory subunit 7 homolog

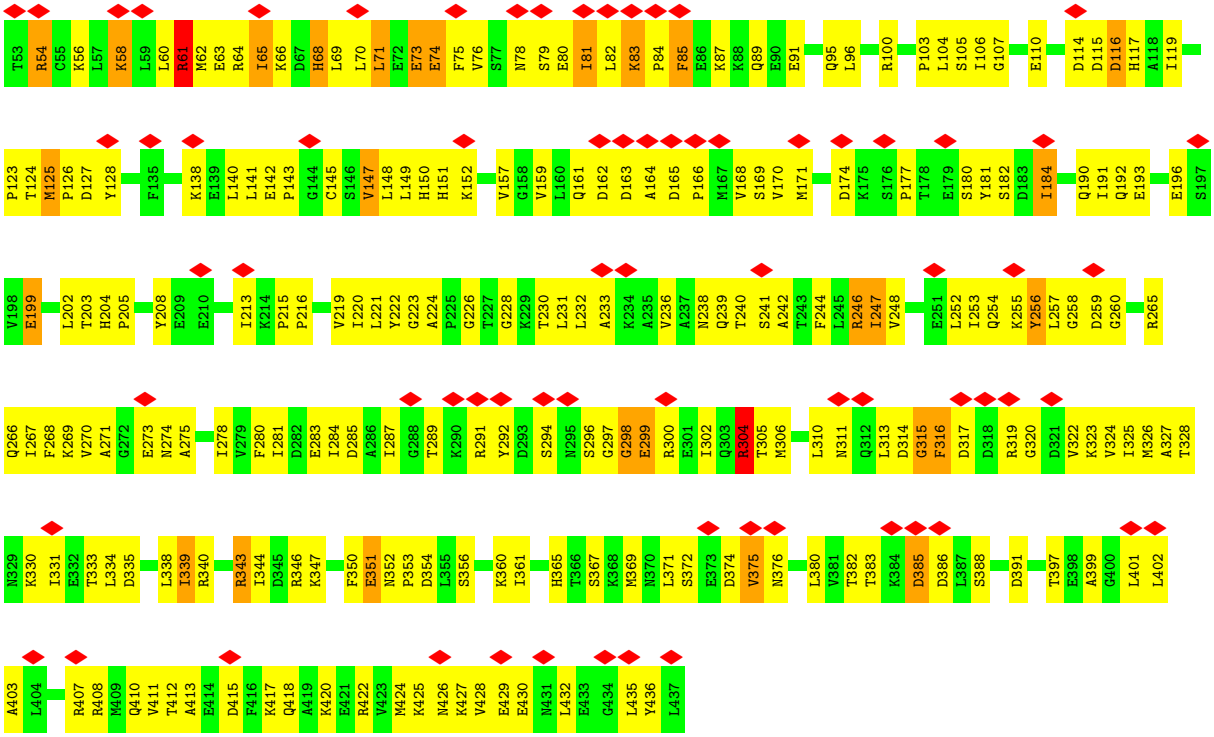
Chain H:





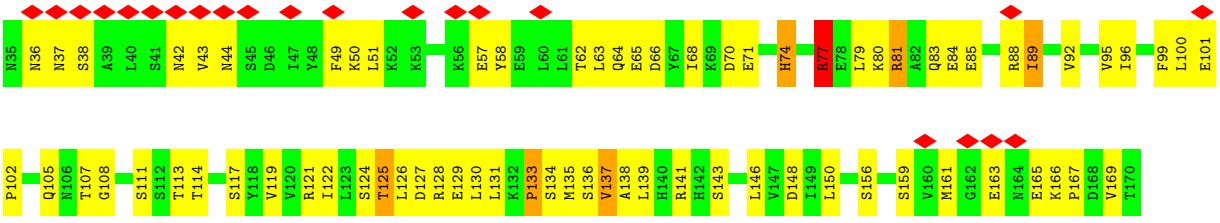
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

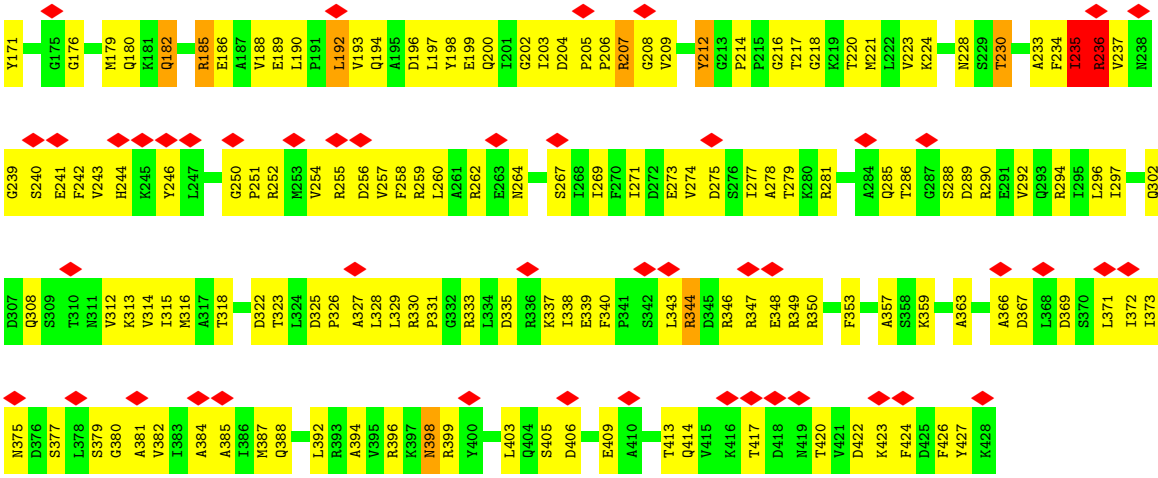
Chain I:



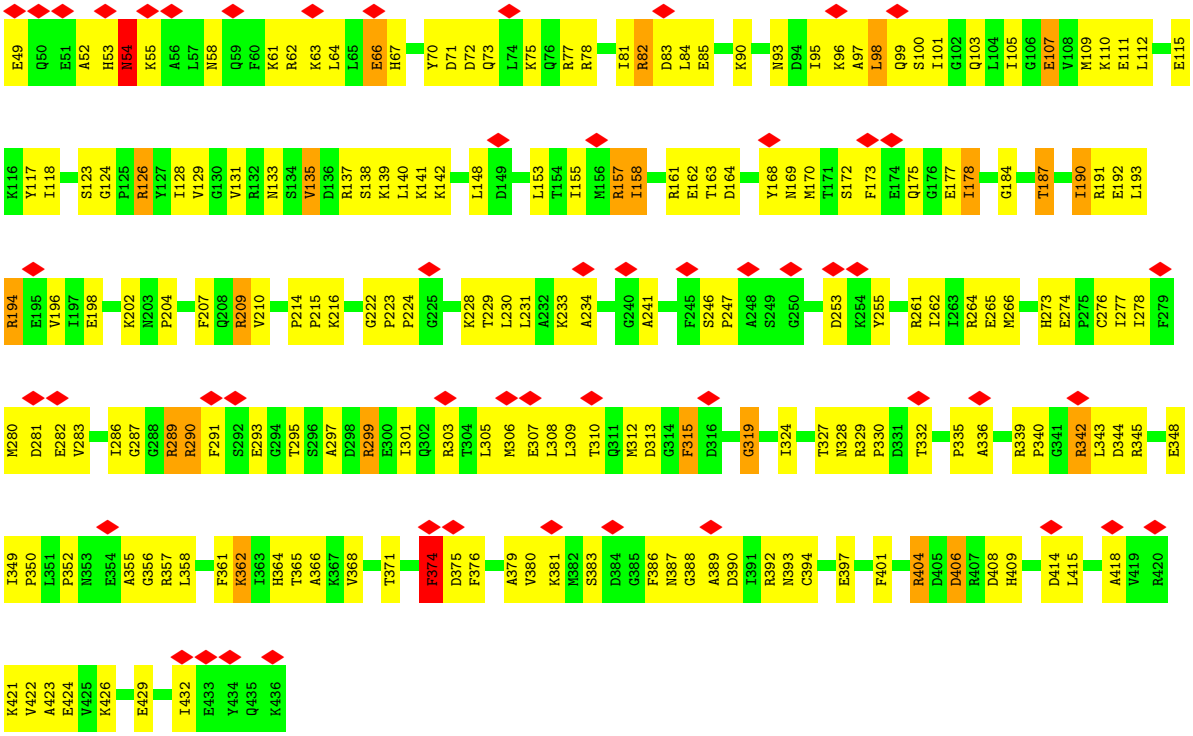
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

Chain K:

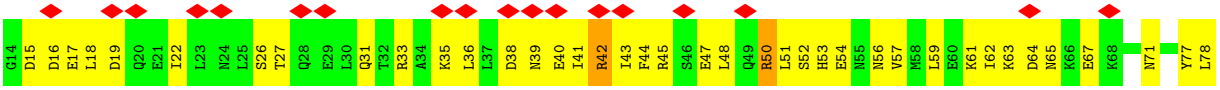


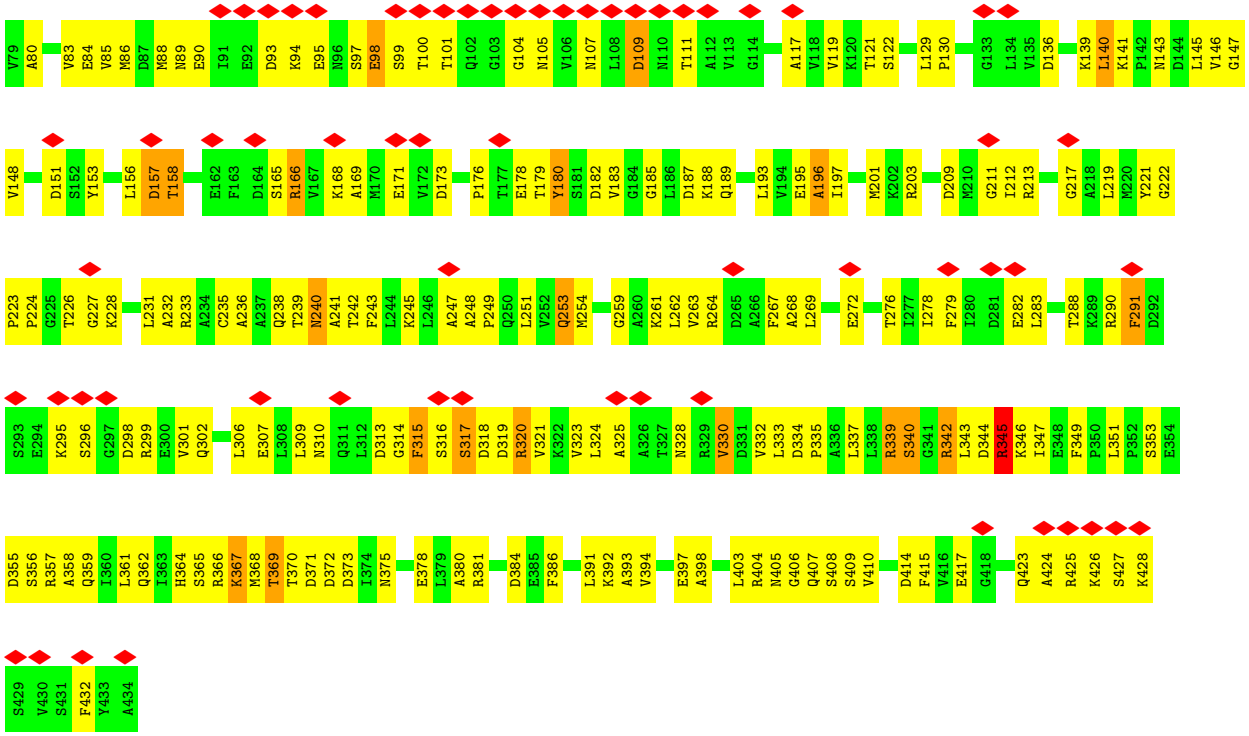


• Molecule 31: 26S proteasome subunit RPT4



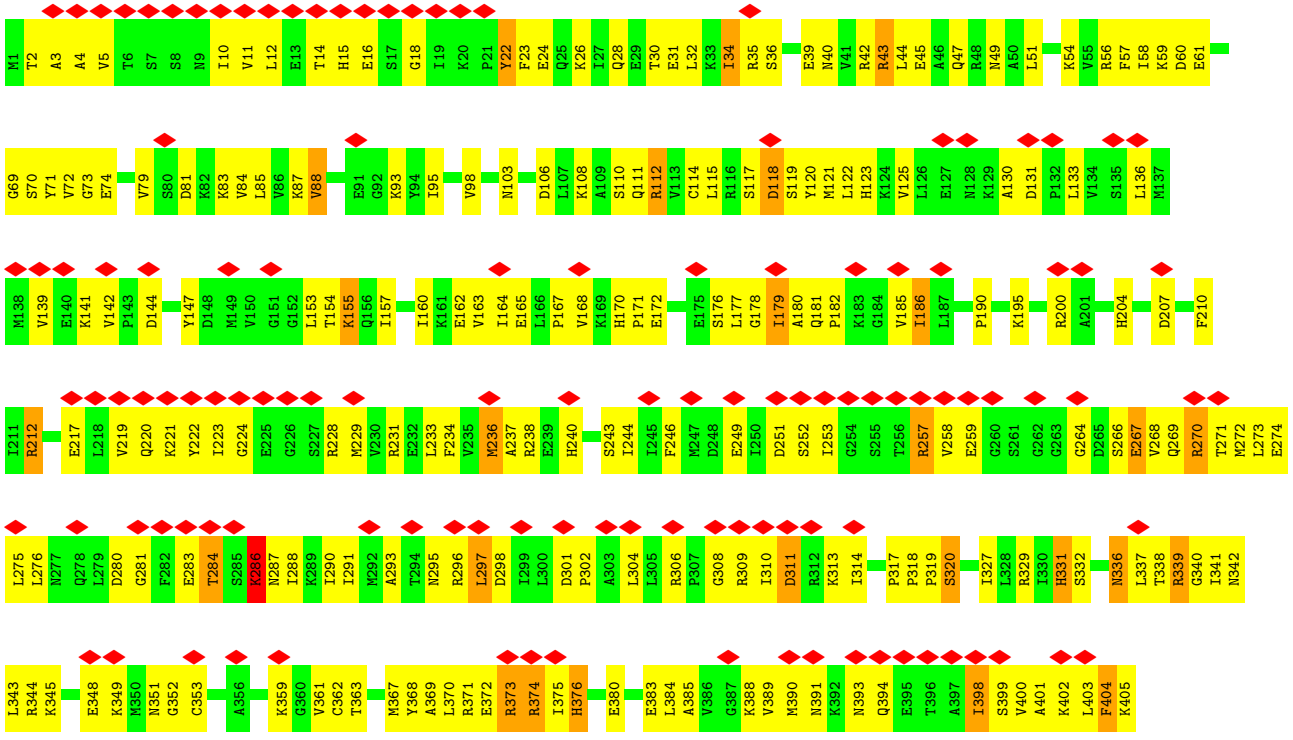
• Molecule 32: 26S proteasome regulatory subunit 6A





• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146519	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	0.181	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	2.28	72/1951 (3.7%)	2.46	124/2641 (4.7%)
1	a	2.23	57/1951 (2.9%)	2.42	129/2641 (4.9%)
2	B	2.27	60/1918 (3.1%)	2.43	122/2597 (4.7%)
2	b	2.26	66/1918 (3.4%)	2.47	130/2597 (5.0%)
3	C	2.29	73/1914 (3.8%)	2.37	98/2591 (3.8%)
3	c	2.27	65/1914 (3.4%)	2.41	109/2591 (4.2%)
4	D	2.30	72/1892 (3.8%)	2.46	130/2562 (5.1%)
4	d	2.32	83/2016 (4.1%)	2.51	137/2723 (5.0%)
5	E	2.36	80/1909 (4.2%)	2.45	130/2571 (5.1%)
5	e	2.29	69/1909 (3.6%)	2.44	120/2571 (4.7%)
6	F	2.24	69/1811 (3.8%)	2.39	108/2447 (4.4%)
6	f	2.25	65/1811 (3.6%)	2.49	128/2447 (5.2%)
7	G	2.27	80/1937 (4.1%)	2.50	122/2614 (4.7%)
7	g	2.24	63/1937 (3.3%)	2.54	137/2614 (5.2%)
8	1	2.22	52/1541 (3.4%)	2.41	93/2087 (4.5%)
8	h	2.34	65/1541 (4.2%)	2.44	93/2087 (4.5%)
9	2	2.32	73/1751 (4.2%)	2.39	109/2373 (4.6%)
9	i	2.26	62/1751 (3.5%)	2.39	100/2373 (4.2%)
10	3	2.28	69/1611 (4.3%)	2.42	112/2174 (5.2%)
10	j	2.25	51/1611 (3.2%)	2.43	86/2174 (4.0%)
11	4	2.27	58/1590 (3.6%)	2.35	105/2142 (4.9%)
11	k	2.29	64/1590 (4.0%)	2.40	91/2142 (4.2%)
12	5	2.25	61/1681 (3.6%)	2.34	97/2274 (4.3%)
12	l	2.24	62/1681 (3.7%)	2.42	103/2274 (4.5%)
13	6	2.29	81/1795 (4.5%)	2.40	102/2420 (4.2%)
13	m	2.31	73/1795 (4.1%)	2.40	105/2420 (4.3%)
14	7	2.28	78/1821 (4.3%)	2.38	91/2470 (3.7%)
14	n	2.31	76/1847 (4.1%)	2.43	123/2503 (4.9%)
15	W	2.17	46/1558 (3.0%)	2.48	107/2111 (5.1%)
16	V	2.26	86/2309 (3.7%)	2.55	185/3115 (5.9%)
17	T	2.20	70/2236 (3.1%)	2.61	205/3017 (6.8%)
18	X	2.34	41/1059 (3.9%)	2.40	58/1432 (4.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
19	Y	2.20	25/741 (3.4%)	2.57	60/1000 (6.0%)
20	Z	3.17	19/7123 (0.3%)	1.90	157/9645 (1.6%)
21	N	2.24	255/7273 (3.5%)	2.53	575/9822 (5.9%)
22	S	2.19	132/3967 (3.3%)	2.54	306/5355 (5.7%)
23	P	2.18	117/3664 (3.2%)	2.53	274/4940 (5.5%)
24	Q	2.23	134/3556 (3.8%)	2.54	259/4787 (5.4%)
25	R	2.24	113/3314 (3.4%)	2.52	269/4469 (6.0%)
26	U	2.25	80/2461 (3.3%)	2.52	196/3327 (5.9%)
27	O	2.27	109/3247 (3.4%)	2.52	229/4380 (5.2%)
28	H	2.29	138/3363 (4.1%)	2.53	238/4532 (5.3%)
29	I	2.22	104/3061 (3.4%)	2.51	225/4121 (5.5%)
30	K	2.30	133/3156 (4.2%)	2.41	202/4261 (4.7%)
31	L	2.28	111/3129 (3.5%)	2.41	193/4204 (4.6%)
32	M	2.32	144/3323 (4.3%)	2.42	214/4478 (4.8%)
33	J	2.30	125/3212 (3.9%)	2.52	223/4316 (5.2%)
All	All	2.33	3881/112146 (3.5%)	2.44	7309/151432 (4.8%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	6
11	4	0	7
11	k	0	7
12	5	0	7
12	l	0	7
13	6	0	6
13	m	0	6
14	7	0	10
14	n	0	4
15	W	0	1
16	V	0	6
17	T	0	7
18	X	0	4
19	Y	0	2
20	Z	1	7
21	N	0	18
22	S	0	18
23	P	0	10
24	Q	0	14
25	R	0	12
26	U	0	3
27	O	0	6
28	H	0	15
29	I	0	7
30	K	0	10
31	L	0	10
32	M	0	13
33	J	0	13
All	All	1	355

All (3881) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	748	LEU	CA-C	217.61	4.46	1.52
20	Z	255	LEU	CB-CG	73.72	3.00	1.53
20	Z	748	LEU	N-CA	54.11	2.15	1.46
20	Z	728	LYS	CG-CD	48.53	2.98	1.52
20	Z	738	TYR	CZ-OH	37.64	2.17	1.38
20	Z	255	LEU	CG-CD1	29.20	2.48	1.52
20	Z	748	LEU	CA-CB	18.34	1.83	1.53
20	Z	728	LYS	CB-CG	16.58	2.02	1.52
3	C	8	SER	CA-C	-13.78	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	391	ILE	CA-C	-13.39	1.35	1.52
14	7	76	ILE	N-CA	-12.53	1.36	1.45
26	U	267	VAL	CA-CB	-12.10	1.40	1.54
8	h	47	HIS	ND1-CE1	12.01	1.44	1.32
9	i	223	ASN	CA-C	-12.01	1.37	1.52
20	Z	728	LYS	CA-CB	11.61	1.73	1.53
20	Z	747	ALA	C-N	11.22	1.49	1.34
2	B	226	GLY	C-N	11.14	1.43	1.33
24	Q	190	ASN	CA-C	-11.14	1.38	1.52
8	1	112	ASP	CA-C	-11.02	1.39	1.52
30	K	259	ARG	CD-NE	10.79	1.61	1.46
3	c	106	ILE	CA-C	-10.75	1.41	1.52
27	O	268	SER	CA-C	-10.70	1.39	1.52
27	O	34	GLU	CA-C	-10.68	1.39	1.52
33	J	170	HIS	C-N	-10.56	1.25	1.33
28	H	234	ARG	CD-NE	10.44	1.60	1.46
2	b	124	SER	CA-C	-10.31	1.40	1.52
31	L	83	ASP	CA-C	-10.29	1.39	1.52
6	F	154	THR	N-CA	-10.27	1.33	1.46
24	Q	50	ARG	CZ-NH2	10.14	1.46	1.33
7	g	87	HIS	ND1-CE1	9.98	1.42	1.32
11	4	26	SER	CA-C	-9.97	1.40	1.52
7	g	47	VAL	C-N	9.97	1.46	1.33
10	3	39	LYS	CA-C	-9.95	1.40	1.52
30	K	108	GLY	CA-C	-9.94	1.43	1.52
28	H	273	ARG	CA-C	-9.93	1.39	1.52
14	n	205	VAL	CA-CB	-9.93	1.42	1.54
18	X	60	GLU	CA-C	-9.80	1.40	1.52
21	N	234	ASP	N-CA	-9.79	1.34	1.46
13	6	36	ARG	NE-CZ	9.77	1.43	1.33
12	l	161	LEU	N-CA	-9.77	1.34	1.46
23	P	211	PRO	CA-CB	9.77	1.67	1.53
29	I	316	PHE	CA-C	-9.76	1.40	1.52
4	d	195	THR	C-N	9.65	1.46	1.33
11	4	36	ARG	CD-NE	9.64	1.59	1.46
3	c	59	GLN	CA-C	-9.60	1.42	1.52
18	X	130	ASN	N-CA	-9.60	1.34	1.46
31	L	82	ARG	NE-CZ	9.57	1.43	1.33
14	n	136	ARG	NE-CZ	9.56	1.43	1.33
5	E	156	PHE	CA-C	-9.54	1.41	1.52
16	V	190	HIS	CB-CG	9.53	1.63	1.50
25	R	183	ASP	CA-C	-9.52	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	241	PHE	N-CA	-9.51	1.34	1.46
23	P	402	PHE	CA-CB	9.46	1.66	1.53
32	M	368	MET	C-N	9.44	1.46	1.33
12	l	263	HIS	ND1-CE1	9.42	1.42	1.32
33	J	178	GLY	C-N	9.32	1.44	1.33
13	m	84	HIS	CB-CG	9.30	1.63	1.50
33	J	185	VAL	C-N	9.30	1.45	1.33
9	i	104	ARG	NE-CZ	9.27	1.43	1.33
27	O	367	LYS	CA-C	-9.27	1.40	1.52
8	1	127	SER	CA-CB	9.26	1.62	1.54
2	B	235	PHE	N-CA	-9.26	1.34	1.46
15	W	196	SER	CA-CB	9.24	1.60	1.53
12	l	116	LEU	CA-C	-9.19	1.41	1.52
27	O	189	TYR	CA-C	-9.19	1.41	1.52
21	N	616	HIS	ND1-CE1	9.15	1.41	1.32
4	D	119	ARG	NE-CZ	9.14	1.43	1.33
24	Q	186	HIS	ND1-CE1	9.14	1.41	1.32
7	G	82	ILE	CA-CB	9.11	1.59	1.54
25	R	303	SER	N-CA	-9.10	1.33	1.46
11	4	100	VAL	CA-C	-9.08	1.41	1.52
27	O	78	VAL	C-N	9.08	1.45	1.33
9	2	191	GLY	CA-C	-9.07	1.41	1.51
24	Q	299	MET	CA-C	-9.03	1.41	1.52
27	O	126	ILE	CA-C	-9.03	1.41	1.52
12	l	153	ALA	CA-C	-9.02	1.41	1.52
29	I	407	ARG	CD-NE	9.01	1.58	1.46
28	H	95	HIS	ND1-CE1	9.01	1.41	1.32
8	h	58	ALA	CA-C	-9.01	1.41	1.52
5	E	50	VAL	CA-C	-9.00	1.43	1.52
7	G	130	ARG	CA-C	-8.93	1.42	1.52
14	7	69	PHE	N-CA	-8.90	1.35	1.46
28	H	340	LEU	C-N	8.89	1.45	1.33
32	M	272	GLU	CA-C	-8.88	1.41	1.52
17	T	77	SER	CA-C	-8.87	1.41	1.52
27	O	208	ALA	CA-C	-8.86	1.41	1.52
5	E	114	GLN	C-N	8.83	1.45	1.33
31	L	63	LYS	N-CA	-8.83	1.35	1.46
11	k	22	THR	CA-C	-8.80	1.42	1.52
22	S	80	VAL	CA-C	-8.80	1.45	1.52
13	6	47	TYR	N-CA	-8.79	1.34	1.46
25	R	252	TYR	C-N	8.79	1.45	1.33
8	h	194	ARG	NE-CZ	8.78	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	20	LYS	C-N	8.78	1.45	1.33
9	i	95	HIS	ND1-CE1	8.78	1.41	1.32
14	n	65	SER	CA-CB	8.73	1.66	1.53
24	Q	124	PHE	CA-C	-8.71	1.40	1.52
5	e	114	GLN	CA-C	-8.71	1.41	1.52
9	2	115	HIS	ND1-CE1	8.70	1.41	1.32
12	l	77	THR	CA-C	-8.69	1.42	1.52
6	f	160	ALA	CA-C	-8.67	1.41	1.52
1	A	194	ILE	CA-C	-8.65	1.42	1.52
16	V	100	ARG	CZ-NH2	8.63	1.44	1.33
1	a	207	ILE	CA-C	-8.62	1.42	1.52
11	k	105	GLY	C-N	8.62	1.42	1.33
3	c	125	HIS	ND1-CE1	8.61	1.41	1.32
2	b	208	THR	CA-C	-8.60	1.41	1.52
29	I	325	ILE	CA-C	-8.59	1.42	1.52
21	N	444	HIS	ND1-CE1	8.58	1.41	1.32
3	c	244	ILE	N-CA	-8.57	1.36	1.46
25	R	402	LEU	CA-C	-8.57	1.42	1.52
30	K	252	ARG	CZ-NH1	8.57	1.44	1.32
4	d	114	ALA	N-CA	-8.56	1.34	1.46
9	2	234	PHE	CA-C	8.56	1.60	1.52
22	S	456	ASP	CA-C	8.56	1.63	1.52
28	H	147	ILE	CA-C	-8.55	1.41	1.52
5	e	122	ARG	CA-CB	8.54	1.63	1.53
8	h	137	GLY	CA-C	-8.54	1.42	1.52
22	S	121	VAL	CA-CB	-8.53	1.44	1.54
3	C	152	ASN	C-N	8.52	1.43	1.34
31	L	390	ASP	C-N	8.51	1.44	1.33
29	I	141	LEU	CA-C	-8.51	1.42	1.52
24	Q	250	THR	CA-C	-8.49	1.40	1.52
21	N	331	ALA	CA-C	-8.49	1.41	1.52
14	n	148	ILE	CA-C	-8.48	1.41	1.52
10	3	125	ASP	CA-C	8.46	1.58	1.53
33	J	5	VAL	N-CA	-8.45	1.35	1.46
6	f	101	ARG	N-CA	-8.45	1.35	1.45
5	e	130	GLU	CA-C	-8.45	1.42	1.52
15	W	55	ALA	CA-C	-8.44	1.42	1.52
30	K	294	ARG	NE-CZ	8.43	1.42	1.33
33	J	267	GLU	C-N	8.43	1.44	1.33
4	d	133	THR	CA-C	-8.43	1.42	1.52
13	6	169	GLU	CA-C	8.42	1.62	1.53
4	D	234	THR	CA-C	-8.41	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	124	TYR	C-N	8.39	1.45	1.33
21	N	220	CYS	CA-C	-8.39	1.42	1.52
13	m	22	GLY	CA-C	8.39	1.60	1.52
11	k	37	GLN	C-N	8.38	1.45	1.33
5	E	203	ILE	CA-CB	-8.36	1.43	1.54
21	N	531	LEU	C-N	8.35	1.45	1.33
5	E	151	ASP	C-N	8.35	1.43	1.33
16	V	96	LYS	CA-CB	8.35	1.66	1.53
5	e	39	GLY	CA-C	-8.34	1.44	1.51
26	U	94	HIS	ND1-CE1	8.33	1.40	1.32
21	N	162	ARG	CA-C	-8.33	1.42	1.52
30	K	205	PRO	CA-C	8.33	1.59	1.52
30	K	111	SER	CA-CB	8.32	1.64	1.53
1	a	212	ASP	CA-CB	8.32	1.66	1.53
3	C	5	ARG	CD-NE	8.32	1.57	1.46
3	c	244	ILE	CA-CB	-8.32	1.43	1.54
21	N	678	ILE	CA-CB	-8.31	1.44	1.54
5	E	159	GLU	CA-C	-8.31	1.46	1.52
1	a	233	PHE	CA-C	-8.31	1.42	1.52
25	R	417	TYR	C-N	8.30	1.45	1.33
32	M	279	PHE	CA-C	-8.30	1.42	1.52
4	D	181	ARG	NE-CZ	8.29	1.42	1.33
18	X	100	TRP	CA-C	-8.28	1.42	1.52
5	e	44	GLU	CA-C	-8.27	1.41	1.52
33	J	290	ILE	CA-C	-8.26	1.42	1.52
7	G	234	ASP	CA-C	-8.24	1.42	1.52
21	N	649	VAL	N-CA	-8.24	1.35	1.46
31	L	315	PHE	C-N	8.24	1.44	1.33
2	b	68	THR	CA-C	8.24	1.63	1.52
26	U	254	ARG	CZ-NH2	8.24	1.44	1.33
5	e	143	LEU	CA-C	-8.24	1.42	1.52
16	V	68	VAL	CA-C	-8.23	1.42	1.52
3	c	46	LEU	N-CA	-8.23	1.35	1.46
3	C	129	ARG	NE-CZ	8.23	1.42	1.33
33	J	16	GLU	CA-C	-8.22	1.42	1.52
3	C	206	LEU	CA-CB	8.20	1.63	1.53
27	O	237	PRO	CA-C	8.20	1.66	1.52
24	Q	13	ARG	NE-CZ	8.20	1.42	1.33
31	L	356	GLY	CA-C	-8.20	1.40	1.51
26	U	46	ILE	CA-C	-8.18	1.42	1.52
6	f	137	TYR	CA-C	-8.18	1.43	1.52
33	J	171	PRO	N-CA	-8.18	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	224	LEU	CA-C	-8.16	1.42	1.52
31	L	282	GLU	CA-C	-8.16	1.44	1.53
9	2	109	LEU	CA-C	-8.15	1.42	1.52
28	H	400	ARG	CD-NE	8.15	1.57	1.46
29	I	411	VAL	CA-C	8.15	1.62	1.52
7	g	167	LYS	N-CA	-8.14	1.36	1.46
15	W	163	ASN	CA-C	-8.13	1.42	1.52
14	7	194	ARG	CA-C	-8.11	1.42	1.52
9	i	84	VAL	CA-CB	-8.11	1.44	1.54
30	K	318	THR	CA-C	-8.09	1.42	1.52
22	S	478	SER	CA-C	-8.09	1.42	1.52
12	5	181	ARG	CD-NE	8.09	1.57	1.46
26	U	218	GLU	N-CA	-8.09	1.35	1.46
5	e	77	ALA	C-N	8.09	1.43	1.33
30	K	347	ARG	CD-NE	8.09	1.57	1.46
7	G	20	ARG	NE-CZ	8.09	1.42	1.33
15	W	122	ARG	N-CA	-8.07	1.36	1.46
31	L	329	ARG	NE-CZ	8.07	1.42	1.33
23	P	389	ILE	CA-C	-8.06	1.43	1.53
24	Q	182	SER	CA-C	-8.05	1.42	1.52
31	L	97	ALA	C-N	8.05	1.44	1.33
14	n	162	TYR	CA-C	-8.04	1.42	1.52
27	O	172	TYR	N-CA	8.04	1.56	1.46
12	5	247	GLY	N-CA	-8.04	1.33	1.45
8	h	133	TYR	CA-C	-8.04	1.42	1.52
12	l	210	PHE	N-CA	-8.03	1.35	1.46
3	c	222	ASP	N-CA	-8.03	1.35	1.46
14	7	50	ASP	N-CA	-8.03	1.36	1.46
23	P	314	VAL	N-CA	-8.03	1.36	1.46
22	S	233	LEU	CA-C	-8.02	1.42	1.52
3	C	211	LEU	CA-C	-8.02	1.42	1.52
21	N	207	LEU	N-CA	-7.99	1.36	1.46
8	1	57	SER	C-N	7.99	1.44	1.33
21	N	629	CYS	CA-CB	7.98	1.64	1.53
9	i	217	ARG	CD-NE	7.98	1.57	1.46
16	V	255	ILE	CA-C	7.98	1.63	1.53
31	L	299	ARG	NE-CZ	7.98	1.41	1.33
30	K	350	ARG	NE-CZ	7.97	1.41	1.33
5	e	157	HIS	ND1-CE1	7.97	1.40	1.32
13	m	36	ARG	NE-CZ	7.97	1.41	1.33
7	G	93	ARG	CD-NE	7.96	1.57	1.46
23	P	279	ASP	C-N	-7.96	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	PHE	CA-CB	7.95	1.66	1.53
7	G	177	GLU	C-N	7.95	1.44	1.33
6	F	101	ARG	CD-NE	7.95	1.57	1.46
4	d	49	ARG	NE-CZ	7.94	1.41	1.33
9	i	97	LEU	CA-C	7.94	1.63	1.52
25	R	96	GLN	CA-C	-7.93	1.41	1.52
5	e	64	ILE	C-N	7.93	1.43	1.33
11	4	50	ALA	N-CA	-7.92	1.36	1.46
21	N	633	GLY	CA-C	-7.92	1.45	1.52
33	J	181	GLN	CA-CB	7.91	1.65	1.53
2	B	236	ARG	N-CA	-7.91	1.36	1.46
24	Q	404	ASN	CA-C	-7.91	1.43	1.52
30	K	204	ASP	C-N	7.90	1.42	1.33
27	O	127	LEU	C-N	7.89	1.44	1.33
32	M	129	LEU	C-N	-7.89	1.24	1.33
12	5	247	GLY	CA-C	-7.89	1.40	1.51
32	M	290	ARG	CD-NE	7.88	1.57	1.46
27	O	362	GLN	C-N	7.88	1.43	1.33
33	J	125	VAL	CA-CB	-7.88	1.45	1.54
6	f	161	ILE	N-CA	-7.87	1.37	1.46
22	S	216	LYS	C-N	7.86	1.44	1.33
1	a	60	PRO	N-CA	-7.86	1.37	1.47
26	U	283	ARG	NE-CZ	7.86	1.41	1.33
14	n	98	ARG	NE-CZ	7.86	1.41	1.33
1	A	152	PRO	CA-CB	-7.86	1.43	1.53
21	N	765	ASP	CA-C	-7.85	1.42	1.52
4	d	71	VAL	CA-C	-7.85	1.43	1.52
4	D	35	GLY	CA-C	-7.84	1.44	1.51
15	W	169	SER	C-O	-7.84	1.14	1.23
7	G	136	THR	N-CA	-7.84	1.37	1.46
9	2	113	LYS	CA-C	-7.83	1.42	1.52
28	H	206	VAL	CA-C	-7.83	1.43	1.52
23	P	392	LYS	CA-C	-7.83	1.43	1.52
2	b	99	ARG	NE-CZ	7.82	1.41	1.33
18	X	17	TYR	C-N	7.82	1.43	1.33
1	A	193	HIS	ND1-CE1	7.82	1.40	1.32
13	m	99	ARG	CD-NE	7.82	1.57	1.46
10	3	166	THR	N-CA	-7.82	1.36	1.46
19	Y	66	ASP	C-N	7.82	1.40	1.33
25	R	324	ARG	NE-CZ	7.81	1.41	1.33
1	a	152	PRO	CA-C	-7.81	1.43	1.52
12	5	121	ALA	CA-C	-7.81	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	VAL	CA-C	-7.79	1.43	1.52
27	O	369	ARG	NE-CZ	7.79	1.41	1.33
13	6	84	HIS	CB-CG	7.78	1.61	1.50
26	U	60	GLU	CA-C	-7.78	1.42	1.52
14	n	179	PHE	N-CA	-7.78	1.36	1.46
7	G	54	ILE	CA-C	-7.78	1.42	1.52
26	U	193	GLN	C-N	7.78	1.44	1.33
32	M	264	ARG	CD-NE	7.78	1.57	1.46
1	a	137	LEU	C-N	7.77	1.42	1.33
31	L	62	ARG	NE-CZ	7.77	1.41	1.33
33	J	15	HIS	CB-CG	-7.76	1.39	1.50
16	V	20	ARG	NE-CZ	7.76	1.41	1.33
3	c	89	ASN	CA-CB	7.76	1.65	1.53
4	d	151	GLU	C-N	7.76	1.43	1.33
2	B	185	LEU	N-CA	-7.75	1.37	1.46
14	7	88	GLY	CA-C	-7.75	1.41	1.51
4	d	67	ILE	CA-C	-7.75	1.43	1.52
6	f	128	TYR	CA-C	-7.75	1.42	1.52
11	k	11	ASP	CA-C	-7.75	1.43	1.52
16	V	49	VAL	C-N	7.75	1.43	1.33
12	l	247	GLY	CA-C	-7.75	1.41	1.51
6	f	81	ALA	CA-C	-7.74	1.42	1.52
6	F	208	VAL	CA-CB	-7.74	1.44	1.54
13	m	74	LYS	CA-C	7.74	1.63	1.52
32	M	424	ALA	C-N	7.74	1.43	1.33
7	G	50	VAL	CA-C	-7.73	1.43	1.52
20	Z	748	LEU	CB-CG	7.73	1.69	1.53
27	O	245	ASP	CA-C	-7.73	1.42	1.53
8	h	197	PHE	N-CA	-7.73	1.36	1.46
17	T	24	GLU	N-CA	-7.73	1.36	1.46
17	T	14	ALA	CA-C	-7.72	1.42	1.52
10	j	34	LEU	C-N	7.72	1.38	1.33
7	G	93	ARG	NE-CZ	7.72	1.41	1.33
4	D	42	VAL	CA-C	-7.72	1.43	1.52
10	3	34	LEU	CA-C	-7.72	1.43	1.52
14	7	40	THR	C-N	7.72	1.41	1.33
26	U	34	VAL	N-CA	-7.72	1.37	1.46
31	L	215	PRO	CA-CB	7.72	1.64	1.54
2	b	180	ASN	CA-C	-7.71	1.42	1.52
10	3	202	MET	C-N	7.71	1.43	1.33
26	U	47	ARG	CZ-NH1	7.71	1.43	1.32
31	L	266	MET	CA-C	-7.71	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	110	ASP	CA-C	-7.71	1.42	1.52
6	F	137	TYR	C-N	7.70	1.41	1.33
21	N	421	ASP	CA-CB	7.70	1.65	1.53
3	C	91	ALA	N-CA	-7.70	1.37	1.46
23	P	113	ASN	N-CA	-7.69	1.37	1.46
14	7	56	ALA	CA-C	-7.69	1.43	1.52
17	T	132	HIS	CB-CG	7.68	1.60	1.50
25	R	422	ARG	NE-CZ	7.68	1.41	1.33
23	P	52	LEU	C-N	7.68	1.44	1.34
30	K	267	SER	C-N	7.67	1.43	1.33
2	b	82	TYR	CA-CB	7.67	1.65	1.53
10	j	170	ALA	CA-C	-7.67	1.43	1.52
21	N	638	ILE	N-CA	-7.66	1.38	1.46
13	6	99	ARG	NE-CZ	7.66	1.41	1.33
4	D	200	LEU	CA-C	-7.66	1.42	1.52
19	Y	58	ASN	CA-C	-7.65	1.44	1.53
7	g	60	VAL	CA-C	7.65	1.59	1.53
22	S	185	PHE	N-CA	-7.65	1.37	1.46
4	D	6	ARG	C-N	7.65	1.43	1.33
24	Q	130	ARG	CA-C	-7.65	1.42	1.53
26	U	126	LYS	N-CA	-7.64	1.35	1.45
30	K	381	ALA	CA-C	-7.64	1.42	1.52
3	C	149	TYR	CA-C	-7.63	1.43	1.52
7	g	232	LYS	CA-C	-7.63	1.43	1.52
12	5	281	SER	CA-C	-7.62	1.43	1.53
23	P	88	GLN	CA-CB	7.62	1.64	1.53
11	k	95	ARG	CZ-NH1	7.62	1.43	1.32
3	c	188	ASP	CA-C	7.62	1.63	1.52
7	g	123	HIS	CB-CG	7.61	1.60	1.50
14	7	201	THR	N-CA	-7.60	1.36	1.46
9	2	45	ALA	C-N	7.60	1.43	1.33
21	N	258	ALA	N-CA	-7.60	1.37	1.46
29	I	219	VAL	C-N	7.58	1.43	1.33
9	2	97	LEU	CA-C	-7.58	1.43	1.52
14	n	136	ARG	CD-NE	7.57	1.56	1.46
29	I	371	LEU	CA-C	-7.57	1.42	1.53
9	2	65	ARG	NE-CZ	7.57	1.41	1.33
10	j	198	ARG	CD-NE	7.56	1.56	1.46
21	N	173	LYS	CA-C	-7.56	1.41	1.52
4	D	56	ASP	CA-C	-7.56	1.43	1.53
21	N	500	ASP	CA-C	7.56	1.62	1.52
15	W	122	ARG	CD-NE	7.56	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	184	LEU	CA-C	-7.56	1.42	1.52
2	b	129	PRO	CA-C	7.55	1.61	1.52
21	N	217	MET	CA-C	-7.55	1.45	1.53
14	n	124	TYR	CA-C	-7.55	1.43	1.52
33	J	18	GLY	C-N	7.54	1.42	1.34
33	J	35	ARG	NE-CZ	7.53	1.41	1.33
29	I	76	VAL	CA-CB	-7.53	1.44	1.54
11	k	27	VAL	CA-C	-7.52	1.44	1.52
12	l	97	ALA	C-N	7.52	1.44	1.33
27	O	210	ARG	NE-CZ	7.52	1.41	1.33
7	g	132	PHE	N-CA	-7.51	1.35	1.45
24	Q	405	GLN	CA-CB	7.51	1.66	1.53
14	7	83	VAL	CA-C	-7.50	1.43	1.52
32	M	227	GLY	C-N	7.50	1.43	1.33
27	O	284	GLU	N-CA	-7.50	1.37	1.46
5	e	140	VAL	N-CA	-7.50	1.37	1.46
7	g	20	ARG	NE-CZ	7.50	1.41	1.33
11	k	133	HIS	CA-C	-7.50	1.43	1.52
31	L	291	PHE	CA-C	-7.50	1.46	1.53
13	m	193	ARG	NE-CZ	7.49	1.41	1.33
7	g	9	ASP	CA-CB	7.49	1.65	1.53
8	1	43	LEU	CA-C	-7.49	1.43	1.52
25	R	416	LYS	CA-C	-7.48	1.43	1.52
32	M	380	ALA	CA-C	-7.48	1.43	1.52
28	H	434	ARG	NE-CZ	7.48	1.41	1.33
27	O	235	HIS	CE1-NE2	-7.47	1.25	1.32
3	c	216	ILE	CA-C	-7.47	1.43	1.52
13	m	125	ASP	CA-C	-7.47	1.42	1.52
8	h	13	MET	CA-CB	7.46	1.66	1.53
25	R	51	LEU	CA-C	-7.46	1.43	1.52
14	7	63	TYR	CA-C	-7.46	1.43	1.52
25	R	348	LEU	CA-C	-7.46	1.43	1.52
29	I	422	ARG	NE-CZ	7.46	1.41	1.33
9	i	87	LEU	CA-C	-7.45	1.43	1.52
14	7	232	ILE	CA-C	-7.45	1.43	1.52
18	X	26	PRO	CA-C	-7.45	1.43	1.52
10	3	80	ARG	CD-NE	7.44	1.56	1.46
12	l	146	LYS	C-N	7.44	1.42	1.33
29	I	281	ILE	CA-C	-7.43	1.44	1.52
20	Z	728	LYS	CA-C	7.43	1.62	1.52
5	e	36	THR	CA-C	7.42	1.62	1.52
11	k	141	PHE	N-CA	-7.42	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	420	THR	N-CA	-7.42	1.37	1.46
4	D	215	VAL	CA-C	-7.42	1.43	1.52
21	N	917	ILE	N-CA	-7.41	1.35	1.46
8	h	201	GLU	N-CA	-7.41	1.37	1.46
32	M	166	ARG	NE-CZ	7.41	1.41	1.33
26	U	214	VAL	C-N	7.40	1.41	1.33
8	1	130	LYS	C-N	7.40	1.42	1.33
31	L	53	HIS	CA-C	-7.40	1.42	1.52
30	K	57	GLU	CA-C	-7.40	1.42	1.52
31	L	61	LYS	C-N	7.40	1.43	1.33
30	K	42	ASN	C-N	7.40	1.43	1.33
12	l	100	TRP	N-CA	-7.39	1.36	1.46
25	R	383	ARG	NE-CZ	7.38	1.41	1.33
21	N	676	ALA	CA-C	-7.38	1.43	1.52
2	B	243	ILE	C-N	7.38	1.44	1.33
28	H	368	PRO	N-CD	7.38	1.58	1.47
33	J	162	GLU	CA-C	-7.38	1.43	1.52
9	2	215	TYR	CA-CB	7.38	1.62	1.52
21	N	561	GLY	CA-C	-7.38	1.41	1.51
30	K	148	ASP	CA-C	-7.38	1.43	1.52
19	Y	12	SER	N-CA	-7.37	1.37	1.46
32	M	248	ALA	C-O	-7.37	1.17	1.24
5	e	60	GLU	CA-C	-7.37	1.43	1.52
13	m	206	VAL	C-N	7.36	1.40	1.32
23	P	3	ARG	CD-NE	7.36	1.56	1.46
29	I	208	TYR	C-N	7.35	1.45	1.33
4	d	254	HIS	CD2-NE2	7.35	1.46	1.37
1	a	213	ALA	N-CA	-7.34	1.37	1.46
25	R	237	THR	N-CA	-7.34	1.37	1.46
7	g	123	HIS	ND1-CE1	7.34	1.39	1.32
21	N	577	SER	CA-C	-7.34	1.42	1.52
5	e	142	LEU	CA-C	-7.33	1.43	1.52
1	A	209	HIS	ND1-CE1	7.33	1.39	1.32
4	D	5	ASP	N-CA	-7.33	1.36	1.46
19	Y	43	TRP	NE1-CE2	-7.33	1.29	1.37
27	O	353	VAL	N-CA	-7.33	1.37	1.46
11	4	39	SER	CA-C	7.32	1.59	1.52
9	i	104	ARG	N-CA	-7.32	1.37	1.45
11	4	42	THR	CA-C	-7.32	1.43	1.52
14	n	66	LEU	C-N	7.31	1.44	1.33
5	E	44	GLU	CA-C	-7.31	1.42	1.52
8	1	95	CYS	N-CA	-7.31	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	408	THR	CA-C	7.31	1.62	1.52
32	M	40	GLU	C-N	7.30	1.42	1.33
12	l	215	LEU	CA-C	-7.30	1.43	1.52
2	B	100	ILE	N-CA	-7.29	1.36	1.46
11	4	97	PRO	CA-CB	-7.29	1.45	1.54
13	6	90	LYS	C-N	7.29	1.43	1.33
21	N	189	LEU	CA-CB	7.29	1.64	1.53
17	T	45	SER	CA-C	7.29	1.62	1.52
6	f	130	VAL	N-CA	-7.28	1.37	1.46
11	k	96	ARG	CD-NE	7.28	1.56	1.46
1	A	131	ARG	NE-CZ	7.28	1.41	1.33
22	S	153	GLU	CA-C	7.28	1.60	1.53
33	J	339	ARG	CA-C	-7.28	1.44	1.53
28	H	387	ASN	C-N	7.28	1.43	1.33
5	E	16	SER	CA-C	7.28	1.61	1.52
5	e	53	ARG	CZ-NH1	7.27	1.43	1.32
10	3	52	GLY	CA-C	-7.27	1.44	1.52
22	S	261	HIS	CE1-NE2	7.27	1.39	1.32
31	L	335	PRO	C-N	7.26	1.43	1.33
25	R	291	SER	CA-C	-7.26	1.43	1.52
1	A	136	PRO	CA-C	-7.26	1.43	1.52
14	7	81	ASN	CA-C	-7.26	1.43	1.53
5	E	166	ARG	CZ-NH2	7.25	1.42	1.33
22	S	309	PHE	C-N	7.25	1.43	1.33
29	I	429	GLU	CA-C	-7.25	1.43	1.53
16	V	28	TYR	CA-CB	7.25	1.63	1.53
12	5	258	ASP	C-N	7.25	1.42	1.33
33	J	43	ARG	NE-CZ	7.24	1.41	1.33
21	N	72	LEU	N-CA	7.24	1.55	1.46
6	F	107	ARG	CD-NE	7.24	1.56	1.46
1	A	56	GLN	CA-CB	7.24	1.65	1.53
21	N	167	GLU	CA-C	-7.24	1.43	1.52
3	c	143	ARG	CD-NE	7.24	1.56	1.46
33	J	399	SER	CA-C	-7.24	1.43	1.52
28	H	164	SER	CA-C	-7.23	1.43	1.52
25	R	392	ARG	NE-CZ	7.23	1.41	1.33
3	C	186	VAL	CA-C	-7.23	1.43	1.52
22	S	38	LEU	N-CA	-7.23	1.37	1.46
2	B	180	ASN	CA-C	-7.23	1.43	1.52
7	G	156	SER	CA-C	-7.23	1.43	1.52
3	c	133	VAL	CA-C	-7.22	1.43	1.52
6	f	82	ARG	N-CA	7.22	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	13	SER	CA-C	-7.22	1.43	1.52
12	l	131	GLU	C-N	7.22	1.44	1.34
25	R	376	GLN	N-CA	-7.22	1.39	1.46
24	Q	76	GLU	N-CA	-7.21	1.37	1.46
4	d	45	GLY	CA-C	-7.21	1.46	1.52
2	B	42	GLY	CA-C	-7.21	1.43	1.51
31	L	339	ARG	NE-CZ	7.21	1.41	1.33
21	N	742	TRP	N-CA	-7.21	1.36	1.46
22	S	343	LEU	C-N	7.20	1.42	1.34
25	R	340	GLN	CA-C	7.20	1.62	1.52
28	H	275	ILE	CA-C	7.20	1.61	1.52
30	K	117	SER	CA-C	-7.20	1.43	1.52
21	N	880	ARG	CD-NE	7.19	1.56	1.46
21	N	626	GLY	CA-C	-7.19	1.43	1.51
23	P	285	GLN	C-N	7.19	1.43	1.33
33	J	286	LYS	CA-CB	7.19	1.64	1.53
9	2	230	LYS	CA-C	-7.19	1.43	1.52
7	g	81	LEU	CA-CB	7.19	1.63	1.53
26	U	135	ASP	CA-C	-7.18	1.44	1.52
28	H	60	GLU	CA-C	-7.18	1.43	1.52
9	i	236	ARG	NE-CZ	7.17	1.41	1.33
5	E	200	VAL	N-CA	7.17	1.55	1.46
21	N	498	ILE	N-CA	-7.17	1.37	1.46
27	O	169	ASN	CA-CB	7.17	1.64	1.53
9	2	198	SER	CA-C	7.17	1.61	1.52
10	j	155	GLU	CA-C	-7.16	1.47	1.52
21	N	618	ARG	NE-CZ	7.16	1.41	1.33
9	i	225	ARG	CZ-NH2	7.16	1.42	1.33
3	C	47	ALA	CA-C	-7.16	1.43	1.52
5	E	129	GLY	CA-C	-7.16	1.41	1.51
30	K	38	SER	N-CA	-7.15	1.37	1.46
31	L	137	ARG	CA-C	7.15	1.62	1.53
9	2	131	GLY	CA-C	-7.15	1.43	1.51
15	W	94	ALA	N-CA	7.15	1.55	1.46
4	D	169	LYS	N-CA	-7.15	1.37	1.46
13	6	113	TYR	CA-C	-7.15	1.43	1.53
28	H	428	MET	CA-C	-7.15	1.42	1.52
11	4	115	GLU	C-N	7.14	1.43	1.33
4	D	120	TYR	CA-C	-7.14	1.43	1.52
25	R	64	LYS	CA-C	-7.14	1.43	1.52
8	h	114	LYS	CA-CB	7.14	1.65	1.53
9	2	107	SER	CA-C	-7.14	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	343	LYS	CA-C	-7.14	1.43	1.52
32	M	323	VAL	CA-C	-7.14	1.44	1.52
3	c	132	GLY	CA-C	7.14	1.61	1.51
15	W	109	ARG	NE-CZ	7.13	1.40	1.33
27	O	241	THR	C-N	7.13	1.41	1.33
32	M	107	ASN	CA-C	-7.13	1.43	1.52
26	U	113	TYR	CA-C	-7.13	1.43	1.52
17	T	19	ASP	CA-C	-7.13	1.44	1.52
23	P	160	LEU	C-N	7.12	1.43	1.33
30	K	169	VAL	N-CA	7.12	1.54	1.46
8	1	44	THR	CA-C	-7.12	1.44	1.52
28	H	357	ARG	CD-NE	7.11	1.56	1.46
32	M	333	LEU	CA-C	-7.11	1.43	1.52
5	e	162	GLY	CA-C	-7.11	1.41	1.51
24	Q	135	HIS	ND1-CE1	7.11	1.39	1.32
26	U	197	LEU	CA-CB	7.11	1.64	1.53
22	S	70	ASN	N-CA	-7.10	1.38	1.46
11	k	149	ARG	NE-CZ	7.10	1.40	1.33
3	c	114	ARG	CD-NE	7.10	1.56	1.46
14	7	210	ILE	N-CA	-7.10	1.37	1.46
11	4	78	GLN	CA-CB	7.10	1.64	1.53
31	L	303	ARG	CZ-NH1	7.10	1.42	1.32
2	B	164	ILE	C-N	7.09	1.41	1.33
24	Q	74	LEU	C-N	7.09	1.42	1.33
9	2	64	HIS	CG-CD2	7.09	1.43	1.35
6	f	187	ASP	N-CA	-7.09	1.37	1.46
22	S	464	ARG	NE-CZ	7.09	1.40	1.33
8	h	154	ASN	CA-CB	7.09	1.64	1.53
3	C	57	LEU	CA-C	-7.09	1.44	1.52
7	G	214	LEU	N-CA	-7.09	1.37	1.46
32	M	268	ALA	N-CA	-7.09	1.37	1.46
19	Y	83	ARG	NE-CZ	7.08	1.40	1.33
8	h	140	SER	CA-C	-7.08	1.42	1.52
22	S	321	GLN	CA-C	-7.08	1.43	1.52
3	c	231	LYS	CA-CB	7.08	1.63	1.53
4	D	39	LYS	CA-C	-7.08	1.43	1.52
8	1	13	MET	CA-C	-7.08	1.44	1.52
27	O	166	ARG	NE-CZ	7.07	1.40	1.33
6	f	103	LEU	C-N	7.07	1.43	1.33
21	N	919	THR	CA-CB	7.07	1.64	1.53
13	m	191	LEU	C-N	7.07	1.42	1.33
6	F	43	HIS	CD2-NE2	7.07	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	167	LYS	CA-C	-7.07	1.43	1.52
19	Y	45	ASN	CA-C	-7.07	1.44	1.52
25	R	360	SER	CA-CB	7.07	1.64	1.53
25	R	128	LEU	CA-C	-7.06	1.46	1.52
33	J	329	ARG	CZ-NH2	7.06	1.42	1.33
28	H	194	SER	CA-CB	7.06	1.65	1.53
25	R	165	GLY	C-N	7.06	1.43	1.33
21	N	690	HIS	ND1-CE1	7.06	1.39	1.32
24	Q	364	LYS	N-CA	7.06	1.54	1.46
7	g	178	LYS	CA-CB	7.05	1.64	1.53
7	G	218	TRP	CA-C	-7.05	1.44	1.52
10	3	156	PRO	CA-C	-7.05	1.43	1.52
32	M	39	ASN	CA-C	-7.05	1.43	1.52
5	E	57	PRO	CA-C	-7.05	1.41	1.52
30	K	220	THR	C-N	7.05	1.43	1.33
11	4	189	ILE	N-CA	-7.05	1.38	1.46
17	T	259	ILE	N-CA	-7.04	1.38	1.46
13	m	75	ARG	CD-NE	7.04	1.56	1.46
14	n	116	ALA	C-N	7.04	1.43	1.33
12	5	106	VAL	C-O	-7.04	1.17	1.24
23	P	288	ASN	N-CA	7.04	1.55	1.46
32	M	251	LEU	C-N	7.03	1.42	1.33
32	M	345	ARG	NE-CZ	7.03	1.40	1.33
29	I	408	ARG	CA-CB	7.02	1.65	1.53
27	O	115	ARG	NE-CZ	7.02	1.40	1.33
3	C	24	TYR	CA-CB	7.02	1.65	1.53
21	N	838	GLU	CA-C	-7.02	1.43	1.52
27	O	288	ARG	N-CA	-7.02	1.37	1.46
32	M	209	ASP	CA-CB	7.02	1.64	1.53
17	T	57	ILE	CA-C	-7.02	1.44	1.52
14	n	76	ILE	CA-CB	-7.02	1.45	1.54
5	E	73	HIS	ND1-CE1	7.02	1.39	1.32
5	E	51	GLU	N-CA	-7.01	1.37	1.46
16	V	29	ILE	C-O	-7.01	1.16	1.24
14	n	77	PRO	CA-CB	7.01	1.62	1.53
3	c	125	HIS	N-CA	-7.01	1.37	1.45
28	H	123	GLY	CA-C	-7.01	1.42	1.52
24	Q	69	GLY	C-N	7.00	1.43	1.33
17	T	139	ASP	CA-C	-7.00	1.44	1.52
5	E	135	SER	CA-C	-7.00	1.43	1.52
7	G	93	ARG	CA-C	-7.00	1.43	1.52
1	a	77	ARG	NE-CZ	7.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	176	LEU	N-CA	-7.00	1.38	1.46
8	1	153	GLU	CA-C	-7.00	1.43	1.53
21	N	635	GLN	C-N	7.00	1.43	1.33
23	P	432	LEU	N-CA	-7.00	1.36	1.46
33	J	85	LEU	C-N	7.00	1.42	1.33
21	N	757	THR	N-CA	-6.99	1.37	1.46
10	j	14	ALA	C-N	6.99	1.42	1.33
16	V	157	ARG	NE-CZ	6.99	1.40	1.33
10	3	105	VAL	CA-C	-6.98	1.45	1.52
8	1	108	VAL	CA-C	-6.98	1.44	1.52
24	Q	163	ARG	NE-CZ	6.98	1.40	1.33
1	A	93	ALA	N-CA	-6.97	1.38	1.46
7	G	162	GLY	C-N	6.97	1.43	1.33
21	N	429	GLU	CA-C	-6.97	1.43	1.52
28	H	104	LYS	C-N	6.97	1.40	1.33
28	H	436	LYS	CA-C	-6.97	1.43	1.52
1	A	202	VAL	CA-CB	-6.97	1.45	1.54
6	f	60	GLN	CA-C	-6.97	1.44	1.52
11	k	12	SER	CA-C	-6.96	1.44	1.52
2	B	142	PHE	N-CA	-6.96	1.37	1.46
32	M	425	ARG	NE-CZ	6.96	1.40	1.33
32	M	156	LEU	C-N	6.96	1.42	1.33
26	U	143	VAL	CA-CB	6.96	1.62	1.54
12	l	174	THR	CA-C	-6.96	1.44	1.52
10	3	88	THR	N-CA	-6.96	1.38	1.46
13	6	103	HIS	ND1-CE1	6.95	1.39	1.32
23	P	44	LYS	C-N	6.95	1.42	1.33
24	Q	172	PRO	N-CA	-6.95	1.39	1.47
10	3	130	ILE	CA-C	-6.95	1.44	1.52
21	N	63	LEU	C-N	6.95	1.42	1.33
16	V	216	LEU	N-CA	-6.95	1.40	1.46
15	W	170	HIS	CG-CD2	-6.94	1.28	1.35
22	S	274	PHE	N-CA	-6.94	1.37	1.46
4	D	75	PHE	CA-C	-6.94	1.44	1.52
21	N	499	HIS	ND1-CE1	6.94	1.39	1.32
28	H	71	GLU	CA-C	-6.94	1.43	1.52
30	K	63	LEU	CA-C	-6.94	1.43	1.52
11	k	192	VAL	C-N	6.93	1.42	1.33
11	4	67	TYR	CA-CB	6.93	1.64	1.53
28	H	182	ASN	C-N	6.93	1.42	1.33
30	K	246	TYR	C-N	6.93	1.43	1.33
19	Y	66	ASP	N-CA	-6.93	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	204	GLN	CA-C	-6.93	1.43	1.52
15	W	36	ILE	CA-CB	-6.93	1.45	1.54
21	N	602	VAL	CA-CB	6.93	1.58	1.54
5	E	40	ILE	CA-C	-6.93	1.44	1.52
26	U	282	VAL	C-N	6.93	1.43	1.33
33	J	190	PRO	C-O	-6.93	1.19	1.25
6	f	121	GLN	C-N	6.92	1.42	1.33
1	A	27	GLN	N-CA	-6.92	1.37	1.46
12	5	104	GLN	C-N	6.92	1.43	1.33
28	H	329	VAL	CA-C	6.92	1.61	1.52
13	m	221	ARG	NE-CZ	6.92	1.40	1.33
31	L	157	ARG	CD-NE	6.92	1.55	1.46
2	b	86	VAL	CA-C	-6.92	1.44	1.52
6	f	131	GLY	CA-C	-6.92	1.45	1.52
13	6	161	GLN	C-N	6.92	1.40	1.33
30	K	373	ILE	CA-CB	-6.91	1.46	1.54
25	R	82	ASP	CA-C	-6.91	1.43	1.53
26	U	102	SER	C-N	6.90	1.43	1.33
30	K	244	HIS	CD2-NE2	6.90	1.45	1.37
11	k	5	LEU	CA-C	-6.90	1.44	1.52
30	K	340	PHE	C-O	-6.90	1.19	1.25
27	O	13	THR	CA-C	6.90	1.61	1.52
27	O	33	TYR	CA-C	-6.90	1.44	1.52
8	h	54	ARG	NE-CZ	6.89	1.40	1.33
28	H	354	ALA	CA-CB	6.89	1.62	1.53
33	J	190	PRO	CA-C	6.89	1.55	1.51
21	N	208	ARG	CD-NE	6.89	1.55	1.46
33	J	23	PHE	CA-C	-6.89	1.44	1.52
33	J	93	LYS	C-O	6.89	1.32	1.23
6	f	191	LYS	C-O	-6.89	1.16	1.24
12	5	179	TYR	N-CA	-6.89	1.38	1.46
5	e	31	ILE	C-N	6.88	1.43	1.33
16	V	114	PHE	CA-C	-6.88	1.43	1.53
13	6	220	VAL	CA-C	-6.88	1.44	1.52
7	G	115	ARG	CZ-NH2	6.88	1.42	1.33
7	g	148	LEU	CA-C	-6.87	1.44	1.52
8	h	117	GLY	N-CA	-6.87	1.35	1.45
7	g	73	HIS	ND1-CE1	6.87	1.39	1.32
28	H	85	MET	CA-C	-6.87	1.44	1.52
16	V	195	HIS	ND1-CE1	6.87	1.39	1.32
9	2	140	PHE	CA-C	-6.87	1.44	1.52
25	R	207	ARG	CZ-NH2	6.87	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	91	SER	CA-CB	6.87	1.64	1.53
9	2	167	LEU	CA-C	-6.87	1.44	1.52
25	R	345	TYR	CA-C	-6.86	1.44	1.52
13	m	134	ASP	C-N	6.86	1.41	1.34
10	j	28	ARG	CD-NE	6.86	1.55	1.46
14	n	96	ILE	CA-CB	-6.86	1.45	1.54
16	V	190	HIS	ND1-CE1	6.86	1.39	1.32
2	b	194	LEU	CA-CB	6.85	1.64	1.53
17	T	228	ILE	CA-C	-6.85	1.45	1.52
21	N	329	HIS	ND1-CE1	6.85	1.39	1.32
12	5	113	ASN	CA-C	6.84	1.61	1.52
28	H	324	GLY	N-CA	-6.84	1.37	1.45
2	B	99	ARG	CD-NE	6.83	1.55	1.46
16	V	251	TYR	CA-C	-6.83	1.43	1.52
4	d	116	VAL	CA-CB	-6.83	1.45	1.54
8	h	26	ASP	CA-C	-6.83	1.44	1.52
8	h	79	TYR	N-CA	-6.83	1.39	1.46
5	e	123	PHE	C-N	6.83	1.41	1.33
3	C	171	ALA	C-N	6.83	1.42	1.33
7	G	85	GLY	N-CA	-6.83	1.37	1.45
30	K	250	GLY	C-N	-6.83	1.25	1.33
33	J	155	LYS	C-N	6.83	1.44	1.33
7	G	86	ARG	CD-NE	6.83	1.55	1.46
13	6	187	GLU	C-N	6.83	1.42	1.33
5	E	84	ASP	CA-CB	6.83	1.65	1.53
21	N	548	ARG	CZ-NH1	6.83	1.42	1.32
10	j	64	ASN	C-N	6.82	1.42	1.33
1	a	128	TYR	C-N	6.82	1.44	1.33
30	K	128	ARG	CD-NE	6.82	1.55	1.46
22	S	142	VAL	C-O	-6.81	1.16	1.24
25	R	352	SER	CA-CB	6.81	1.64	1.53
29	I	316	PHE	CA-CB	6.81	1.64	1.53
2	b	157	PHE	CA-C	-6.81	1.45	1.52
3	c	165	VAL	CA-C	-6.81	1.45	1.53
32	M	394	VAL	CA-C	-6.81	1.43	1.52
4	d	49	ARG	CD-NE	6.81	1.55	1.46
8	h	157	LYS	N-CA	-6.81	1.38	1.46
24	Q	294	ARG	NE-CZ	6.81	1.40	1.33
32	M	221	TYR	CA-C	-6.81	1.44	1.52
11	k	152	MET	CA-CB	6.81	1.66	1.53
11	4	74	GLU	CA-C	-6.81	1.44	1.52
25	R	260	THR	C-N	6.80	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	64	ILE	CA-C	-6.80	1.44	1.52
17	T	271	GLU	CA-CB	6.80	1.63	1.53
30	K	89	ILE	N-CA	-6.80	1.38	1.46
7	G	75	GLY	CA-C	-6.79	1.43	1.52
10	j	68	ARG	CD-NE	6.79	1.55	1.46
7	G	22	PHE	CA-C	-6.79	1.44	1.52
5	e	235	LYS	N-CA	-6.79	1.38	1.46
8	1	183	ARG	NE-CZ	6.79	1.40	1.33
13	6	228	LYS	CA-C	-6.79	1.44	1.52
23	P	326	ASP	C-N	6.79	1.43	1.33
8	1	37	ASN	CA-C	-6.78	1.43	1.52
22	S	465	ILE	N-CA	-6.78	1.38	1.46
4	d	20	VAL	CA-CB	-6.78	1.45	1.54
19	Y	64	TRP	CA-CB	6.78	1.62	1.53
32	M	370	THR	N-CA	-6.78	1.37	1.46
14	7	183	MET	CA-C	-6.78	1.44	1.53
31	L	157	ARG	NE-CZ	6.78	1.40	1.33
11	k	87	GLU	CA-C	-6.78	1.44	1.52
10	3	71	THR	CA-C	-6.77	1.44	1.52
33	J	302	PRO	N-CA	-6.77	1.38	1.47
7	g	190	ARG	CZ-NH2	6.77	1.42	1.33
2	B	214	ILE	CA-C	-6.77	1.44	1.52
13	6	204	ILE	N-CA	6.77	1.53	1.46
16	V	40	HIS	CG-ND1	-6.77	1.30	1.38
31	L	95	ILE	CA-C	6.76	1.61	1.52
3	C	23	GLU	CA-CB	6.76	1.64	1.53
28	H	322	GLY	C-N	6.76	1.43	1.33
7	G	190	ARG	CA-C	-6.76	1.44	1.52
22	S	405	ARG	CD-NE	6.76	1.55	1.46
3	c	118	ILE	C-N	6.75	1.43	1.33
14	7	187	LEU	CA-C	-6.75	1.44	1.52
18	X	12	ALA	C-N	6.75	1.41	1.33
4	D	178	ASN	CA-C	-6.74	1.44	1.52
33	J	212	ARG	CD-NE	6.74	1.55	1.46
14	n	175	LEU	CA-C	-6.74	1.44	1.52
27	O	196	LEU	CA-C	-6.74	1.44	1.52
1	a	67	THR	C-N	6.74	1.42	1.33
21	N	714	THR	CA-C	-6.74	1.44	1.52
21	N	443	LEU	CA-CB	6.74	1.64	1.53
1	a	199	TRP	CZ2-CH2	6.73	1.50	1.37
27	O	66	VAL	CA-CB	-6.73	1.46	1.54
8	h	72	LEU	CA-C	-6.73	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	266	HIS	CG-CD2	6.73	1.43	1.35
29	I	202	LEU	CA-CB	6.73	1.64	1.53
32	M	98	GLU	CA-CB	6.73	1.63	1.53
17	T	219	LYS	C-N	6.73	1.43	1.33
3	C	180	TYR	C-O	-6.73	1.15	1.23
31	L	374	PHE	CA-C	-6.73	1.43	1.52
13	m	73	VAL	CA-CB	-6.72	1.45	1.54
15	W	150	ASN	CA-C	-6.72	1.43	1.52
29	I	107	GLY	CA-C	6.72	1.59	1.52
33	J	288	ILE	CA-CB	-6.72	1.45	1.53
5	E	220	SER	CA-C	-6.72	1.44	1.52
10	3	36	VAL	CA-CB	-6.72	1.48	1.55
16	V	131	GLN	CA-CB	6.72	1.63	1.53
21	N	810	ALA	N-CA	-6.72	1.37	1.46
32	M	182	ASP	CA-CB	6.72	1.64	1.53
10	j	85	GLU	C-N	6.71	1.43	1.34
5	E	154	GLN	C-N	6.71	1.42	1.33
22	S	431	VAL	N-CA	-6.71	1.38	1.46
23	P	182	GLU	C-O	-6.71	1.16	1.24
25	R	269	LYS	CA-C	6.71	1.61	1.52
30	K	192	LEU	C-N	6.71	1.41	1.33
4	d	58	ARG	C-N	6.71	1.41	1.33
4	d	213	THR	CA-C	6.71	1.60	1.52
6	F	5	ASN	CA-CB	6.71	1.62	1.53
17	T	161	TRP	CA-C	-6.71	1.44	1.52
25	R	420	ALA	C-O	-6.71	1.16	1.24
1	A	226	GLY	CA-C	-6.71	1.46	1.52
11	4	2	ASP	CA-C	-6.71	1.43	1.52
4	D	83	ARG	NE-CZ	6.70	1.40	1.33
21	N	584	ARG	CZ-NH2	6.70	1.42	1.33
21	N	668	THR	C-N	6.70	1.43	1.33
29	I	399	ALA	CA-C	-6.70	1.44	1.52
4	d	222	VAL	N-CA	-6.70	1.38	1.46
30	K	273	GLU	CA-C	-6.70	1.44	1.52
1	a	120	ARG	CA-CB	6.70	1.64	1.53
33	J	234	PHE	C-N	6.70	1.42	1.33
24	Q	25	GLN	N-CA	-6.70	1.38	1.46
21	N	688	ASN	CA-C	-6.69	1.44	1.52
21	N	832	HIS	N-CA	-6.69	1.37	1.46
6	F	47	VAL	CA-CB	-6.69	1.45	1.54
2	b	120	GLU	C-N	6.69	1.43	1.33
2	b	139	HIS	C-N	6.68	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	89	ASN	CA-CB	6.68	1.64	1.53
33	J	274	GLU	N-CA	-6.68	1.38	1.46
11	k	65	GLN	CA-CB	6.68	1.63	1.53
23	P	348	HIS	CG-CD2	6.68	1.43	1.35
28	H	273	ARG	N-CA	-6.68	1.37	1.46
23	P	135	GLU	N-CA	-6.68	1.37	1.46
8	h	22	ILE	CA-C	-6.67	1.44	1.52
21	N	767	ALA	C-O	-6.67	1.15	1.23
24	Q	145	HIS	ND1-CE1	6.67	1.39	1.32
16	V	267	LYS	C-N	6.67	1.42	1.33
32	M	19	ASP	CA-C	6.67	1.61	1.52
6	F	112	LEU	CA-C	-6.67	1.44	1.52
22	S	115	PRO	C-N	6.67	1.43	1.33
28	H	370	ARG	NE-CZ	6.67	1.40	1.33
12	5	282	PHE	CA-CB	6.67	1.63	1.53
24	Q	336	ASN	CA-C	-6.67	1.44	1.52
11	4	73	TYR	N-CA	-6.67	1.37	1.46
29	I	171	MET	CA-C	6.67	1.61	1.52
23	P	151	GLY	C-N	6.67	1.42	1.33
18	X	111	LEU	CA-CB	6.66	1.61	1.52
21	N	885	ILE	CA-C	-6.66	1.44	1.52
22	S	415	SER	N-CA	-6.66	1.37	1.45
1	A	131	ARG	CA-C	-6.66	1.43	1.53
14	7	257	ASP	CA-C	-6.66	1.44	1.52
16	V	238	LEU	C-N	6.66	1.42	1.33
7	G	195	GLN	N-CA	-6.65	1.38	1.46
27	O	330	ARG	CA-C	-6.65	1.44	1.52
14	7	144	TRP	CA-CB	6.65	1.61	1.53
25	R	340	GLN	N-CA	-6.65	1.38	1.46
32	M	414	ASP	CA-C	-6.65	1.44	1.52
13	m	229	ARG	NE-CZ	6.64	1.40	1.33
2	B	182	GLU	CA-C	-6.64	1.44	1.52
26	U	53	ALA	CA-C	-6.64	1.44	1.52
2	B	187	ASP	CA-CB	6.64	1.63	1.53
10	3	29	LEU	C-N	6.64	1.42	1.33
14	n	223	ARG	CD-NE	6.64	1.55	1.46
31	L	98	LEU	N-CA	6.64	1.54	1.46
12	l	154	ALA	CA-CB	-6.64	1.43	1.53
25	R	245	SER	CA-C	-6.64	1.44	1.52
1	A	80	GLY	C-N	6.64	1.42	1.33
5	E	213	ASP	N-CA	-6.63	1.37	1.45
29	I	190	GLN	N-CA	-6.63	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	31	THR	CA-C	6.63	1.60	1.52
17	T	78	PHE	CA-CB	6.63	1.63	1.53
13	6	211	GLU	CA-C	-6.63	1.44	1.52
16	V	32	ILE	CA-C	-6.63	1.44	1.52
9	2	91	ASN	C-N	6.63	1.41	1.33
32	M	166	ARG	CD-NE	6.63	1.55	1.46
10	j	135	ASP	C-N	6.63	1.41	1.33
31	L	84	LEU	CA-C	6.63	1.61	1.52
18	X	59	ARG	N-CA	-6.62	1.37	1.46
16	V	106	GLY	CA-C	-6.62	1.44	1.52
31	L	281	ASP	C-N	6.62	1.42	1.33
33	J	270	ARG	CA-CB	6.62	1.64	1.53
7	g	58	LEU	CA-C	-6.62	1.43	1.52
3	C	50	ARG	NE-CZ	6.62	1.40	1.33
9	2	183	LEU	C-N	6.62	1.43	1.33
21	N	398	ARG	NE-CZ	6.62	1.40	1.33
10	j	57	ALA	N-CA	-6.62	1.38	1.46
31	L	324	ILE	CA-CB	6.62	1.62	1.54
30	K	105	GLN	C-N	6.62	1.42	1.33
4	D	165	GLY	CA-C	-6.61	1.42	1.51
11	4	162	LYS	CA-CB	6.61	1.63	1.53
20	Z	248	TYR	CA-C	-6.61	1.44	1.52
25	R	20	ARG	C-N	6.61	1.40	1.33
29	I	162	ASP	C-N	6.61	1.43	1.33
5	e	152	GLY	CA-C	-6.61	1.44	1.52
13	6	136	VAL	CA-C	-6.61	1.44	1.52
21	N	313	LEU	N-CA	-6.61	1.38	1.46
27	O	236	HIS	CB-CG	6.61	1.59	1.50
21	N	537	THR	C-N	6.60	1.43	1.34
4	D	205	THR	CA-C	-6.60	1.44	1.52
23	P	104	LEU	CA-C	6.60	1.61	1.52
2	b	28	VAL	CA-CB	6.60	1.62	1.54
21	N	87	ASP	CA-C	-6.60	1.44	1.52
23	P	382	ASP	C-N	6.60	1.43	1.33
31	L	336	ALA	CA-C	-6.60	1.44	1.52
6	f	74	LEU	N-CA	-6.59	1.37	1.45
8	1	152	ARG	CZ-NH1	6.59	1.42	1.32
12	5	234	ARG	NE-CZ	6.59	1.40	1.33
13	6	172	THR	N-CA	-6.59	1.37	1.46
28	H	190	ARG	N-CA	-6.59	1.37	1.46
28	H	300	THR	CA-C	6.59	1.61	1.52
2	b	43	VAL	CA-C	-6.59	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	88	ILE	CA-CB	-6.59	1.46	1.54
21	N	458	ALA	CA-CB	6.59	1.63	1.53
3	C	69	LEU	CA-CB	-6.59	1.42	1.53
7	G	60	VAL	CA-C	-6.59	1.47	1.53
22	S	157	GLU	CA-CB	6.58	1.63	1.53
27	O	290	LYS	CA-CB	6.58	1.63	1.53
23	P	178	GLN	C-N	6.58	1.42	1.33
7	g	169	ARG	CZ-NH2	6.58	1.42	1.33
21	N	476	THR	C-N	6.58	1.43	1.33
21	N	762	ARG	NE-CZ	6.58	1.40	1.33
7	G	161	LYS	N-CA	-6.58	1.37	1.46
8	h	28	ARG	C-N	6.57	1.42	1.33
17	T	256	LYS	CA-CB	6.57	1.63	1.53
9	i	220	LEU	CA-C	-6.57	1.44	1.52
27	O	161	ASP	N-CA	-6.57	1.37	1.46
13	m	229	ARG	C-N	6.56	1.42	1.33
14	7	185	ASN	CA-C	6.56	1.61	1.52
1	a	32	PHE	N-CA	-6.56	1.37	1.46
14	n	129	LEU	N-CA	-6.56	1.38	1.46
21	N	636	SER	CA-CB	6.56	1.63	1.53
32	M	340	SER	CA-C	-6.56	1.44	1.52
29	I	117	HIS	CA-C	-6.56	1.44	1.52
9	i	43	ILE	N-CA	-6.56	1.38	1.46
16	V	25	GLU	CA-C	-6.56	1.44	1.52
22	S	55	ARG	C-N	6.56	1.42	1.33
1	a	76	SER	CA-C	-6.55	1.45	1.53
6	f	136	GLY	N-CA	-6.55	1.38	1.45
13	6	209	GLY	C-N	6.55	1.42	1.33
29	I	422	ARG	CZ-NH2	6.55	1.42	1.33
31	L	303	ARG	CD-NE	6.55	1.55	1.46
3	c	9	ARG	CA-C	-6.55	1.44	1.53
3	c	92	ARG	CD-NE	6.55	1.55	1.46
5	E	72	ARG	CD-NE	6.55	1.55	1.46
1	a	152	PRO	CA-CB	6.54	1.62	1.53
10	j	46	TYR	N-CA	-6.54	1.38	1.46
25	R	130	GLN	C-N	6.54	1.42	1.33
5	E	47	VAL	CA-C	-6.54	1.44	1.52
32	M	57	VAL	CA-C	-6.54	1.44	1.52
32	M	386	PHE	C-N	6.54	1.42	1.33
9	2	89	GLY	CA-C	-6.54	1.44	1.51
25	R	300	ASP	CA-C	-6.54	1.44	1.52
28	H	419	LEU	CA-CB	6.54	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	118	GLN	CA-CB	6.53	1.62	1.53
21	N	610	SER	C-N	6.53	1.42	1.33
26	U	295	LYS	N-CA	-6.53	1.38	1.46
33	J	339	ARG	CD-NE	6.53	1.55	1.46
14	7	136	ARG	NE-CZ	6.53	1.40	1.33
23	P	319	GLU	C-O	-6.53	1.18	1.24
33	J	374	ARG	CA-C	-6.53	1.44	1.52
6	F	16	THR	N-CA	-6.52	1.37	1.46
25	R	277	LEU	C-N	6.52	1.43	1.33
24	Q	248	ASN	CA-CB	6.52	1.65	1.53
28	H	249	TYR	N-CA	6.52	1.54	1.46
1	A	49	ASP	CA-CB	6.52	1.64	1.53
10	3	125	ASP	N-CA	-6.52	1.42	1.46
2	B	204	PHE	N-CA	-6.52	1.37	1.46
4	D	226	SER	CA-C	-6.52	1.44	1.52
25	R	273	SER	C-O	-6.52	1.18	1.24
27	O	177	GLN	CA-CB	6.52	1.63	1.53
11	k	168	LEU	N-CA	-6.52	1.38	1.46
3	C	214	ALA	CA-C	-6.51	1.44	1.52
13	6	181	LYS	CA-C	-6.51	1.44	1.52
18	X	8	ILE	CA-C	-6.51	1.44	1.52
25	R	333	MET	CA-C	-6.51	1.44	1.52
12	5	242	ARG	CZ-NH2	6.51	1.42	1.33
23	P	47	ARG	CD-NE	6.51	1.55	1.46
6	f	129	GLY	CA-C	-6.51	1.44	1.51
21	N	329	HIS	N-CA	-6.51	1.38	1.46
10	j	28	ARG	NE-CZ	6.51	1.40	1.33
14	n	226	ARG	C-N	6.51	1.42	1.33
9	2	203	ASP	CA-C	-6.51	1.44	1.52
30	K	239	GLY	C-N	6.51	1.43	1.33
6	f	178	THR	N-CA	-6.51	1.38	1.46
12	l	202	PHE	CA-C	-6.51	1.44	1.52
5	E	55	THR	CA-C	6.51	1.61	1.52
21	N	570	ARG	CA-C	-6.51	1.44	1.52
6	f	91	GLN	CA-CB	6.50	1.64	1.53
14	n	53	VAL	C-N	6.50	1.41	1.33
1	A	140	ILE	CA-CB	-6.50	1.46	1.54
22	S	94	LYS	CA-C	-6.50	1.44	1.52
22	S	473	ASP	C-N	6.50	1.42	1.33
2	b	218	ASN	CA-C	-6.50	1.45	1.52
25	R	110	ILE	CA-C	-6.50	1.45	1.52
27	O	46	THR	CA-CB	6.50	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	31	THR	N-CA	-6.50	1.38	1.46
6	F	35	THR	CA-C	-6.50	1.44	1.52
17	T	170	ASN	CA-CB	6.50	1.61	1.52
1	A	179	THR	CA-C	6.50	1.61	1.52
17	T	59	LYS	CA-C	-6.50	1.44	1.52
29	I	291	ARG	CZ-NH2	6.50	1.41	1.33
12	l	134	LEU	CA-CB	6.50	1.63	1.53
3	c	91	ALA	N-CA	-6.49	1.38	1.46
8	1	129	HIS	CA-CB	6.49	1.62	1.52
28	H	101	ARG	CZ-NH1	6.49	1.41	1.32
32	M	386	PHE	CA-C	-6.49	1.45	1.52
14	n	198	ILE	C-N	6.49	1.41	1.34
4	D	172	ARG	CZ-NH1	6.49	1.41	1.32
9	2	194	ASN	CA-C	-6.49	1.43	1.52
7	g	169	ARG	CD-NE	6.49	1.55	1.46
11	4	34	LYS	N-CA	-6.49	1.39	1.46
6	F	83	VAL	CA-C	-6.48	1.44	1.52
22	S	471	LEU	C-N	6.48	1.42	1.33
24	Q	149	LYS	CA-C	-6.48	1.44	1.52
21	N	368	THR	C-N	6.48	1.43	1.33
18	X	48	PHE	N-CA	-6.48	1.38	1.46
25	R	293	THR	CA-C	-6.48	1.44	1.52
5	e	114	GLN	C-N	6.48	1.42	1.33
9	2	181	ILE	C-N	6.48	1.42	1.33
16	V	67	ASP	CA-C	-6.48	1.44	1.52
21	N	155	GLY	C-N	6.48	1.41	1.33
8	h	123	PRO	N-CD	6.47	1.56	1.47
6	F	136	GLY	CA-C	-6.47	1.44	1.51
4	d	71	VAL	C-O	-6.47	1.17	1.24
9	i	186	ASP	CA-C	-6.47	1.44	1.52
20	Z	918	ASP	CA-C	-6.47	1.47	1.52
23	P	168	TYR	CA-C	-6.47	1.44	1.52
33	J	3	ALA	CA-C	-6.47	1.45	1.52
33	J	270	ARG	NE-CZ	6.47	1.40	1.33
13	6	10	PHE	CA-C	-6.47	1.44	1.52
28	H	302	LYS	N-CA	-6.47	1.38	1.46
6	F	15	PRO	CA-CB	6.47	1.62	1.53
21	N	208	ARG	CA-C	-6.46	1.44	1.52
27	O	141	ASN	C-N	6.46	1.43	1.33
18	X	124	LYS	N-CA	-6.46	1.38	1.46
28	H	188	PRO	CA-CB	-6.46	1.48	1.53
30	K	198	TYR	CA-C	6.46	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	93	ASN	N-CA	6.46	1.54	1.46
32	M	117	ALA	CA-C	-6.46	1.44	1.52
14	7	211	VAL	CA-CB	-6.46	1.46	1.54
33	J	87	LYS	CA-CB	6.46	1.60	1.52
32	M	203	ARG	NE-CZ	6.46	1.40	1.33
15	W	101	ARG	CD-NE	6.45	1.55	1.46
13	m	199	ALA	CA-C	-6.45	1.44	1.52
1	A	120	ARG	NE-CZ	6.45	1.40	1.33
10	j	18	LYS	CA-CB	6.45	1.61	1.53
2	B	157	PHE	CA-C	-6.45	1.46	1.52
27	O	373	TRP	N-CA	-6.45	1.37	1.46
12	l	89	VAL	N-CA	-6.45	1.38	1.46
4	D	17	ILE	CA-CB	-6.45	1.46	1.53
19	Y	18	LYS	C-N	6.45	1.43	1.33
21	N	102	VAL	CA-CB	-6.45	1.46	1.54
4	d	223	ALA	N-CA	-6.45	1.38	1.46
21	N	510	HIS	N-CA	-6.45	1.38	1.46
29	I	105	SER	CA-C	-6.45	1.45	1.52
32	M	291	PHE	N-CA	-6.45	1.41	1.47
3	c	31	HIS	CD2-NE2	6.45	1.45	1.37
10	j	137	ILE	C-N	6.45	1.42	1.33
5	E	53	ARG	CA-C	-6.45	1.44	1.52
2	b	57	MET	CA-C	-6.44	1.44	1.52
13	m	193	ARG	C-N	6.44	1.42	1.34
31	L	62	ARG	CD-NE	6.44	1.55	1.46
2	B	240	SER	CA-C	-6.44	1.44	1.52
25	R	107	GLU	C-N	6.44	1.41	1.33
11	4	70	ARG	CA-C	-6.44	1.44	1.52
5	E	157	HIS	CA-C	-6.43	1.45	1.52
6	F	81	ALA	CA-C	-6.43	1.44	1.52
23	P	213	TYR	CA-CB	6.43	1.63	1.53
26	U	4	GLN	CA-C	-6.43	1.44	1.52
28	H	297	MET	N-CA	-6.43	1.38	1.46
30	K	363	ALA	N-CA	-6.43	1.41	1.46
31	L	307	GLU	C-N	6.43	1.42	1.33
30	K	122	ILE	CA-C	6.43	1.61	1.52
24	Q	410	ASP	CA-CB	6.43	1.63	1.53
9	i	160	SER	CA-C	-6.42	1.44	1.52
14	7	98	ARG	NE-CZ	6.42	1.40	1.33
12	l	110	ILE	CA-C	-6.42	1.44	1.52
3	C	7	ASP	C-N	6.42	1.38	1.33
32	M	369	THR	C-N	6.42	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	212	ILE	CA-C	6.42	1.60	1.52
21	N	594	VAL	CA-CB	-6.42	1.46	1.54
31	L	424	GLU	N-CA	-6.42	1.38	1.46
13	m	194	ASP	N-CA	-6.42	1.38	1.46
2	b	189	ILE	CA-C	6.42	1.61	1.52
8	h	28	ARG	N-CA	-6.42	1.37	1.46
23	P	381	SER	CA-C	-6.42	1.44	1.52
28	H	350	LYS	C-N	6.42	1.41	1.33
1	A	69	VAL	CA-C	-6.42	1.45	1.52
25	R	83	GLU	CA-CB	6.42	1.66	1.54
28	H	183	ILE	CA-C	-6.42	1.45	1.52
30	K	267	SER	N-CA	-6.42	1.38	1.45
30	K	254	VAL	N-CA	-6.42	1.39	1.46
14	n	98	ARG	CZ-NH2	6.41	1.41	1.33
13	6	187	GLU	CA-C	-6.41	1.44	1.52
16	V	144	ILE	CA-CB	-6.41	1.46	1.54
24	Q	191	LEU	CA-C	-6.41	1.44	1.52
5	E	225	GLN	C-N	6.41	1.43	1.33
9	i	248	ASN	N-CA	6.41	1.54	1.45
31	L	129	VAL	C-N	6.41	1.41	1.33
31	L	313	ASP	CA-C	-6.41	1.44	1.52
33	J	120	TYR	CA-CB	6.41	1.63	1.53
5	e	166	ARG	NE-CZ	6.41	1.40	1.33
29	I	328	THR	N-CA	-6.41	1.38	1.46
30	K	208	GLY	N-CA	-6.41	1.36	1.45
32	M	232	ALA	CA-C	-6.41	1.44	1.52
11	4	190	ARG	NE-CZ	6.41	1.40	1.33
24	Q	359	ILE	C-N	6.40	1.42	1.33
8	h	194	ARG	CA-C	-6.40	1.44	1.52
10	j	183	TRP	CA-CB	6.40	1.63	1.53
16	V	117	TRP	CA-C	-6.40	1.44	1.52
22	S	290	ASN	CA-CB	6.40	1.63	1.53
27	O	30	GLU	CA-CB	6.40	1.63	1.53
2	b	90	ARG	CA-CB	6.40	1.63	1.53
9	2	158	SER	CA-CB	6.40	1.63	1.53
21	N	905	LEU	CA-C	-6.40	1.44	1.52
6	f	104	ALA	N-CA	-6.40	1.37	1.45
14	n	114	ALA	CA-C	6.40	1.61	1.52
10	j	80	ARG	CD-NE	6.39	1.55	1.46
32	M	366	ARG	CA-C	-6.39	1.46	1.53
25	R	27	SER	CA-C	-6.39	1.44	1.52
25	R	388	VAL	C-O	-6.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	209	ASP	CA-C	6.39	1.60	1.52
33	J	344	ARG	CD-NE	6.39	1.55	1.46
32	M	278	ILE	CA-C	-6.39	1.44	1.52
33	J	72	VAL	C-O	-6.39	1.17	1.24
3	c	104	GLU	CA-C	-6.38	1.44	1.52
10	3	80	ARG	CZ-NH2	6.38	1.41	1.33
28	H	169	GLU	CA-C	6.38	1.60	1.52
33	J	399	SER	C-N	6.38	1.42	1.33
5	E	214	GLU	CA-CB	6.38	1.64	1.53
7	G	111	ALA	CA-C	-6.38	1.44	1.52
22	S	391	GLY	C-N	6.38	1.42	1.33
31	L	290	ARG	CZ-NH1	6.38	1.41	1.32
14	7	220	ARG	NE-CZ	6.38	1.40	1.33
33	J	275	LEU	CA-CB	6.38	1.63	1.53
16	V	135	ARG	NE-CZ	6.38	1.40	1.33
31	L	139	LYS	N-CA	-6.38	1.38	1.46
8	h	161	VAL	CA-C	-6.38	1.45	1.52
21	N	740	TRP	NE1-CE2	6.38	1.44	1.37
11	k	68	SER	N-CA	-6.37	1.38	1.46
13	m	20	ILE	C-N	6.37	1.41	1.33
10	3	84	PRO	N-CA	-6.37	1.39	1.47
27	O	228	TYR	CA-CB	6.37	1.61	1.53
21	N	509	GLN	N-CA	-6.37	1.37	1.45
23	P	232	ARG	NE-CZ	6.37	1.40	1.33
10	3	32	GLN	CA-C	-6.37	1.44	1.52
6	F	133	LEU	C-N	6.37	1.41	1.33
9	2	172	LYS	CA-C	-6.37	1.44	1.52
8	1	85	GLU	N-CA	-6.36	1.38	1.46
25	R	422	ARG	CA-C	-6.36	1.44	1.52
10	j	14	ALA	CA-C	-6.36	1.44	1.52
7	G	223	GLU	CA-C	-6.36	1.44	1.52
28	H	287	GLY	C-N	6.36	1.42	1.33
28	H	382	LEU	C-N	6.36	1.43	1.33
21	N	150	LEU	N-CA	-6.36	1.37	1.46
23	P	3	ARG	CA-C	6.36	1.60	1.52
27	O	45	LEU	CA-C	-6.36	1.44	1.52
2	b	186	GLU	CA-C	-6.36	1.44	1.52
18	X	123	ASN	C-N	6.36	1.42	1.33
25	R	338	TYR	N-CA	-6.36	1.38	1.46
18	X	69	ILE	CA-C	-6.35	1.47	1.53
33	J	219	VAL	C-N	6.35	1.41	1.33
3	C	208	TYR	CA-CB	6.35	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	93	SER	CA-C	-6.35	1.44	1.53
16	V	288	LEU	C-N	6.35	1.42	1.34
22	S	211	ARG	CD-NE	6.35	1.55	1.46
10	3	43	ILE	N-CA	-6.35	1.38	1.46
21	N	908	ARG	CD-NE	6.34	1.55	1.46
10	3	178	ASP	N-CA	6.34	1.53	1.46
21	N	147	ALA	CA-C	-6.34	1.43	1.52
10	j	126	LEU	CB-CG	6.34	1.66	1.53
1	A	75	ILE	CA-C	-6.34	1.46	1.52
10	3	28	ARG	CA-C	-6.34	1.44	1.52
30	K	399	ARG	N-CA	-6.34	1.37	1.45
2	B	128	ARG	CA-C	-6.34	1.45	1.53
16	V	285	ASP	CA-CB	6.34	1.63	1.53
30	K	294	ARG	C-N	6.34	1.41	1.33
30	K	405	SER	C-N	6.34	1.42	1.33
22	S	428	ARG	NE-CZ	6.34	1.40	1.33
25	R	124	ASP	CA-CB	6.34	1.63	1.53
31	L	126	ARG	CZ-NH1	6.34	1.41	1.32
5	e	201	LEU	C-N	6.33	1.42	1.33
5	e	47	VAL	CA-C	-6.33	1.44	1.52
8	h	202	TYR	C-O	-6.33	1.16	1.24
7	G	90	ASN	CA-C	-6.33	1.44	1.52
29	I	271	ALA	C-N	6.33	1.41	1.34
30	K	209	VAL	N-CA	-6.33	1.38	1.46
5	E	143	LEU	C-O	-6.33	1.16	1.24
26	U	47	ARG	CA-CB	6.33	1.62	1.53
2	b	97	TYR	CA-CB	6.32	1.61	1.53
12	l	126	ASP	N-CA	-6.32	1.38	1.46
1	A	131	ARG	CD-NE	6.32	1.55	1.46
21	N	786	ARG	CD-NE	6.32	1.55	1.46
30	K	62	THR	C-N	6.32	1.42	1.33
5	e	145	ALA	CA-C	-6.32	1.45	1.52
5	E	209	GLU	CA-C	-6.32	1.44	1.52
33	J	81	ASP	C-N	6.32	1.42	1.33
7	G	155	GLY	CA-C	-6.32	1.43	1.51
13	m	46	ARG	NE-CZ	6.32	1.40	1.33
13	m	105	LEU	CA-C	-6.32	1.44	1.52
15	W	123	ASP	CA-C	-6.32	1.44	1.52
21	N	631	GLY	C-N	6.32	1.42	1.33
22	S	479	MET	N-CA	-6.32	1.38	1.46
2	B	190	HIS	ND1-CE1	6.31	1.38	1.32
2	B	200	VAL	CA-CB	-6.31	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	25	CYS	C-N	6.31	1.42	1.33
2	b	236	ARG	CD-NE	6.31	1.55	1.46
13	m	57	ASN	CA-C	-6.31	1.44	1.53
6	F	39	ARG	CZ-NH2	6.31	1.41	1.33
18	X	113	GLU	CA-C	6.31	1.61	1.52
21	N	335	ALA	C-O	6.31	1.31	1.24
4	D	170	THR	N-CA	-6.31	1.38	1.46
21	N	327	LEU	CA-C	-6.31	1.44	1.52
3	c	85	GLU	C-O	-6.31	1.16	1.24
10	j	129	CYS	CA-C	-6.31	1.44	1.52
5	E	145	ALA	C-N	6.31	1.40	1.33
21	N	121	GLU	N-CA	-6.31	1.38	1.46
32	M	243	PHE	CA-CB	6.31	1.61	1.53
4	d	30	GLY	C-N	6.31	1.41	1.33
31	L	142	LYS	CA-C	-6.31	1.44	1.52
24	Q	368	LEU	CA-CB	6.31	1.62	1.53
25	R	183	ASP	N-CA	-6.30	1.39	1.46
2	b	234	ARG	NE-CZ	6.30	1.40	1.33
8	h	29	THR	CA-C	-6.30	1.45	1.52
28	H	254	THR	CA-C	-6.30	1.44	1.52
11	k	119	ILE	CA-CB	-6.30	1.46	1.54
10	3	199	TYR	CA-CB	6.30	1.63	1.53
16	V	123	VAL	CA-CB	-6.30	1.46	1.54
8	h	179	GLY	CA-C	-6.30	1.43	1.51
31	L	58	ASN	CA-CB	6.30	1.63	1.53
2	B	94	HIS	ND1-CE1	6.29	1.38	1.32
22	S	446	THR	C-N	6.29	1.42	1.33
13	6	175	LYS	N-CA	-6.29	1.38	1.46
18	X	113	GLU	CA-CB	6.29	1.64	1.53
2	b	246	ARG	NE-CZ	6.29	1.40	1.33
5	e	201	LEU	CA-C	-6.29	1.44	1.52
22	S	285	ASP	CA-C	-6.29	1.45	1.52
29	I	141	LEU	CA-CB	6.29	1.62	1.53
8	1	51	TRP	C-N	6.29	1.42	1.33
30	K	396	ARG	NE-CZ	6.29	1.40	1.33
22	S	232	MET	C-N	6.29	1.42	1.33
8	1	161	VAL	N-CA	6.28	1.53	1.46
10	3	50	PHE	C-N	6.28	1.42	1.33
21	N	45	ASP	N-CA	-6.28	1.38	1.46
22	S	382	ARG	CD-NE	6.28	1.55	1.46
31	L	418	ALA	C-N	6.28	1.41	1.33
2	b	217	GLU	CA-C	6.28	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	333	ARG	N-CA	-6.28	1.38	1.46
9	i	238	THR	CA-C	-6.28	1.44	1.52
11	k	34	LYS	CA-C	-6.28	1.47	1.52
6	F	163	ALA	CA-C	-6.28	1.44	1.52
8	h	38	ARG	NE-CZ	6.28	1.40	1.33
2	B	246	ARG	CZ-NH1	6.28	1.41	1.32
33	J	74	GLU	C-N	6.28	1.40	1.33
4	d	175	LEU	C-N	6.27	1.41	1.33
27	O	49	PHE	N-CA	-6.27	1.37	1.46
13	m	64	GLY	N-CA	-6.27	1.36	1.45
9	2	108	ALA	N-CA	-6.27	1.38	1.46
13	6	203	HIS	CB-CG	6.27	1.58	1.50
19	Y	26	LYS	N-CA	-6.27	1.38	1.46
17	T	186	ARG	NE-CZ	6.27	1.40	1.33
9	2	48	ARG	CZ-NH1	6.27	1.41	1.32
22	S	326	ASP	C-N	6.27	1.40	1.33
28	H	190	ARG	CD-NE	6.27	1.55	1.46
33	J	144	ASP	CA-CB	6.27	1.62	1.53
9	i	163	ALA	CA-C	-6.27	1.44	1.52
28	H	168	ILE	C-N	6.27	1.41	1.33
28	H	337	ILE	C-N	6.27	1.43	1.33
21	N	712	ASN	N-CA	6.27	1.54	1.45
14	n	132	VAL	CA-C	-6.26	1.44	1.52
5	E	66	LYS	CA-C	-6.26	1.44	1.53
9	2	130	ALA	C-O	-6.26	1.16	1.23
12	5	79	LEU	N-CA	-6.26	1.38	1.46
30	K	218	GLY	C-N	6.26	1.41	1.33
16	V	299	GLY	CA-C	-6.26	1.44	1.51
13	m	75	ARG	C-N	6.26	1.42	1.33
11	4	171	ARG	CZ-NH1	6.26	1.41	1.32
30	K	65	GLU	CA-C	-6.26	1.44	1.52
18	X	78	ILE	N-CA	-6.26	1.38	1.46
11	k	106	GLY	CA-C	-6.26	1.46	1.52
17	T	238	GLN	N-CA	-6.26	1.38	1.46
27	O	15	ARG	CA-C	-6.26	1.44	1.52
31	L	53	HIS	C-O	-6.26	1.16	1.24
33	J	39	GLU	C-N	6.26	1.42	1.33
4	d	148	TYR	N-CA	6.25	1.53	1.45
2	B	234	ARG	N-CA	-6.25	1.38	1.46
18	X	59	ARG	CZ-NH1	6.25	1.41	1.32
1	A	223	LEU	CA-C	-6.25	1.44	1.52
21	N	517	LEU	CA-C	-6.25	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	206	PRO	CA-CB	6.25	1.62	1.53
30	K	371	LEU	C-N	6.25	1.40	1.33
32	M	325	ALA	N-CA	-6.25	1.38	1.46
3	c	96	GLN	N-CA	6.25	1.54	1.46
14	n	41	GLY	C-N	6.25	1.41	1.33
30	K	121	ARG	CA-CB	6.25	1.63	1.53
32	M	201	MET	CA-C	-6.25	1.44	1.52
26	U	207	VAL	C-N	6.25	1.41	1.33
28	H	420	ARG	NE-CZ	6.25	1.40	1.33
2	b	83	ARG	CD-NE	6.25	1.54	1.46
31	L	93	ASN	C-N	6.25	1.42	1.33
7	g	170	GLN	N-CA	-6.24	1.38	1.46
26	U	129	GLY	CA-C	-6.24	1.43	1.52
9	i	86	GLN	CA-CB	6.24	1.63	1.53
7	G	91	ARG	CZ-NH2	6.24	1.41	1.33
24	Q	71	LYS	N-CA	-6.24	1.37	1.45
11	k	149	ARG	C-N	6.24	1.41	1.34
27	O	285	SER	C-N	6.24	1.42	1.33
28	H	380	PRO	C-N	6.24	1.42	1.33
30	K	207	ARG	NE-CZ	6.24	1.40	1.33
32	M	52	SER	CA-C	-6.24	1.45	1.52
7	G	192	ALA	N-CA	-6.23	1.38	1.46
26	U	24	ARG	CD-NE	6.23	1.54	1.46
23	P	123	ARG	NE-CZ	6.23	1.40	1.33
11	4	17	SER	C-O	-6.23	1.16	1.23
11	4	97	PRO	CA-C	-6.23	1.45	1.52
16	V	60	ASP	C-N	6.23	1.42	1.33
23	P	334	ASN	CA-CB	6.23	1.64	1.53
26	U	119	LEU	CA-C	-6.23	1.44	1.52
31	L	262	ILE	N-CA	6.23	1.53	1.46
32	M	364	HIS	ND1-CE1	6.23	1.38	1.32
3	c	217	ARG	CZ-NH2	6.23	1.41	1.33
10	j	163	LEU	C-N	6.23	1.42	1.33
8	h	118	GLU	CA-CB	6.22	1.64	1.53
2	B	91	LYS	N-CA	-6.22	1.38	1.46
9	2	205	CYS	C-O	-6.22	1.16	1.23
11	4	36	ARG	NE-CZ	6.22	1.39	1.33
12	5	148	ARG	CZ-NH1	6.22	1.41	1.32
30	K	399	ARG	NE-CZ	6.22	1.39	1.33
4	d	127	ARG	CD-NE	6.22	1.54	1.46
5	e	20	ARG	CA-C	-6.22	1.44	1.52
12	l	242	ARG	CD-NE	6.22	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	10	ARG	CZ-NH1	6.22	1.41	1.32
6	F	144	LEU	CA-C	6.22	1.59	1.52
21	N	329	HIS	CA-C	-6.22	1.44	1.52
15	W	141	ILE	C-N	6.22	1.40	1.33
23	P	29	GLN	C-N	6.22	1.42	1.33
28	H	136	ALA	C-N	6.22	1.41	1.33
29	I	241	SER	C-N	6.22	1.41	1.33
33	J	34	ILE	C-N	6.22	1.42	1.33
22	S	311	GLN	C-N	6.21	1.42	1.33
32	M	384	ASP	CA-C	-6.21	1.45	1.52
33	J	167	PRO	C-N	6.21	1.41	1.33
5	e	219	LEU	CA-C	-6.21	1.45	1.52
6	f	43	HIS	C-N	6.21	1.42	1.33
12	l	260	TRP	CZ2-CH2	6.21	1.49	1.37
6	F	107	ARG	NE-CZ	6.21	1.39	1.33
22	S	399	TYR	CA-C	-6.21	1.45	1.52
29	I	424	MET	C-N	6.21	1.42	1.33
33	J	290	ILE	C-N	6.21	1.41	1.33
8	1	87	ALA	CA-C	-6.21	1.44	1.52
10	3	77	LYS	CA-C	6.21	1.60	1.52
25	R	226	GLU	N-CA	-6.21	1.38	1.46
28	H	442	ASP	C-N	6.21	1.42	1.33
7	g	16	SER	C-N	6.20	1.40	1.34
8	h	44	THR	N-CA	-6.20	1.38	1.46
21	N	36	TRP	NE1-CE2	6.20	1.44	1.37
1	A	167	LYS	CA-C	-6.20	1.45	1.53
14	7	251	LYS	CA-C	-6.20	1.45	1.52
13	m	86	ASP	C-N	6.19	1.41	1.33
5	E	240	ILE	CB-CG1	6.19	1.65	1.53
26	U	259	ASN	N-CA	-6.19	1.39	1.46
2	B	159	TRP	NE1-CE2	6.19	1.44	1.37
28	H	62	ARG	CD-NE	6.19	1.54	1.46
1	A	211	ILE	CA-C	-6.19	1.45	1.52
2	B	98	LYS	CA-C	-6.19	1.45	1.52
9	i	239	THR	CA-C	6.19	1.60	1.52
29	I	265	ARG	NE-CZ	6.19	1.39	1.33
33	J	306	ARG	C-N	6.19	1.41	1.33
3	c	9	ARG	CD-NE	6.19	1.54	1.46
10	j	69	TYR	C-N	6.18	1.42	1.33
1	a	158	ASP	CA-C	-6.18	1.44	1.52
21	N	488	CYS	CA-CB	6.18	1.62	1.53
22	S	445	THR	C-N	6.18	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	211	VAL	N-CA	-6.18	1.38	1.46
28	H	237	THR	CA-C	6.18	1.60	1.52
4	d	181	ARG	CZ-NH2	6.18	1.41	1.33
27	O	356	ARG	NE-CZ	6.18	1.39	1.33
25	R	386	GLY	CA-C	-6.18	1.42	1.51
30	K	139	LEU	CA-C	-6.18	1.45	1.52
3	C	240	VAL	N-CA	-6.18	1.39	1.46
26	U	277	TYR	N-CA	-6.18	1.38	1.46
33	J	182	PRO	C-O	-6.18	1.17	1.23
8	h	45	ARG	CZ-NH1	6.17	1.41	1.32
23	P	336	HIS	CA-C	-6.17	1.44	1.52
29	I	319	ARG	CZ-NH1	6.17	1.41	1.32
2	b	137	ALA	C-N	6.17	1.39	1.33
21	N	567	ALA	CA-C	-6.17	1.44	1.52
29	I	256	TYR	C-N	6.17	1.42	1.33
5	e	153	TYR	N-CA	-6.16	1.38	1.46
9	2	137	SER	CA-C	-6.16	1.44	1.52
14	7	207	GLU	CA-C	6.16	1.60	1.52
27	O	315	LYS	N-CA	-6.16	1.39	1.46
32	M	233	ARG	NE-CZ	6.16	1.39	1.33
33	J	372	GLU	N-CA	-6.16	1.39	1.46
9	i	77	THR	CA-C	-6.16	1.45	1.52
12	l	260	TRP	N-CA	-6.16	1.38	1.46
14	7	162	TYR	N-CA	-6.16	1.38	1.45
16	V	285	ASP	CA-C	-6.16	1.44	1.52
32	M	404	ARG	CA-C	-6.16	1.44	1.52
33	J	283	GLU	CA-CB	6.16	1.63	1.53
22	S	281	ALA	CA-C	6.16	1.60	1.52
25	R	216	ILE	C-N	6.16	1.42	1.33
21	N	188	TYR	N-CA	-6.15	1.38	1.46
24	Q	168	LEU	CA-C	-6.15	1.44	1.53
6	f	29	ILE	N-CA	-6.15	1.39	1.46
16	V	107	TRP	NE1-CE2	6.15	1.44	1.37
22	S	99	ASN	N-CA	-6.15	1.38	1.46
16	V	218	LYS	N-CA	-6.15	1.39	1.46
23	P	181	LEU	CA-CB	6.15	1.63	1.53
28	H	353	PHE	CA-C	-6.15	1.45	1.52
29	I	103	PRO	N-CA	-6.15	1.36	1.47
13	m	90	LYS	N-CA	6.15	1.53	1.45
2	B	45	ILE	C-O	-6.15	1.17	1.24
4	D	53	LYS	CA-C	-6.15	1.43	1.52
4	D	127	ARG	CZ-NH1	6.15	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	125	VAL	N-CA	-6.14	1.38	1.46
24	Q	424	ASP	CA-C	6.14	1.60	1.52
2	B	86	VAL	CA-CB	-6.14	1.46	1.54
5	E	248	ALA	CA-C	-6.14	1.44	1.52
27	O	23	HIS	C-N	6.14	1.41	1.34
16	V	28	TYR	CA-C	-6.14	1.45	1.52
23	P	400	VAL	N-CA	-6.14	1.39	1.46
6	F	100	ASN	CA-C	-6.14	1.45	1.53
5	e	188	HIS	CA-C	-6.14	1.45	1.52
7	g	179	LEU	C-N	6.14	1.41	1.33
22	S	36	LYS	C-N	6.14	1.41	1.33
23	P	80	THR	N-CA	-6.14	1.39	1.46
28	H	426	ALA	CA-CB	6.14	1.63	1.53
33	J	401	ALA	N-CA	-6.14	1.38	1.46
20	Z	727	GLU	C-N	6.13	1.42	1.33
23	P	248	ASP	C-N	6.13	1.41	1.33
32	M	122	SER	C-N	6.13	1.41	1.33
25	R	140	TYR	N-CA	-6.13	1.38	1.46
28	H	113	ASP	N-CA	-6.13	1.38	1.46
10	3	75	LYS	C-O	-6.13	1.17	1.24
4	D	203	VAL	C-N	6.13	1.42	1.33
17	T	186	ARG	CD-NE	6.13	1.54	1.46
23	P	242	GLN	C-N	6.13	1.41	1.33
33	J	195	LYS	CA-CB	6.13	1.62	1.53
6	f	181	LYS	C-N	6.13	1.40	1.33
12	l	241	HIS	CD2-NE2	6.13	1.44	1.37
21	N	650	ASP	CA-C	-6.13	1.44	1.52
9	i	81	THR	N-CA	-6.12	1.39	1.46
1	A	187	LYS	CA-CB	6.12	1.63	1.53
6	F	89	ARG	NE-CZ	6.12	1.39	1.33
21	N	524	ILE	CA-CB	-6.12	1.46	1.54
21	N	626	GLY	C-N	6.12	1.41	1.33
29	I	304	ARG	CD-NE	6.12	1.54	1.46
33	J	314	ILE	N-CA	-6.12	1.38	1.46
5	e	213	ASP	N-CA	-6.12	1.37	1.46
7	g	224	THR	N-CA	6.12	1.53	1.46
7	G	98	SER	CA-C	-6.12	1.45	1.52
31	L	139	LYS	CA-C	6.12	1.60	1.52
33	J	223	ILE	C-N	6.12	1.42	1.33
3	c	61	THR	N-CA	-6.12	1.39	1.46
9	i	44	ALA	CA-C	-6.12	1.45	1.52
13	m	38	ILE	CA-C	-6.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	140	VAL	C-N	6.12	1.41	1.33
9	i	143	HIS	CG-CD2	6.12	1.42	1.35
21	N	265	ALA	CA-CB	-6.12	1.43	1.53
23	P	186	LEU	C-O	-6.12	1.16	1.24
30	K	414	GLN	CA-CB	6.12	1.62	1.53
8	h	67	ILE	CA-CB	6.12	1.61	1.54
28	H	352	MET	CA-C	-6.12	1.45	1.52
27	O	372	GLU	C-N	6.12	1.42	1.33
4	d	222	VAL	C-O	-6.11	1.18	1.24
10	j	39	LYS	C-N	6.11	1.42	1.33
22	S	276	LEU	C-N	6.11	1.42	1.33
24	Q	100	LEU	CA-C	-6.11	1.45	1.52
22	S	215	MET	N-CA	-6.11	1.38	1.46
6	f	196	ALA	CA-CB	6.11	1.62	1.53
11	k	72	ASP	C-N	-6.11	1.25	1.33
9	2	243	LYS	CA-C	-6.11	1.45	1.52
17	T	21	ALA	CA-C	-6.11	1.44	1.52
23	P	254	GLU	CA-C	-6.11	1.44	1.52
27	O	356	ARG	CD-NE	6.11	1.54	1.46
32	M	95	GLU	CA-C	-6.11	1.45	1.52
33	J	123	HIS	ND1-CE1	6.11	1.38	1.32
32	M	321	VAL	C-N	6.10	1.42	1.33
3	c	111	LEU	C-N	6.10	1.41	1.33
11	k	16	ALA	CA-C	-6.10	1.45	1.52
13	m	227	LEU	CA-C	-6.10	1.45	1.52
14	n	220	ARG	NE-CZ	6.10	1.39	1.33
21	N	242	PHE	CA-C	-6.10	1.44	1.52
24	Q	308	ASN	CA-CB	6.10	1.62	1.53
32	M	267	PHE	CA-C	-6.10	1.44	1.52
6	F	51	ARG	CD-NE	6.10	1.54	1.46
1	a	190	LYS	CA-C	-6.10	1.44	1.53
1	A	58	LYS	CA-C	-6.10	1.45	1.52
29	I	242	ALA	CA-CB	6.10	1.63	1.53
6	F	160	ALA	N-CA	-6.10	1.38	1.45
8	1	165	LYS	CA-C	-6.10	1.44	1.52
26	U	267	VAL	CA-C	-6.10	1.45	1.52
1	A	74	CYS	CA-C	-6.10	1.45	1.52
23	P	3	ARG	N-CA	-6.09	1.38	1.46
31	L	101	ILE	CA-CB	-6.09	1.48	1.54
12	5	195	THR	C-N	6.09	1.41	1.33
29	I	291	ARG	CZ-NH1	6.09	1.41	1.32
30	K	330	ARG	NE-CZ	6.09	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	165	TYR	CA-C	-6.09	1.45	1.52
11	k	11	ASP	N-CA	-6.09	1.39	1.46
11	k	32	ASP	N-CA	-6.09	1.38	1.46
4	D	225	SER	N-CA	-6.09	1.38	1.46
22	S	423	VAL	CA-CB	-6.09	1.46	1.54
25	R	150	ALA	N-CA	-6.09	1.39	1.46
5	E	219	LEU	CA-CB	6.09	1.63	1.53
4	d	147	LEU	C-N	6.09	1.41	1.33
21	N	305	ASN	CA-C	-6.09	1.44	1.52
31	L	231	LEU	CA-C	-6.09	1.44	1.52
22	S	407	ILE	CA-C	-6.08	1.45	1.52
12	l	148	ARG	C-N	6.08	1.42	1.33
13	6	210	LEU	C-N	6.08	1.41	1.33
21	N	471	TYR	C-N	6.08	1.42	1.33
32	M	50	ARG	CD-NE	6.08	1.54	1.46
14	n	227	ASN	C-N	6.08	1.41	1.33
6	F	110	HIS	CG-CD2	6.08	1.42	1.35
6	f	51	ARG	CA-C	-6.08	1.45	1.52
8	1	135	ILE	C-N	6.08	1.41	1.33
12	l	79	LEU	CA-C	-6.08	1.45	1.52
7	G	14	VAL	CA-CB	-6.07	1.46	1.54
8	1	144	TYR	N-CA	-6.07	1.39	1.46
14	7	145	ASN	N-CA	-6.07	1.38	1.46
13	m	178	LYS	CA-C	6.07	1.59	1.52
28	H	88	ARG	NE-CZ	6.07	1.39	1.33
28	H	97	LEU	N-CA	-6.07	1.38	1.46
33	J	257	ARG	CD-NE	6.07	1.54	1.46
22	S	277	SER	C-N	6.07	1.41	1.33
29	I	436	TYR	CA-C	-6.07	1.45	1.52
2	b	191	ILE	C-N	6.07	1.41	1.33
6	F	69	HIS	CD2-NE2	6.07	1.44	1.37
14	7	105	THR	CA-C	-6.07	1.44	1.52
21	N	9	LEU	CA-CB	6.07	1.63	1.53
3	c	5	ARG	NE-CZ	6.06	1.39	1.33
8	1	194	ARG	NE-CZ	6.06	1.39	1.33
12	5	174	THR	CA-C	-6.06	1.45	1.52
32	M	424	ALA	CA-CB	-6.06	1.46	1.54
11	4	118	GLN	CA-C	-6.06	1.45	1.52
24	Q	120	LYS	C-N	6.06	1.42	1.33
5	e	139	GLY	C-N	6.06	1.40	1.33
10	3	198	ARG	NE-CZ	6.06	1.39	1.33
9	i	248	ASN	CA-C	-6.06	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	39	GLY	CA-C	-6.06	1.43	1.51
9	2	239	THR	N-CA	-6.06	1.39	1.46
3	c	160	TRP	CA-C	6.05	1.60	1.52
13	m	120	ALA	C-N	6.05	1.39	1.33
24	Q	258	ALA	C-N	6.05	1.41	1.33
21	N	162	ARG	CZ-NH2	6.05	1.41	1.33
21	N	205	SER	N-CA	-6.05	1.39	1.46
24	Q	153	ASP	N-CA	-6.05	1.38	1.46
27	O	371	VAL	C-N	6.05	1.41	1.33
12	l	82	ARG	NE-CZ	6.05	1.39	1.33
4	D	69	SER	C-N	6.05	1.42	1.33
21	N	860	LYS	CA-C	6.05	1.60	1.52
26	U	93	TYR	CA-CB	6.05	1.62	1.53
16	V	146	SER	CA-CB	6.05	1.63	1.53
19	Y	40	ILE	N-CA	-6.05	1.39	1.46
26	U	152	LYS	C-N	6.05	1.41	1.33
5	E	166	ARG	CD-NE	6.05	1.54	1.46
15	W	81	ILE	CA-CB	-6.05	1.46	1.54
26	U	43	SER	CA-C	-6.05	1.45	1.52
30	K	426	PHE	C-O	-6.05	1.19	1.23
27	O	306	ARG	NE-CZ	6.04	1.39	1.33
12	l	158	LEU	N-CA	-6.04	1.38	1.46
8	h	71	HIS	ND1-CE1	6.04	1.38	1.32
29	I	162	ASP	CA-C	-6.04	1.44	1.52
4	d	113	VAL	CA-C	-6.04	1.45	1.52
6	f	39	ARG	CD-NE	6.04	1.54	1.46
13	m	224	PHE	CA-C	-6.04	1.45	1.52
9	2	65	ARG	C-O	-6.04	1.16	1.24
30	K	223	VAL	N-CA	6.04	1.53	1.46
30	K	396	ARG	CZ-NH1	6.04	1.41	1.32
24	Q	108	PRO	N-CD	-6.04	1.39	1.47
32	M	15	ASP	N-CA	-6.04	1.38	1.46
11	k	96	ARG	C-O	-6.03	1.17	1.24
4	D	151	GLU	N-CA	-6.03	1.41	1.46
12	l	268	VAL	CA-CB	6.03	1.62	1.54
16	V	215	ASN	CA-CB	6.03	1.61	1.53
11	k	43	LEU	N-CA	-6.03	1.38	1.46
22	S	419	VAL	CA-CB	-6.03	1.46	1.54
25	R	365	ASP	C-N	6.03	1.41	1.33
4	d	91	VAL	C-N	6.03	1.42	1.33
4	D	6	ARG	CA-C	-6.03	1.44	1.52
21	N	108	MET	CA-CB	6.03	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	392	ILE	C-N	6.03	1.42	1.34
23	P	292	LYS	N-CA	-6.03	1.39	1.46
29	I	82	LEU	N-CA	-6.03	1.39	1.46
9	i	170	HIS	ND1-CE1	6.02	1.38	1.32
2	b	234	ARG	CZ-NH1	6.02	1.41	1.32
21	N	277	LEU	C-N	6.02	1.42	1.34
32	M	22	ILE	CA-C	-6.02	1.45	1.52
32	M	296	SER	C-O	-6.02	1.16	1.23
1	A	105	ARG	N-CA	-6.02	1.39	1.46
9	i	233	LYS	C-O	-6.02	1.16	1.23
3	C	244	ILE	CA-C	6.02	1.58	1.52
22	S	166	ASN	CG-ND2	6.02	1.45	1.33
23	P	348	HIS	ND1-CE1	6.02	1.38	1.32
24	Q	332	ARG	NE-CZ	6.02	1.39	1.33
31	L	194	ARG	NE-CZ	6.02	1.39	1.33
33	J	293	ALA	C-N	6.02	1.41	1.33
3	C	117	ASP	CA-CB	6.01	1.62	1.53
10	3	154	TYR	CA-C	-6.01	1.44	1.52
21	N	924	LYS	C-N	6.01	1.41	1.33
22	S	184	TRP	CA-C	-6.01	1.44	1.52
11	4	170	LYS	C-N	6.01	1.42	1.33
31	L	111	GLU	CA-CB	6.01	1.63	1.53
6	F	6	TYR	C-N	6.01	1.41	1.33
24	Q	162	LEU	CA-C	-6.01	1.45	1.52
9	i	166	VAL	CA-CB	-6.01	1.46	1.54
14	n	191	VAL	C-N	6.01	1.41	1.33
4	D	116	VAL	C-O	-6.01	1.17	1.24
9	2	130	ALA	CA-C	-6.01	1.45	1.52
13	6	209	GLY	CA-C	-6.01	1.45	1.51
23	P	70	ASN	C-N	6.01	1.42	1.33
7	g	12	ASN	CA-CB	6.01	1.61	1.53
9	2	244	GLU	C-N	6.01	1.41	1.33
31	L	273	HIS	ND1-CE1	6.01	1.38	1.32
9	i	233	LYS	CA-C	-6.00	1.45	1.52
28	H	186	PRO	CA-C	6.00	1.60	1.52
21	N	572	LEU	CB-CG	6.00	1.65	1.53
32	M	353	SER	CA-C	-6.00	1.44	1.53
14	n	182	HIS	CA-C	-6.00	1.45	1.52
8	1	135	ILE	N-CA	-6.00	1.39	1.46
3	c	109	GLU	C-N	6.00	1.41	1.33
8	h	49	LYS	CA-C	6.00	1.60	1.52
14	7	216	VAL	CA-CB	-6.00	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	41	VAL	C-N	6.00	1.42	1.33
14	n	66	LEU	CA-CB	6.00	1.62	1.53
26	U	108	GLU	C-N	-6.00	1.25	1.34
29	I	322	VAL	CA-CB	-6.00	1.46	1.54
1	a	53	VAL	CA-C	-6.00	1.45	1.52
6	F	12	THR	C-N	6.00	1.41	1.33
7	G	41	LYS	CA-C	-5.99	1.44	1.52
22	S	43	LYS	C-N	5.99	1.42	1.33
7	g	49	ALA	C-N	5.99	1.40	1.33
11	4	3	ILE	C-O	-5.99	1.17	1.23
25	R	222	ARG	CZ-NH2	5.99	1.41	1.33
29	I	180	SER	CA-CB	5.99	1.62	1.53
4	d	144	GLU	CA-C	-5.99	1.44	1.52
9	i	186	ASP	CA-CB	5.99	1.62	1.53
13	6	118	ILE	CA-CB	-5.99	1.47	1.54
14	n	73	GLU	C-N	5.99	1.41	1.33
3	C	240	VAL	CA-C	-5.99	1.45	1.52
4	D	183	GLU	CA-CB	5.99	1.60	1.53
5	E	150	ASP	CA-CB	5.99	1.63	1.53
8	1	152	ARG	CD-NE	5.99	1.54	1.46
21	N	461	GLU	CA-C	-5.99	1.45	1.52
1	A	145	SER	CA-C	-5.99	1.45	1.52
14	7	259	LYS	CA-C	-5.99	1.44	1.52
21	N	234	ASP	CA-CB	5.99	1.61	1.53
22	S	162	VAL	C-N	5.99	1.41	1.33
24	Q	58	ILE	CA-CB	-5.99	1.46	1.54
9	i	171	TRP	N-CA	-5.99	1.38	1.45
7	G	129	VAL	N-CA	-5.99	1.39	1.46
22	S	120	SER	C-N	5.99	1.41	1.33
24	Q	319	LYS	CA-C	-5.99	1.45	1.52
6	F	46	LEU	CA-C	-5.98	1.45	1.52
23	P	58	VAL	C-N	5.98	1.41	1.33
9	2	46	ASP	C-N	5.98	1.43	1.33
15	W	159	ALA	CA-C	-5.98	1.45	1.52
21	N	376	LYS	CA-C	5.98	1.60	1.52
24	Q	33	LYS	CA-CB	5.98	1.62	1.53
1	a	162	TYR	CA-C	-5.98	1.44	1.52
11	4	39	SER	CA-CB	-5.98	1.45	1.53
12	5	184	GLY	CA-C	-5.98	1.43	1.51
13	6	71	ALA	CA-CB	-5.98	1.43	1.53
28	H	152	ILE	CA-C	-5.98	1.45	1.52
9	i	74	GLY	CA-C	-5.98	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	182	ASN	N-CA	-5.98	1.39	1.46
21	N	419	THR	CA-C	-5.98	1.44	1.52
13	6	122	LEU	C-N	5.97	1.41	1.33
14	7	166	LEU	CA-CB	5.97	1.63	1.53
22	S	105	PRO	C-N	5.97	1.42	1.33
33	J	181	GLN	CD-NE2	5.97	1.45	1.33
4	d	251	LYS	N-CA	-5.97	1.39	1.46
6	F	21	GLN	C-O	-5.97	1.17	1.24
16	V	73	GLN	CA-C	-5.97	1.44	1.53
27	O	60	ARG	CA-C	-5.97	1.45	1.52
28	H	116	THR	CA-C	-5.97	1.45	1.52
4	d	61	PRO	N-CD	-5.97	1.39	1.47
7	g	176	LEU	CA-C	-5.97	1.44	1.52
13	m	220	VAL	CA-CB	-5.97	1.46	1.54
14	n	77	PRO	CA-C	-5.97	1.45	1.52
9	2	175	LEU	C-N	5.97	1.41	1.33
16	V	305	ILE	C-N	5.97	1.41	1.33
28	H	382	LEU	CA-C	5.97	1.60	1.52
13	m	161	GLN	CA-C	-5.97	1.45	1.52
22	S	359	LYS	C-N	5.97	1.42	1.33
5	e	241	LYS	C-N	5.97	1.41	1.33
7	g	233	GLY	C-N	5.97	1.41	1.33
1	a	86	PRO	CA-CB	5.96	1.61	1.53
22	S	265	SER	CA-CB	5.96	1.63	1.53
30	K	194	GLN	CA-C	-5.96	1.45	1.53
12	l	281	SER	C-N	5.96	1.42	1.33
13	m	211	GLU	C-O	5.96	1.30	1.24
1	A	185	HIS	CE1-NE2	-5.96	1.26	1.32
16	V	204	HIS	CA-C	-5.96	1.45	1.52
25	R	291	SER	CA-CB	5.96	1.62	1.53
32	M	169	ALA	CA-C	-5.96	1.44	1.52
17	T	28	PRO	N-CD	-5.96	1.39	1.47
3	c	6	TYR	CZ-OH	5.96	1.50	1.38
4	d	28	LYS	C-N	5.96	1.42	1.33
14	7	45	ILE	C-N	5.96	1.41	1.33
6	f	14	SER	CA-CB	5.96	1.61	1.53
2	B	212	ALA	CA-C	-5.96	1.45	1.52
10	3	199	TYR	C-N	5.96	1.41	1.33
17	T	36	LYS	C-N	5.96	1.41	1.33
18	X	110	PRO	CA-C	5.96	1.59	1.52
11	4	81	SER	CA-C	-5.96	1.45	1.52
18	X	119	LYS	CA-C	-5.96	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	94	GLU	CA-C	-5.95	1.45	1.52
32	M	83	VAL	CA-C	-5.95	1.45	1.52
32	M	299	ARG	CZ-NH2	5.95	1.41	1.33
32	M	346	LYS	CA-C	-5.95	1.45	1.53
33	J	320	SER	C-N	5.95	1.41	1.33
27	O	238	ILE	CA-CB	-5.95	1.47	1.54
14	n	217	LEU	C-O	-5.95	1.17	1.24
23	P	252	SER	C-N	5.95	1.41	1.33
22	S	223	LEU	CA-C	-5.95	1.44	1.52
28	H	212	GLY	CA-C	-5.95	1.45	1.52
7	G	185	GLU	CA-C	-5.95	1.44	1.52
21	N	91	ILE	N-CA	-5.95	1.39	1.46
11	4	167	GLU	N-CA	5.94	1.53	1.46
30	K	259	ARG	C-N	5.94	1.41	1.33
12	5	144	ARG	CD-NE	5.94	1.54	1.46
17	T	40	LEU	C-N	5.94	1.40	1.33
17	T	245	TYR	CA-CB	5.94	1.62	1.53
21	N	263	SER	N-CA	-5.94	1.39	1.46
28	H	187	LEU	CA-C	5.94	1.60	1.52
1	A	197	GLU	N-CA	-5.94	1.39	1.46
15	W	61	VAL	N-CA	-5.94	1.39	1.46
26	U	55	PRO	N-CD	-5.94	1.39	1.47
29	I	302	ILE	N-CA	-5.94	1.39	1.46
1	A	192	ASP	CA-CB	5.94	1.61	1.53
4	D	94	GLN	N-CA	-5.94	1.39	1.46
4	D	140	PRO	CA-C	-5.94	1.44	1.52
21	N	433	THR	N-CA	-5.94	1.38	1.45
11	k	32	ASP	C-N	5.93	1.41	1.33
21	N	664	LEU	CA-CB	5.93	1.61	1.53
27	O	95	SER	C-N	5.93	1.41	1.33
4	d	219	SER	CA-CB	5.93	1.62	1.53
1	A	244	ARG	CZ-NH2	5.93	1.41	1.33
12	5	196	ARG	CZ-NH1	5.93	1.41	1.32
2	B	224	TYR	N-CA	-5.93	1.38	1.45
31	L	77	ARG	CD-NE	5.93	1.54	1.46
24	Q	169	ASP	CA-C	-5.93	1.45	1.52
32	M	357	ARG	NE-CZ	5.93	1.39	1.33
5	e	63	SER	N-CA	-5.93	1.39	1.46
9	2	234	PHE	N-CA	5.92	1.50	1.46
21	N	657	MET	CA-C	5.92	1.60	1.52
24	Q	217	GLU	CA-C	-5.92	1.45	1.52
32	M	17	GLU	N-CA	-5.92	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	84	HIS	C-O	-5.92	1.17	1.24
22	S	55	ARG	CZ-NH1	5.92	1.41	1.32
9	i	154	LEU	CA-C	-5.92	1.45	1.52
23	P	275	ASN	C-N	5.92	1.41	1.33
5	E	86	ARG	NE-CZ	5.92	1.39	1.33
16	V	228	TYR	C-N	5.92	1.42	1.33
25	R	21	VAL	CA-C	5.92	1.59	1.52
25	R	404	VAL	C-N	5.92	1.42	1.33
32	M	140	LEU	N-CA	-5.92	1.39	1.46
8	h	65	ALA	CA-CB	5.92	1.63	1.53
18	X	11	ARG	C-N	5.92	1.40	1.33
24	Q	90	LYS	C-N	5.92	1.41	1.33
12	l	260	TRP	NE1-CE2	5.92	1.44	1.37
3	C	24	TYR	CA-C	-5.92	1.44	1.52
5	e	13	SER	N-CA	-5.91	1.39	1.46
9	i	184	ALA	CA-C	-5.91	1.45	1.52
10	3	174	ALA	CA-C	5.91	1.60	1.52
8	h	79	TYR	CA-C	-5.91	1.45	1.53
2	b	31	GLY	N-CA	-5.91	1.37	1.45
4	d	42	VAL	CA-CB	-5.91	1.46	1.54
16	V	125	THR	N-CA	-5.91	1.39	1.46
21	N	566	SER	CA-CB	5.91	1.62	1.53
8	h	28	ARG	NE-CZ	5.91	1.39	1.33
13	m	53	ASP	CA-CB	5.91	1.61	1.53
2	B	62	SER	CA-C	-5.91	1.45	1.52
1	A	91	ARG	CD-NE	5.91	1.54	1.46
1	A	120	ARG	CZ-NH2	5.91	1.41	1.33
6	F	49	LEU	CA-CB	5.91	1.61	1.53
7	G	190	ARG	NE-CZ	5.91	1.39	1.33
13	6	80	VAL	CA-C	-5.90	1.45	1.52
22	S	267	SER	CA-CB	5.90	1.62	1.53
14	n	239	LEU	CA-CB	5.90	1.61	1.53
7	G	8	TYR	CA-CB	5.90	1.62	1.54
10	3	27	LEU	C-N	5.90	1.41	1.33
12	5	230	TYR	CA-CB	-5.90	1.43	1.53
12	l	100	TRP	CD2-CE2	5.90	1.51	1.41
12	l	132	THR	CA-C	-5.90	1.44	1.52
14	7	137	ARG	NE-CZ	5.90	1.39	1.33
18	X	92	SER	CA-C	-5.90	1.45	1.52
7	g	59	LEU	C-N	5.90	1.39	1.33
4	D	189	GLU	C-N	5.90	1.42	1.34
19	Y	81	LEU	C-N	5.90	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	158	PHE	CA-CB	-5.90	1.44	1.53
23	P	350	LEU	C-N	5.90	1.41	1.33
2	b	27	ALA	CA-CB	5.90	1.62	1.53
14	n	226	ARG	CZ-NH1	5.90	1.41	1.32
14	7	92	ASP	N-CA	-5.90	1.38	1.46
12	5	89	VAL	C-N	5.89	1.41	1.33
14	7	58	ASP	C-N	5.89	1.41	1.33
23	P	418	ASN	C-N	5.89	1.41	1.33
24	Q	75	ARG	CD-NE	5.89	1.54	1.46
3	C	66	LEU	C-N	5.89	1.42	1.33
12	5	280	GLY	CA-C	5.89	1.60	1.51
15	W	170	HIS	ND1-CE1	5.89	1.38	1.32
22	S	85	SER	CA-CB	5.89	1.62	1.53
32	M	295	LYS	CA-C	-5.89	1.47	1.53
10	3	136	PHE	N-CA	-5.89	1.38	1.46
16	V	163	ALA	CA-C	-5.89	1.44	1.52
30	K	96	ILE	CA-CB	-5.89	1.47	1.54
32	M	307	GLU	CA-C	-5.89	1.44	1.52
1	a	49	ASP	N-CA	-5.89	1.39	1.46
2	b	136	ILE	CA-C	-5.89	1.45	1.52
6	F	112	LEU	CA-CB	5.89	1.62	1.53
14	7	60	LEU	N-CA	-5.89	1.38	1.45
29	I	114	ASP	N-CA	-5.89	1.39	1.46
11	k	78	GLN	CA-CB	5.89	1.62	1.53
30	K	126	LEU	C-N	5.89	1.42	1.33
8	1	129	HIS	ND1-CE1	5.89	1.38	1.32
12	5	88	ILE	CB-CG1	5.89	1.65	1.53
16	V	65	VAL	CA-CB	-5.89	1.46	1.53
22	S	455	GLU	C-N	5.89	1.41	1.33
1	A	135	ARG	N-CA	-5.88	1.36	1.45
10	3	66	MET	N-CA	-5.88	1.39	1.46
30	K	85	GLU	CA-CB	5.88	1.62	1.53
10	j	128	GLY	CA-C	-5.88	1.43	1.51
3	C	101	THR	C-N	5.88	1.43	1.33
7	G	52	LYS	CA-CB	5.88	1.62	1.53
28	H	392	HIS	ND1-CE1	5.88	1.38	1.32
1	A	105	ARG	NE-CZ	5.88	1.39	1.33
8	1	39	VAL	CA-CB	5.88	1.62	1.54
32	M	219	LEU	CA-CB	5.88	1.62	1.53
2	b	234	ARG	CA-C	-5.88	1.45	1.52
14	n	57	ALA	N-CA	-5.88	1.38	1.46
8	1	182	ILE	C-N	5.88	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	32	ALA	CA-C	-5.88	1.45	1.52
3	c	117	ASP	N-CA	-5.88	1.39	1.46
3	C	64	GLU	CA-CB	5.88	1.63	1.53
6	F	174	ARG	CA-C	-5.88	1.45	1.52
17	T	109	TYR	CA-C	-5.88	1.45	1.52
22	S	181	ALA	CA-C	-5.88	1.44	1.52
4	d	120	TYR	N-CA	5.87	1.53	1.46
10	j	93	SER	N-CA	-5.87	1.39	1.46
28	H	265	ASN	CA-CB	5.87	1.62	1.53
1	a	120	ARG	CD-NE	5.87	1.54	1.46
11	k	17	SER	N-CA	5.87	1.53	1.45
6	F	16	THR	C-N	5.87	1.41	1.33
12	5	168	ALA	CA-C	5.87	1.58	1.52
13	6	88	ASN	CA-CB	5.87	1.62	1.53
32	M	50	ARG	N-CA	-5.87	1.39	1.46
8	h	191	GLY	CA-C	-5.87	1.43	1.51
14	n	102	ASP	CA-CB	5.87	1.63	1.53
9	2	65	ARG	CA-CB	5.87	1.60	1.53
12	5	144	ARG	NE-CZ	5.87	1.39	1.33
15	W	127	ARG	NE-CZ	5.87	1.39	1.33
28	H	373	ARG	NE-CZ	5.87	1.39	1.33
4	D	131	VAL	CA-C	-5.87	1.45	1.52
17	T	122	PHE	CA-CB	5.87	1.62	1.53
22	S	338	MET	CA-CB	5.87	1.61	1.53
6	F	24	TYR	C-N	5.87	1.42	1.34
21	N	336	ASN	C-N	5.87	1.41	1.33
21	N	604	ARG	CZ-NH2	5.87	1.41	1.33
12	l	263	HIS	CA-CB	5.86	1.61	1.53
24	Q	326	MET	N-CA	-5.86	1.39	1.46
32	M	269	LEU	N-CA	-5.86	1.39	1.46
1	a	193	HIS	CB-CG	5.86	1.58	1.50
11	k	120	ASP	CA-C	-5.86	1.44	1.53
4	D	152	PRO	N-CA	-5.86	1.39	1.47
6	F	163	ALA	CA-CB	5.86	1.61	1.53
9	2	130	ALA	N-CA	-5.86	1.38	1.45
11	4	23	ARG	NE-CZ	5.86	1.39	1.33
13	6	23	ILE	CA-CB	5.86	1.62	1.54
24	Q	13	ARG	CD-NE	5.86	1.54	1.46
32	M	43	ILE	N-CA	-5.86	1.39	1.46
23	P	69	ARG	NE-CZ	5.86	1.39	1.33
2	b	221	LEU	CA-C	5.86	1.60	1.52
6	F	126	ARG	CA-C	-5.86	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	126	GLY	C-N	-5.86	1.28	1.33
21	N	882	ILE	CA-C	-5.86	1.46	1.52
25	R	299	SER	CA-CB	5.86	1.62	1.53
31	L	214	PRO	CA-C	-5.86	1.46	1.52
9	i	48	ARG	CD-NE	5.86	1.54	1.46
6	F	93	ASN	CA-CB	5.86	1.62	1.53
14	7	228	PHE	N-CA	-5.86	1.38	1.46
21	N	31	VAL	CA-CB	-5.86	1.46	1.54
28	H	430	ALA	C-O	-5.86	1.17	1.24
15	W	4	GLU	C-N	5.85	1.41	1.33
14	n	239	LEU	CA-C	-5.85	1.45	1.52
4	D	195	THR	CA-C	-5.85	1.45	1.52
24	Q	21	ASN	N-CA	-5.85	1.39	1.46
30	K	252	ARG	CD-NE	5.85	1.54	1.46
30	K	279	THR	CA-C	-5.85	1.45	1.52
9	i	142	ILE	CA-C	-5.85	1.45	1.52
13	6	229	ARG	CZ-NH1	5.85	1.41	1.32
27	O	235	HIS	CD2-NE2	5.85	1.44	1.37
5	e	171	ALA	CA-C	-5.84	1.45	1.52
23	P	284	ILE	CB-CG1	5.84	1.65	1.53
24	Q	10	GLU	N-CA	-5.84	1.39	1.46
26	U	173	HIS	ND1-CE1	5.84	1.38	1.32
12	l	170	LEU	N-CA	-5.84	1.39	1.46
23	P	201	ARG	NE-CZ	5.84	1.39	1.33
28	H	146	VAL	CA-C	-5.84	1.45	1.52
14	n	166	LEU	N-CA	-5.84	1.39	1.46
9	2	112	LEU	C-N	5.84	1.41	1.33
7	G	81	LEU	CA-C	-5.84	1.45	1.52
31	L	342	ARG	CD-NE	5.84	1.54	1.46
7	g	128	SER	N-CA	-5.84	1.39	1.46
16	V	257	GLU	C-N	5.84	1.42	1.33
21	N	884	PHE	CA-C	-5.84	1.45	1.52
31	L	64	LEU	CA-C	-5.84	1.45	1.52
11	4	38	LEU	C-N	5.83	1.40	1.33
32	M	176	PRO	N-CA	-5.83	1.40	1.46
33	J	4	ALA	CA-CB	-5.83	1.44	1.53
4	d	115	GLY	C-N	5.83	1.41	1.33
1	A	120	ARG	C-O	-5.83	1.17	1.24
13	6	87	HIS	ND1-CE1	5.83	1.38	1.32
28	H	289	ARG	C-N	5.83	1.41	1.33
3	C	67	TYR	C-O	-5.83	1.16	1.23
26	U	112	LYS	CA-CB	-5.83	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	362	ASP	CA-C	-5.83	1.47	1.53
7	G	193	VAL	N-CA	-5.83	1.39	1.46
10	j	157	ASN	N-CA	-5.83	1.38	1.46
12	l	196	ARG	CD-NE	5.83	1.54	1.46
8	h	190	ALA	C-N	5.82	1.42	1.33
11	4	99	GLN	CA-C	-5.82	1.45	1.53
12	5	230	TYR	CZ-OH	5.82	1.50	1.38
28	H	226	GLU	CA-C	-5.82	1.45	1.52
30	K	77	ARG	NE-CZ	5.82	1.39	1.33
7	g	176	LEU	CA-CB	5.82	1.62	1.53
16	V	257	GLU	C-O	-5.82	1.16	1.24
23	P	259	PRO	CA-C	5.82	1.61	1.52
25	R	318	PRO	N-CA	-5.82	1.39	1.47
8	h	143	ILE	CA-CB	-5.82	1.47	1.54
1	A	28	VAL	N-CA	-5.82	1.39	1.46
24	Q	372	GLN	N-CA	-5.82	1.39	1.46
18	X	27	ILE	CA-C	-5.82	1.46	1.52
8	h	75	TYR	CA-CB	5.82	1.62	1.53
16	V	52	LEU	CA-C	-5.82	1.45	1.52
21	N	384	LYS	CA-C	-5.82	1.45	1.52
22	S	232	MET	CA-CB	5.82	1.62	1.53
12	l	234	ARG	CZ-NH2	5.82	1.41	1.33
2	B	205	ASN	CA-C	-5.82	1.45	1.52
11	k	24	GLY	C-N	5.81	1.41	1.33
14	n	51	ASN	CA-CB	5.81	1.63	1.54
14	n	225	SER	N-CA	-5.81	1.38	1.45
13	6	212	ILE	CA-CB	-5.81	1.46	1.54
22	S	326	ASP	CA-C	-5.81	1.45	1.52
29	I	270	VAL	N-CA	-5.81	1.39	1.46
2	b	123	GLN	CA-C	-5.81	1.45	1.52
30	K	379	SER	C-N	5.81	1.42	1.33
32	M	187	ASP	C-N	5.81	1.41	1.33
21	N	917	ILE	CA-CB	5.81	1.61	1.53
13	m	99	ARG	CZ-NH1	5.81	1.40	1.32
14	7	65	SER	N-CA	5.81	1.53	1.46
14	7	206	ALA	N-CA	-5.81	1.39	1.46
23	P	263	HIS	C-N	5.81	1.41	1.33
29	I	365	HIS	ND1-CE1	5.81	1.38	1.32
33	J	244	ILE	CA-C	-5.81	1.45	1.52
1	a	169	THR	C-N	5.81	1.40	1.33
21	N	692	GLU	CA-CB	5.80	1.62	1.53
7	g	155	GLY	CA-C	-5.80	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	173	LEU	CA-C	-5.80	1.45	1.53
16	V	171	ARG	NE-CZ	5.80	1.39	1.33
17	T	207	ALA	C-N	-5.80	1.26	1.33
21	N	719	ASN	CA-C	-5.80	1.45	1.52
27	O	376	GLN	CA-CB	5.80	1.62	1.53
28	H	124	ASN	CA-CB	5.80	1.62	1.53
1	a	65	ASP	N-CA	-5.80	1.38	1.45
1	a	91	ARG	NE-CZ	5.80	1.39	1.33
4	d	47	GLU	N-CA	-5.80	1.39	1.46
22	S	372	LEU	CA-C	-5.80	1.45	1.52
25	R	154	LEU	CA-CB	5.80	1.63	1.53
1	a	77	ARG	CA-C	-5.79	1.45	1.52
16	V	269	ARG	CD-NE	5.79	1.54	1.46
8	h	83	SER	CA-C	-5.79	1.45	1.52
1	A	50	CYS	CA-CB	5.79	1.63	1.53
1	A	135	ARG	NE-CZ	5.79	1.39	1.33
22	S	327	ILE	N-CA	5.79	1.53	1.46
6	F	20	PHE	N-CA	-5.79	1.39	1.46
8	1	22	ILE	CA-C	-5.79	1.45	1.52
17	T	45	SER	N-CA	-5.79	1.39	1.46
27	O	387	ARG	CZ-NH1	5.79	1.40	1.32
1	a	135	ARG	CD-NE	5.79	1.54	1.46
22	S	337	ASN	CA-C	-5.79	1.45	1.53
28	H	430	ALA	C-N	5.79	1.41	1.33
7	g	121	GLN	N-CA	-5.79	1.38	1.46
26	U	172	GLU	CA-CB	5.79	1.62	1.53
1	a	238	ALA	N-CA	5.78	1.53	1.46
5	E	53	ARG	NE-CZ	5.78	1.39	1.33
17	T	199	PHE	CG-CD2	5.78	1.50	1.38
21	N	792	SER	N-CA	5.78	1.53	1.46
25	R	270	VAL	CA-C	-5.78	1.47	1.53
33	J	95	ILE	C-N	5.78	1.39	1.33
7	G	188	SER	CA-C	-5.78	1.45	1.53
26	U	283	ARG	CD-NE	5.78	1.54	1.46
7	G	96	ALA	CA-C	5.78	1.60	1.52
23	P	320	PRO	C-N	5.78	1.40	1.33
15	W	82	GLU	C-N	5.78	1.39	1.33
17	T	151	TRP	CZ2-CH2	5.78	1.48	1.37
21	N	479	GLU	CA-C	-5.78	1.45	1.52
21	N	493	GLY	C-N	5.78	1.42	1.33
4	d	20	VAL	CA-C	-5.78	1.45	1.52
5	e	183	LEU	N-CA	-5.78	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ALA	N-CA	-5.78	1.39	1.46
3	c	178	MET	CA-C	-5.77	1.45	1.52
11	4	102	VAL	CA-CB	-5.77	1.45	1.55
14	7	240	THR	N-CA	-5.77	1.39	1.46
33	J	372	GLU	CA-C	5.77	1.60	1.52
14	7	85	GLY	N-CA	-5.77	1.38	1.46
24	Q	271	MET	N-CA	5.77	1.53	1.46
3	c	134	SER	N-CA	-5.77	1.39	1.46
6	f	192	ALA	CA-C	-5.77	1.45	1.52
2	B	71	ILE	C-N	5.77	1.40	1.33
21	N	364	LYS	C-N	-5.77	1.26	1.33
27	O	174	THR	CA-C	-5.77	1.45	1.52
28	H	385	ARG	NE-CZ	5.77	1.39	1.33
1	a	228	ALA	CA-CB	5.77	1.61	1.53
24	Q	122	ILE	N-CA	-5.77	1.39	1.46
4	D	29	ARG	CD-NE	5.76	1.54	1.46
13	6	24	ALA	C-N	5.76	1.42	1.33
13	6	84	HIS	ND1-CE1	5.76	1.38	1.32
15	W	11	ASP	CA-C	-5.76	1.45	1.52
26	U	13	LEU	C-N	5.76	1.41	1.33
11	4	146	HIS	ND1-CE1	5.76	1.38	1.32
21	N	239	LEU	C-N	5.76	1.42	1.34
29	I	222	TYR	N-CA	5.76	1.53	1.46
31	L	103	GLN	CA-C	-5.76	1.45	1.52
4	d	76	SER	CA-C	-5.76	1.45	1.52
31	L	129	VAL	CA-C	-5.76	1.45	1.52
12	l	171	SER	CA-C	5.76	1.59	1.52
18	X	93	SER	CA-C	-5.76	1.46	1.53
32	M	384	ASP	N-CA	5.76	1.53	1.46
33	J	348	GLU	N-CA	-5.76	1.38	1.46
4	d	81	ASP	CA-C	-5.75	1.45	1.52
33	J	291	ILE	N-CA	-5.75	1.39	1.46
5	e	130	GLU	N-CA	-5.75	1.38	1.45
7	G	207	ASN	CA-CB	5.75	1.59	1.53
9	2	101	ARG	NE-CZ	5.75	1.39	1.33
31	L	158	ILE	C-N	5.75	1.40	1.33
31	L	348	GLU	CA-C	-5.75	1.45	1.52
4	D	29	ARG	NE-CZ	5.75	1.39	1.33
5	E	20	ARG	CZ-NH2	5.75	1.41	1.33
9	2	218	ASN	C-N	5.75	1.41	1.34
14	7	141	ASN	CA-CB	5.75	1.62	1.53
30	K	77	ARG	CD-NE	5.75	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	93	ARG	CZ-NH2	5.75	1.41	1.33
10	j	107	PRO	CA-CB	5.75	1.62	1.53
12	5	261	ILE	C-O	-5.75	1.18	1.24
18	X	28	PRO	CA-C	-5.75	1.46	1.52
25	R	43	ARG	CD-NE	5.75	1.54	1.46
12	5	130	TRP	CA-CB	5.75	1.64	1.53
31	L	198	GLU	CA-CB	5.75	1.63	1.53
32	M	145	LEU	CA-C	-5.75	1.45	1.52
33	J	59	LYS	C-N	5.75	1.41	1.34
9	i	133	ASP	C-N	5.74	1.38	1.33
1	A	110	TYR	CA-CB	5.74	1.63	1.53
6	F	101	ARG	CZ-NH2	5.74	1.41	1.33
13	6	223	GLU	N-CA	-5.74	1.38	1.46
21	N	34	GLN	CA-C	-5.74	1.45	1.52
25	R	384	VAL	CA-C	-5.74	1.44	1.52
27	O	282	GLN	CA-C	-5.74	1.44	1.52
32	M	50	ARG	CZ-NH2	5.74	1.41	1.33
33	J	281	GLY	CA-C	-5.74	1.43	1.51
21	N	595	LEU	C-N	5.74	1.41	1.34
22	S	54	TRP	NE1-CE2	5.74	1.43	1.37
1	A	105	ARG	CD-NE	5.74	1.54	1.46
1	A	233	PHE	C-N	5.74	1.40	1.33
29	I	315	GLY	CA-C	-5.74	1.44	1.51
30	K	258	PHE	C-N	5.74	1.41	1.33
6	f	180	ILE	N-CA	-5.74	1.39	1.46
10	j	149	MET	CA-CB	5.74	1.62	1.53
29	I	193	GLU	C-N	5.74	1.40	1.33
32	M	262	LEU	N-CA	-5.74	1.38	1.46
10	j	72	ASN	C-O	-5.74	1.16	1.24
10	j	99	ARG	CZ-NH1	5.74	1.40	1.32
10	3	102	PRO	CA-C	-5.74	1.44	1.52
11	4	189	ILE	C-O	-5.74	1.18	1.24
28	H	443	PHE	CA-CB	5.74	1.62	1.53
10	j	9	GLY	C-N	5.74	1.39	1.33
9	2	238	THR	N-CA	5.74	1.53	1.46
27	O	21	SER	N-CA	-5.74	1.39	1.46
29	I	248	VAL	CA-C	-5.74	1.46	1.52
12	5	260	TRP	N-CA	-5.73	1.38	1.45
16	V	259	LYS	CA-C	-5.73	1.45	1.52
17	T	139	ASP	CA-CB	5.73	1.61	1.53
21	N	602	VAL	N-CA	5.73	1.53	1.46
10	j	109	VAL	CA-CB	5.73	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	109	LEU	C-N	5.73	1.41	1.33
3	c	71	ASP	C-O	-5.73	1.16	1.23
22	S	476	LEU	CA-CB	5.73	1.62	1.53
5	e	126	GLY	CA-C	-5.73	1.43	1.51
6	f	119	ASN	CA-C	-5.73	1.44	1.52
7	g	159	GLY	CA-C	-5.73	1.46	1.52
13	m	123	ASP	CA-CB	5.73	1.63	1.53
5	E	68	VAL	C-N	5.73	1.41	1.33
30	K	51	LEU	CB-CG	5.73	1.65	1.53
5	E	16	SER	CA-CB	5.73	1.61	1.53
11	k	193	ASP	CA-CB	5.72	1.62	1.53
3	C	194	LEU	C-O	5.72	1.30	1.24
28	H	245	GLY	CA-C	-5.72	1.43	1.51
28	H	419	LEU	CA-C	-5.72	1.44	1.52
17	T	163	LEU	CA-C	-5.72	1.45	1.52
17	T	222	LEU	CA-C	-5.72	1.45	1.52
22	S	122	ASN	C-N	5.72	1.41	1.33
33	J	253	ILE	CA-C	5.72	1.59	1.52
6	f	138	ASP	CA-C	-5.72	1.47	1.53
7	g	123	HIS	CA-C	5.72	1.60	1.52
7	G	246	GLU	CA-CB	5.72	1.62	1.53
21	N	323	GLY	C-N	5.72	1.42	1.33
23	P	162	GLU	C-N	5.72	1.41	1.33
24	Q	151	TYR	C-N	5.72	1.42	1.33
24	Q	253	ASN	CG-ND2	5.72	1.45	1.33
26	U	204	LEU	C-N	5.72	1.41	1.33
27	O	220	SER	C-N	5.72	1.42	1.33
10	3	195	VAL	C-N	5.72	1.42	1.33
1	a	191	ILE	N-CA	-5.71	1.39	1.46
13	m	39	THR	CA-CB	5.71	1.62	1.53
14	n	132	VAL	CA-CB	-5.71	1.47	1.54
3	C	5	ARG	NE-CZ	5.71	1.39	1.33
14	7	87	SER	CA-C	-5.71	1.45	1.52
27	O	324	VAL	CA-C	-5.71	1.45	1.52
30	K	289	ASP	C-O	-5.71	1.17	1.24
31	L	210	VAL	CA-CB	-5.71	1.47	1.54
3	C	241	LYS	C-N	5.71	1.42	1.33
21	N	615	ALA	CA-C	-5.71	1.45	1.52
5	E	93	ARG	CZ-NH1	5.71	1.40	1.32
5	E	211	LYS	C-N	5.71	1.41	1.33
8	1	115	ASN	C-N	5.71	1.41	1.33
14	7	169	THR	C-N	5.71	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	172	SER	N-CA	-5.71	1.40	1.46
21	N	380	LEU	CA-C	-5.71	1.45	1.52
21	N	728	LYS	CA-C	-5.71	1.45	1.52
22	S	375	ASP	N-CA	-5.71	1.38	1.46
27	O	147	ARG	CA-CB	5.71	1.62	1.53
9	i	105	VAL	CA-CB	5.71	1.61	1.54
13	m	94	ILE	CA-CB	-5.71	1.47	1.54
13	6	138	SER	CA-CB	5.71	1.63	1.53
18	X	64	ILE	CA-C	-5.71	1.45	1.52
21	N	883	SER	CA-C	-5.71	1.45	1.52
22	S	453	ASP	CA-CB	5.71	1.62	1.53
8	h	115	ASN	C-N	5.71	1.41	1.33
9	i	54	ILE	C-N	5.71	1.40	1.33
2	B	221	LEU	N-CA	-5.71	1.38	1.46
18	X	76	VAL	CA-C	5.71	1.56	1.52
21	N	201	LYS	C-N	5.71	1.42	1.33
15	W	12	ASN	CA-C	-5.71	1.45	1.52
30	K	337	LYS	CA-C	-5.70	1.45	1.53
21	N	28	ILE	CA-CB	-5.70	1.47	1.54
32	M	151	ASP	N-CA	-5.70	1.38	1.45
23	P	126	THR	N-CA	5.70	1.53	1.46
23	P	284	ILE	CA-CB	5.70	1.61	1.54
10	3	187	VAL	N-CA	-5.70	1.39	1.46
16	V	82	ALA	C-N	5.70	1.41	1.33
26	U	239	LEU	C-N	5.70	1.41	1.33
13	m	109	ARG	CZ-NH2	5.70	1.40	1.33
4	d	111	ARG	NE-CZ	5.70	1.39	1.33
5	e	216	ASN	C-N	5.70	1.41	1.33
13	m	141	ARG	CZ-NH2	5.70	1.40	1.33
16	V	121	VAL	C-N	5.70	1.42	1.33
22	S	425	ARG	CD-NE	5.70	1.54	1.46
29	I	61	ARG	NE-CZ	5.70	1.39	1.33
13	6	78	ASN	N-CA	5.69	1.53	1.46
23	P	302	LEU	N-CA	-5.69	1.39	1.46
23	P	353	ILE	CA-C	5.69	1.60	1.52
6	F	125	GLY	N-CA	-5.69	1.37	1.45
21	N	59	GLU	C-N	5.69	1.41	1.33
24	Q	247	HIS	CA-CB	5.69	1.62	1.53
10	j	191	LYS	CA-C	-5.69	1.45	1.52
6	F	49	LEU	CA-C	-5.69	1.45	1.52
1	a	19	PHE	N-CA	-5.69	1.38	1.45
1	a	164	VAL	CA-CB	-5.69	1.47	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	248	ALA	CA-C	5.69	1.60	1.52
21	N	690	HIS	CG-ND1	5.69	1.44	1.38
2	b	132	VAL	N-CA	-5.69	1.39	1.46
1	a	231	ASP	CA-C	-5.68	1.45	1.53
6	f	6	TYR	C-O	-5.68	1.16	1.24
10	3	5	SER	N-CA	-5.68	1.38	1.46
21	N	110	VAL	C-N	5.68	1.41	1.33
12	5	239	ALA	N-CA	-5.68	1.39	1.46
11	4	122	LEU	C-N	5.68	1.41	1.33
14	7	70	ASN	N-CA	-5.68	1.39	1.45
17	T	242	LYS	N-CA	-5.68	1.39	1.46
24	Q	104	PHE	C-N	5.68	1.41	1.33
9	i	117	PHE	N-CA	-5.68	1.39	1.46
8	1	171	ALA	CA-C	-5.68	1.45	1.52
15	W	29	GLN	CA-C	5.68	1.60	1.52
29	I	407	ARG	NE-CZ	5.68	1.39	1.33
2	b	138	GLY	C-N	5.67	1.41	1.33
4	d	180	ASP	C-N	5.67	1.41	1.33
11	k	184	VAL	N-CA	-5.67	1.39	1.46
12	l	180	THR	CB-OG1	-5.67	1.34	1.43
4	D	172	ARG	C-N	5.67	1.41	1.33
9	2	129	VAL	CA-C	-5.67	1.45	1.52
13	6	109	ARG	CD-NE	5.67	1.54	1.46
24	Q	67	THR	C-N	5.67	1.41	1.33
24	Q	279	LYS	CA-C	5.67	1.60	1.52
29	I	259	ASP	CA-CB	5.67	1.62	1.53
14	n	43	SER	C-N	5.67	1.40	1.33
27	O	229	ASN	C-N	5.67	1.41	1.33
14	n	95	HIS	ND1-CE1	5.67	1.38	1.32
7	G	167	LYS	CA-CB	5.67	1.62	1.53
14	7	150	ALA	CA-C	-5.67	1.45	1.52
26	U	8	VAL	CA-C	-5.67	1.45	1.52
30	K	297	ILE	C-N	5.67	1.41	1.34
32	M	264	ARG	CA-C	5.67	1.60	1.52
9	2	63	LEU	N-CA	-5.66	1.39	1.46
2	B	48	GLU	C-N	5.66	1.42	1.33
27	O	58	ARG	CA-CB	5.66	1.62	1.53
3	C	18	ARG	CD-NE	-5.66	1.38	1.46
4	D	200	LEU	CA-CB	5.66	1.62	1.53
16	V	137	VAL	N-CA	-5.66	1.39	1.46
24	Q	349	LYS	N-CA	-5.66	1.39	1.46
29	I	149	LEU	CB-CG	5.66	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	173	ASP	N-CA	-5.66	1.39	1.46
4	D	83	ARG	CD-NE	5.66	1.54	1.46
12	5	243	ASP	CA-CB	5.66	1.62	1.53
30	K	207	ARG	CZ-NH2	5.66	1.40	1.33
20	Z	746	ILE	C-N	5.66	1.41	1.33
23	P	3	ARG	CZ-NH2	5.66	1.40	1.33
16	V	247	ILE	C-N	5.66	1.41	1.34
21	N	58	ARG	NE-CZ	5.66	1.39	1.33
22	S	174	ARG	CZ-NH1	5.66	1.40	1.32
14	n	251	LYS	N-CA	-5.65	1.39	1.46
13	6	44	ASN	C-N	5.65	1.40	1.33
10	j	102	PRO	CA-CB	-5.65	1.45	1.53
10	j	198	ARG	NE-CZ	5.65	1.39	1.33
2	B	131	GLY	N-CA	5.65	1.52	1.45
11	4	85	ARG	CD-NE	5.65	1.54	1.46
13	6	145	ARG	CD-NE	5.65	1.54	1.46
14	7	74	ARG	CZ-NH2	5.65	1.40	1.33
21	N	659	ALA	N-CA	-5.65	1.39	1.46
33	J	42	ARG	CZ-NH1	5.65	1.40	1.32
29	I	147	VAL	CA-C	-5.65	1.45	1.52
15	W	53	SER	C-N	5.65	1.41	1.33
4	d	48	ARG	NE-CZ	5.65	1.39	1.33
11	k	158	LEU	C-N	5.65	1.41	1.33
28	H	340	LEU	CA-C	-5.65	1.45	1.52
31	L	306	MET	CA-CB	5.65	1.62	1.53
11	4	117	TYR	CA-C	-5.65	1.46	1.52
7	G	72	ARG	NE-CZ	5.64	1.39	1.33
13	6	221	ARG	CA-C	-5.64	1.45	1.52
22	S	114	TYR	N-CA	-5.64	1.38	1.46
27	O	191	THR	CA-C	-5.64	1.45	1.52
28	H	193	PRO	N-CD	-5.64	1.39	1.47
5	e	32	LYS	CA-C	-5.64	1.44	1.52
6	f	11	VAL	C-N	5.64	1.41	1.33
9	i	113	LYS	CA-C	-5.64	1.45	1.52
22	S	136	CYS	N-CA	-5.64	1.39	1.46
27	O	257	ALA	C-N	5.64	1.41	1.33
33	J	336	ASN	CA-C	-5.64	1.45	1.52
21	N	867	LYS	N-CA	-5.64	1.39	1.46
22	S	156	VAL	C-N	5.64	1.41	1.33
24	Q	420	ASN	CA-CB	5.64	1.62	1.53
27	O	141	ASN	CA-C	-5.64	1.46	1.53
33	J	372	GLU	C-N	5.64	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	209	ILE	C-N	5.64	1.40	1.33
22	S	272	TYR	N-CA	-5.64	1.39	1.46
2	B	90	ARG	C-N	5.64	1.41	1.33
13	6	28	PHE	N-CA	-5.64	1.38	1.45
29	I	147	VAL	C-N	5.64	1.41	1.33
3	c	225	VAL	C-N	5.63	1.41	1.33
7	g	82	ILE	CA-CB	-5.63	1.50	1.53
6	F	124	GLY	CA-C	-5.63	1.44	1.51
16	V	38	LEU	C-N	5.63	1.41	1.33
33	J	273	LEU	CA-CB	5.63	1.62	1.53
12	5	100	TRP	N-CA	-5.63	1.38	1.45
32	M	298	ASP	CA-CB	5.63	1.63	1.53
6	f	3	ARG	NE-CZ	5.63	1.39	1.33
7	g	206	ASP	C-N	5.63	1.41	1.33
25	R	137	LEU	CB-CG	5.63	1.64	1.53
32	M	313	ASP	C-N	5.63	1.38	1.33
17	T	190	ALA	N-CA	-5.63	1.38	1.46
23	P	417	HIS	CD2-NE2	5.63	1.44	1.37
16	V	279	HIS	ND1-CE1	5.63	1.38	1.32
22	S	151	GLU	CA-C	-5.63	1.46	1.52
32	M	365	SER	N-CA	5.63	1.53	1.46
13	6	52	PHE	C-N	5.63	1.41	1.33
13	6	179	PRO	N-CA	-5.63	1.40	1.46
23	P	431	HIS	ND1-CE1	5.63	1.38	1.32
7	G	169	ARG	CD-NE	5.62	1.54	1.46
7	G	215	GLU	C-N	5.62	1.41	1.33
21	N	786	ARG	NE-CZ	5.62	1.39	1.33
3	c	77	VAL	CA-C	-5.62	1.46	1.52
8	h	120	TYR	CA-C	-5.62	1.45	1.52
9	2	107	SER	C-N	5.62	1.41	1.33
10	j	28	ARG	C-N	5.62	1.40	1.33
9	2	121	GLY	C-N	5.62	1.41	1.33
16	V	262	THR	C-N	5.62	1.41	1.33
19	Y	3	THR	C-O	-5.62	1.17	1.23
3	C	162	ALA	CA-CB	5.62	1.63	1.53
28	H	355	THR	C-N	5.62	1.42	1.33
9	2	62	LYS	CA-C	-5.62	1.45	1.53
22	S	474	GLU	CA-C	-5.62	1.45	1.52
24	Q	189	ARG	CA-C	-5.62	1.45	1.52
25	R	286	LEU	CA-CB	5.62	1.62	1.53
26	U	190	LEU	C-N	5.62	1.41	1.33
28	H	440	GLU	CA-C	-5.62	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	356	SER	C-N	5.62	1.41	1.33
33	J	15	HIS	CG-CD2	-5.62	1.29	1.35
33	J	329	ARG	CD-NE	5.62	1.54	1.46
8	1	54	ARG	CD-NE	5.62	1.54	1.46
25	R	20	ARG	NE-CZ	5.62	1.39	1.33
25	R	132	GLN	C-N	5.62	1.41	1.34
28	H	339	GLN	CA-C	-5.62	1.45	1.52
6	F	105	VAL	C-N	5.61	1.41	1.33
14	7	160	LEU	CA-C	-5.61	1.46	1.52
16	V	175	SER	CA-CB	5.61	1.62	1.53
7	G	72	ARG	CZ-NH1	5.61	1.40	1.32
24	Q	252	HIS	ND1-CE1	5.61	1.38	1.32
28	H	360	THR	C-N	5.61	1.41	1.33
31	L	389	ALA	N-CA	-5.61	1.39	1.46
8	h	161	VAL	CA-CB	-5.61	1.47	1.54
10	j	160	PRO	CA-CB	5.61	1.62	1.53
6	F	115	LYS	CA-C	-5.61	1.45	1.52
6	F	229	ALA	CA-C	-5.61	1.45	1.52
10	3	25	CYS	CA-C	-5.61	1.45	1.52
23	P	357	TYR	C-N	5.61	1.41	1.33
33	J	257	ARG	CA-C	5.61	1.60	1.52
1	a	179	THR	CB-OG1	-5.61	1.34	1.43
5	E	105	GLU	N-CA	-5.61	1.38	1.45
19	Y	86	ARG	NE-CZ	5.61	1.39	1.33
24	Q	332	ARG	CZ-NH1	5.61	1.40	1.32
25	R	185	LEU	CA-C	-5.61	1.45	1.52
28	H	139	ASP	N-CA	-5.61	1.38	1.46
28	H	370	ARG	C-N	5.61	1.41	1.33
2	b	245	ASP	CA-C	5.61	1.60	1.52
8	h	136	ALA	CA-C	-5.61	1.45	1.52
11	k	181	VAL	CA-C	-5.61	1.45	1.52
13	m	56	ASP	CA-CB	5.61	1.62	1.53
4	D	24	LEU	CA-C	-5.61	1.45	1.52
1	a	74	CYS	C-N	5.60	1.40	1.33
14	7	53	VAL	C-N	5.60	1.40	1.33
22	S	122	ASN	CA-C	-5.60	1.45	1.52
25	R	272	ASP	C-N	5.60	1.40	1.33
29	I	78	ASN	CA-C	-5.60	1.45	1.52
32	M	426	LYS	N-CA	-5.60	1.39	1.46
8	h	30	THR	N-CA	-5.60	1.39	1.46
10	3	146	LEU	C-O	-5.60	1.17	1.24
11	4	146	HIS	CG-CD2	5.60	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	578	ASP	CA-C	-5.60	1.45	1.52
5	E	214	GLU	C-N	5.60	1.42	1.33
24	Q	106	GLN	CA-CB	5.60	1.62	1.53
32	M	282	GLU	C-N	5.60	1.41	1.33
2	b	192	ALA	CA-CB	5.60	1.62	1.53
9	i	156	LEU	CA-C	5.60	1.59	1.52
6	F	209	ASP	N-CA	-5.60	1.38	1.45
7	G	101	LYS	CA-C	-5.60	1.45	1.52
32	M	339	ARG	CD-NE	5.60	1.54	1.46
33	J	372	GLU	CA-CB	5.60	1.62	1.53
6	F	171	TYR	CA-CB	5.59	1.62	1.53
8	1	115	ASN	CG-ND2	5.59	1.45	1.33
24	Q	142	ALA	C-N	5.59	1.41	1.33
31	L	319	GLY	N-CA	-5.59	1.37	1.45
33	J	18	GLY	CA-C	-5.59	1.45	1.51
22	S	358	LYS	CA-CB	5.59	1.62	1.53
5	e	69	GLU	CA-CB	5.59	1.61	1.53
8	h	80	GLY	C-N	5.59	1.41	1.33
19	Y	29	LEU	N-CA	-5.59	1.39	1.46
21	N	720	ALA	C-N	5.59	1.40	1.33
25	R	235	LEU	N-CA	-5.59	1.39	1.46
26	U	44	SER	CA-CB	5.59	1.62	1.53
7	G	20	ARG	CD-NE	5.59	1.54	1.46
21	N	833	GLU	N-CA	-5.59	1.38	1.45
25	R	153	THR	CA-CB	5.59	1.62	1.53
26	U	109	LEU	N-CA	-5.59	1.39	1.46
28	H	246	ILE	CA-CB	-5.59	1.47	1.54
29	I	425	LYS	CA-C	-5.59	1.45	1.52
4	d	80	ALA	CA-C	-5.59	1.45	1.52
14	n	118	GLU	CA-C	-5.59	1.45	1.53
1	A	114	CYS	CA-CB	5.59	1.62	1.53
8	1	196	ILE	CA-C	-5.59	1.45	1.52
12	5	196	ARG	CZ-NH2	5.59	1.40	1.33
24	Q	289	GLU	N-CA	-5.59	1.39	1.46
31	L	397	GLU	C-N	5.59	1.42	1.33
14	n	58	ASP	N-CA	-5.58	1.39	1.46
17	T	150	ARG	CD-NE	5.58	1.54	1.46
7	g	213	GLU	CA-C	-5.58	1.45	1.52
14	n	183	MET	CA-C	5.58	1.58	1.53
21	N	656	ALA	C-N	5.58	1.41	1.33
4	D	49	ARG	NE-CZ	5.58	1.39	1.33
31	L	295	THR	N-CA	5.58	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	230	ASP	CA-CB	5.58	1.62	1.53
33	J	240	HIS	CE1-NE2	5.58	1.38	1.32
3	C	129	ARG	CA-C	-5.58	1.47	1.53
21	N	7	ALA	N-CA	-5.58	1.40	1.46
22	S	327	ILE	C-N	5.58	1.40	1.33
26	U	92	TRP	C-N	5.58	1.41	1.33
33	J	257	ARG	CZ-NH1	5.58	1.40	1.32
4	D	84	ILE	N-CA	5.58	1.53	1.46
31	L	264	ARG	NE-CZ	5.58	1.39	1.33
6	F	82	ARG	NE-CZ	5.58	1.39	1.33
2	b	87	ASP	CA-C	5.57	1.60	1.52
21	N	51	ASP	C-N	5.57	1.40	1.33
4	D	97	ARG	NE-CZ	5.57	1.39	1.33
9	2	95	HIS	CA-C	-5.57	1.45	1.52
25	R	30	ALA	N-CA	-5.57	1.39	1.46
6	f	127	PRO	CA-C	-5.57	1.45	1.52
17	T	171	ILE	N-CA	-5.57	1.40	1.46
21	N	222	TYR	C-N	5.57	1.41	1.34
22	S	55	ARG	CD-NE	5.57	1.54	1.46
11	k	41	HIS	CB-CG	5.57	1.57	1.50
8	1	71	HIS	CA-C	-5.57	1.45	1.52
18	X	43	LEU	C-N	5.57	1.40	1.33
1	A	57	LYS	CA-C	-5.57	1.46	1.52
9	2	249	ILE	C-N	5.57	1.40	1.33
10	3	163	LEU	N-CA	-5.57	1.39	1.46
24	Q	309	ARG	CZ-NH2	5.57	1.40	1.33
29	I	230	THR	CA-C	-5.57	1.45	1.52
1	a	15	HIS	ND1-CE1	5.57	1.38	1.32
13	6	143	GLN	N-CA	-5.57	1.39	1.46
4	d	197	ARG	CZ-NH2	5.56	1.40	1.33
1	A	53	VAL	CA-C	-5.56	1.45	1.52
26	U	98	LYS	N-CA	-5.56	1.39	1.46
2	B	215	GLY	CA-C	-5.56	1.44	1.51
22	S	216	LYS	CA-CB	5.56	1.62	1.53
29	I	104	LEU	CA-CB	5.56	1.61	1.53
7	g	70	VAL	CA-CB	5.56	1.61	1.54
13	6	129	ALA	CA-CB	-5.56	1.44	1.53
15	W	23	ARG	CZ-NH2	5.56	1.40	1.33
15	W	109	ARG	CZ-NH1	5.56	1.40	1.32
28	H	79	SER	CA-C	-5.56	1.44	1.52
4	d	50	SER	N-CA	-5.56	1.39	1.46
12	l	221	TRP	NE1-CE2	5.56	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	12	ARG	CD-NE	5.56	1.54	1.46
1	A	155	TYR	N-CA	-5.56	1.39	1.46
22	S	51	ARG	CZ-NH1	5.56	1.40	1.32
26	U	245	ASP	CA-CB	5.56	1.62	1.53
28	H	273	ARG	CD-NE	5.56	1.54	1.46
30	K	312	VAL	CA-CB	5.56	1.61	1.54
12	l	120	MET	CA-C	-5.56	1.46	1.52
1	A	83	VAL	CA-C	-5.56	1.46	1.52
15	W	28	ALA	CA-C	5.56	1.59	1.52
21	N	112	GLU	CA-CB	5.56	1.62	1.53
25	R	192	GLU	C-N	5.56	1.41	1.34
11	k	57	ALA	CA-C	-5.55	1.45	1.52
1	A	92	ASN	C-N	5.55	1.41	1.33
4	D	58	ARG	CD-NE	5.55	1.54	1.46
32	M	129	LEU	N-CA	5.55	1.52	1.45
17	T	79	GLU	CA-C	-5.55	1.45	1.52
26	U	100	ARG	CA-C	-5.55	1.45	1.52
7	g	48	PHE	C-N	5.55	1.41	1.33
14	n	253	ASP	CA-C	-5.55	1.44	1.52
5	E	182	GLU	CA-CB	-5.55	1.44	1.53
16	V	58	VAL	CA-C	-5.55	1.46	1.52
21	N	761	ILE	CA-C	-5.55	1.45	1.52
22	S	332	PHE	N-CA	-5.55	1.39	1.46
26	U	93	TYR	C-N	5.55	1.41	1.33
30	K	81	ARG	NE-CZ	5.55	1.39	1.33
31	L	409	HIS	C-N	5.55	1.40	1.33
2	b	53	SER	N-CA	-5.55	1.38	1.45
3	C	113	ARG	CA-C	-5.55	1.45	1.52
7	G	28	VAL	N-CA	-5.55	1.39	1.46
7	G	116	LEU	C-N	5.55	1.40	1.33
21	N	523	LEU	CA-CB	5.55	1.61	1.53
28	H	343	PHE	C-N	5.55	1.40	1.33
8	h	184	MET	C-N	5.55	1.40	1.33
3	C	221	ASN	CA-C	-5.55	1.45	1.52
7	G	108	PRO	CA-CB	5.55	1.61	1.53
17	T	224	ARG	CZ-NH2	5.55	1.40	1.33
32	M	342	ARG	NE-CZ	5.55	1.39	1.33
10	3	31	SER	CA-CB	5.54	1.59	1.52
1	a	179	THR	CA-C	-5.54	1.45	1.52
7	g	93	ARG	C-N	5.54	1.41	1.33
5	E	231	TYR	C-N	5.54	1.41	1.33
21	N	197	VAL	CA-C	-5.54	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	161	ASP	C-N	5.54	1.41	1.33
28	H	277	SER	N-CA	-5.54	1.39	1.46
29	I	361	ILE	N-CA	-5.54	1.39	1.46
3	c	27	GLU	C-N	5.54	1.41	1.34
5	e	167	TYR	N-CA	-5.54	1.39	1.45
15	W	100	HIS	CG-CD2	5.54	1.42	1.35
24	Q	44	ALA	CA-C	5.54	1.59	1.52
25	R	406	GLN	CA-C	-5.54	1.45	1.52
29	I	267	ILE	C-N	5.54	1.41	1.33
32	M	309	LEU	C-N	5.54	1.41	1.34
2	b	195	THR	C-O	-5.54	1.17	1.24
14	7	215	ARG	CZ-NH2	5.54	1.40	1.33
21	N	254	SER	C-N	5.54	1.41	1.33
29	I	161	GLN	C-N	5.54	1.41	1.33
6	f	132	LEU	CA-C	-5.54	1.46	1.52
13	m	144	CYS	C-N	5.54	1.40	1.33
13	6	44	ASN	CA-C	-5.54	1.45	1.52
24	Q	180	LEU	N-CA	5.54	1.52	1.46
33	J	370	LEU	CA-C	-5.54	1.45	1.52
4	d	90	ARG	N-CA	-5.53	1.39	1.46
4	d	187	THR	C-N	5.53	1.40	1.33
22	S	64	ARG	CD-NE	5.53	1.53	1.46
26	U	95	SER	CA-CB	5.53	1.63	1.53
28	H	50	LYS	N-CA	-5.53	1.39	1.46
29	I	397	THR	CA-C	5.53	1.59	1.52
31	L	290	ARG	NE-CZ	5.53	1.39	1.33
8	h	33	ALA	N-CA	-5.53	1.42	1.47
1	A	121	MET	CA-CB	5.53	1.62	1.53
21	N	597	ARG	CZ-NH1	5.53	1.40	1.32
5	e	173	GLY	C-N	5.53	1.41	1.33
22	S	260	PRO	CA-C	-5.53	1.45	1.52
14	7	198	ILE	CA-C	-5.53	1.47	1.52
24	Q	12	ARG	CZ-NH2	5.53	1.40	1.33
9	i	234	PHE	CA-C	5.53	1.58	1.52
12	l	219	TYR	CZ-OH	5.53	1.49	1.38
26	U	100	ARG	C-N	5.53	1.41	1.33
1	a	91	ARG	CD-NE	5.53	1.53	1.46
10	3	205	ASP	CA-CB	5.53	1.64	1.53
11	4	155	GLU	N-CA	-5.53	1.39	1.46
17	T	237	ASN	CA-CB	5.53	1.61	1.53
18	X	22	ARG	CZ-NH1	5.53	1.40	1.32
24	Q	310	SER	N-CA	-5.53	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	LEU	C-N	5.52	1.40	1.33
18	X	128	VAL	CA-C	-5.52	1.45	1.52
21	N	398	ARG	N-CA	5.52	1.53	1.46
29	I	304	ARG	CZ-NH1	5.52	1.40	1.32
32	M	362	GLN	C-N	5.52	1.40	1.33
28	H	173	ARG	CZ-NH1	5.52	1.40	1.32
30	K	385	ALA	C-N	5.52	1.40	1.33
33	J	228	ARG	N-CA	5.52	1.52	1.46
7	g	116	LEU	C-N	5.52	1.40	1.33
10	j	21	VAL	N-CA	-5.52	1.40	1.46
8	1	134	ALA	CA-C	-5.52	1.45	1.52
11	4	17	SER	CA-C	-5.52	1.45	1.52
21	N	515	ARG	CD-NE	5.52	1.53	1.46
4	d	119	ARG	CZ-NH2	5.52	1.40	1.33
5	E	61	SER	C-O	-5.52	1.16	1.24
10	3	157	ASN	CA-CB	5.52	1.62	1.53
21	N	226	ASN	CA-CB	5.52	1.62	1.53
33	J	15	HIS	CD2-NE2	5.52	1.44	1.37
21	N	268	GLN	N-CA	-5.52	1.39	1.46
24	Q	152	LYS	N-CA	-5.52	1.39	1.46
4	d	154	GLY	C-N	5.51	1.41	1.33
10	j	45	HIS	CG-ND1	-5.51	1.32	1.38
14	7	117	GLU	N-CA	-5.51	1.38	1.46
21	N	185	ILE	C-O	-5.51	1.17	1.24
29	I	401	LEU	C-N	5.51	1.41	1.33
4	d	49	ARG	CZ-NH1	5.51	1.40	1.32
19	Y	81	LEU	CA-C	-5.51	1.45	1.52
28	H	252	PRO	CA-C	-5.51	1.45	1.52
2	b	244	ASN	C-N	5.51	1.41	1.33
21	N	198	THR	N-CA	-5.51	1.40	1.46
32	M	408	SER	C-N	5.51	1.40	1.33
4	d	166	ARG	CZ-NH1	5.51	1.40	1.32
6	f	161	ILE	CA-C	-5.51	1.46	1.52
10	3	28	ARG	NE-CZ	5.51	1.39	1.33
21	N	741	TYR	CA-C	-5.51	1.45	1.52
22	S	456	ASP	CA-CB	5.51	1.61	1.53
23	P	105	LYS	N-CA	-5.51	1.39	1.46
29	I	259	ASP	C-N	5.51	1.41	1.33
3	c	68	LYS	C-N	5.51	1.42	1.33
13	m	153	LEU	C-N	5.51	1.41	1.33
4	D	168	SER	CA-C	5.51	1.60	1.52
16	V	95	LEU	CA-CB	5.50	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	295	GLY	CA-C	5.50	1.58	1.51
29	I	64	ARG	NE-CZ	5.50	1.39	1.33
2	B	178	ARG	NE-CZ	5.50	1.39	1.33
4	D	16	HIS	N-CA	-5.50	1.39	1.46
23	P	69	ARG	N-CA	-5.50	1.39	1.46
24	Q	165	PHE	CA-CB	5.50	1.62	1.53
27	O	183	ASN	CA-CB	5.50	1.62	1.53
30	K	127	ASP	CA-CB	5.50	1.62	1.53
31	L	276	CYS	CA-C	-5.50	1.45	1.52
4	d	98	LEU	N-CA	-5.50	1.39	1.46
27	O	387	ARG	N-CA	5.50	1.52	1.46
7	g	228	HIS	ND1-CE1	5.50	1.38	1.32
2	B	216	ASP	C-N	5.50	1.40	1.33
10	3	24	ALA	N-CA	-5.50	1.39	1.45
15	W	22	PRO	C-N	5.50	1.41	1.33
21	N	747	HIS	C-N	5.50	1.41	1.33
25	R	50	VAL	CA-CB	-5.50	1.47	1.54
27	O	73	ILE	CA-C	-5.50	1.47	1.52
33	J	267	GLU	CA-C	-5.50	1.45	1.52
14	n	215	ARG	CA-C	-5.49	1.46	1.52
5	E	243	LEU	N-CA	-5.49	1.39	1.46
9	2	145	HIS	CG-ND1	5.49	1.44	1.38
10	3	85	GLU	CA-CB	5.49	1.62	1.53
32	M	217	GLY	C-N	5.49	1.41	1.33
11	k	93	ARG	CZ-NH1	5.49	1.40	1.32
13	m	75	ARG	CZ-NH1	5.49	1.40	1.32
27	O	46	THR	CA-C	-5.49	1.45	1.52
30	K	186	GLU	CA-CB	5.49	1.62	1.53
11	k	190	ARG	CZ-NH1	5.49	1.40	1.32
13	m	84	HIS	ND1-CE1	5.49	1.38	1.32
6	F	11	VAL	CA-CB	-5.49	1.48	1.54
9	2	116	LEU	N-CA	-5.49	1.39	1.46
15	W	86	HIS	CB-CG	5.49	1.57	1.50
21	N	858	LYS	C-O	5.49	1.30	1.23
23	P	282	HIS	CB-CG	5.49	1.57	1.50
24	Q	270	ILE	CA-CB	-5.49	1.47	1.54
30	K	138	ALA	CA-C	-5.49	1.46	1.52
31	L	155	ILE	CB-CG1	5.49	1.64	1.53
31	L	289	ARG	C-N	5.49	1.41	1.33
13	6	33	GLY	CA-C	-5.49	1.44	1.51
27	O	281	ALA	N-CA	-5.49	1.39	1.46
5	E	162	GLY	N-CA	5.49	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	22	TYR	C-N	5.49	1.41	1.33
14	n	72	VAL	CA-CB	-5.49	1.46	1.53
14	n	189	ARG	C-N	5.49	1.40	1.33
5	E	223	THR	CA-C	-5.49	1.45	1.52
30	K	377	SER	C-N	5.49	1.40	1.33
29	I	220	ILE	N-CA	5.48	1.52	1.46
2	b	65	SER	CA-C	-5.48	1.45	1.52
4	d	29	ARG	CZ-NH2	5.48	1.40	1.33
6	f	234	ILE	CB-CG1	5.48	1.64	1.53
23	P	425	HIS	ND1-CE1	5.48	1.38	1.32
11	k	113	LYS	C-N	5.48	1.40	1.33
4	D	90	ARG	NE-CZ	5.48	1.39	1.33
25	R	394	ASP	CA-C	-5.48	1.46	1.52
32	M	316	SER	CA-C	-5.48	1.46	1.52
1	a	100	GLU	C-N	5.48	1.41	1.33
9	2	47	THR	C-N	5.48	1.41	1.33
3	c	186	VAL	C-N	5.48	1.41	1.34
21	N	14	ARG	CZ-NH1	5.48	1.40	1.32
24	Q	75	ARG	CZ-NH1	5.48	1.40	1.32
14	7	191	VAL	C-N	5.47	1.40	1.33
21	N	337	GLY	N-CA	-5.47	1.38	1.45
13	m	196	PHE	N-CA	-5.47	1.38	1.46
2	B	94	HIS	CG-ND1	5.47	1.44	1.38
2	b	234	ARG	CD-NE	-5.47	1.38	1.46
3	c	126	GLY	C-N	5.47	1.39	1.33
31	L	135	VAL	CA-C	-5.47	1.46	1.53
6	f	174	ARG	NE-CZ	5.47	1.39	1.33
3	C	83	ASP	C-N	5.47	1.41	1.33
13	6	207	GLY	C-N	5.47	1.41	1.33
28	H	142	ASP	CA-CB	5.47	1.61	1.53
30	K	207	ARG	CA-CB	5.47	1.62	1.53
2	b	8	SER	CA-C	-5.47	1.45	1.52
15	W	60	ARG	CZ-NH1	5.47	1.40	1.32
22	S	24	LYS	CA-C	-5.47	1.45	1.52
11	4	181	VAL	CA-CB	-5.46	1.47	1.54
16	V	192	LEU	CB-CG	5.46	1.64	1.53
31	L	230	LEU	N-CA	-5.46	1.39	1.46
32	M	263	VAL	CA-CB	-5.46	1.47	1.54
2	b	18	LEU	CA-C	-5.46	1.46	1.52
8	1	36	ALA	CA-C	5.46	1.59	1.52
32	M	381	ARG	CZ-NH2	5.46	1.40	1.33
4	d	208	LYS	C-N	5.46	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	187	ILE	C-N	5.46	1.41	1.33
2	B	31	GLY	N-CA	-5.46	1.37	1.44
5	E	148	ASP	C-N	5.46	1.41	1.33
12	5	227	ASP	C-N	5.46	1.41	1.33
17	T	128	TYR	CA-C	5.46	1.59	1.52
28	H	422	VAL	CA-CB	-5.46	1.47	1.54
31	L	67	HIS	CA-CB	5.46	1.61	1.53
6	F	184	GLY	N-CA	-5.46	1.38	1.45
21	N	400	ILE	CA-C	-5.46	1.45	1.52
5	e	53	ARG	C-N	5.46	1.40	1.33
10	3	97	GLU	N-CA	-5.46	1.39	1.46
12	5	191	ASP	CA-C	-5.46	1.46	1.52
12	5	241	HIS	CE1-NE2	-5.46	1.27	1.32
15	W	104	LYS	C-N	5.46	1.40	1.33
17	T	210	PHE	CG-CD2	5.46	1.50	1.38
33	J	269	GLN	CA-C	-5.46	1.45	1.52
9	2	226	GLU	CA-C	5.46	1.59	1.52
18	X	26	PRO	N-CA	-5.46	1.40	1.47
32	M	238	GLN	C-O	-5.46	1.17	1.24
5	e	139	GLY	CA-C	-5.46	1.44	1.51
14	n	207	GLU	CA-C	-5.46	1.45	1.52
2	b	224	TYR	CA-CB	5.45	1.62	1.53
3	c	110	ILE	CA-C	-5.45	1.45	1.52
2	B	231	LYS	N-CA	5.45	1.52	1.45
14	7	90	ILE	N-CA	-5.45	1.39	1.46
32	M	59	LEU	CA-CB	5.45	1.61	1.53
16	V	195	HIS	C-N	5.45	1.40	1.33
25	R	391	ASN	CA-CB	5.45	1.60	1.53
2	b	231	LYS	C-N	5.45	1.41	1.33
5	E	53	ARG	C-N	5.45	1.40	1.33
24	Q	257	LYS	C-O	-5.45	1.17	1.24
26	U	144	LYS	N-CA	-5.45	1.39	1.46
3	c	57	LEU	N-CA	-5.45	1.39	1.46
5	e	242	GLU	CA-C	-5.45	1.45	1.52
10	j	31	SER	N-CA	5.45	1.52	1.46
5	E	109	VAL	N-CA	-5.45	1.40	1.46
17	T	15	PHE	CA-C	-5.45	1.45	1.52
2	b	208	THR	C-N	5.45	1.40	1.33
12	5	196	ARG	C-N	5.45	1.40	1.33
22	S	477	VAL	C-N	5.45	1.41	1.33
27	O	136	THR	CA-C	5.45	1.59	1.52
6	f	150	SER	CA-CB	5.45	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	PRO	CA-CB	5.45	1.61	1.53
9	2	95	HIS	ND1-CE1	5.45	1.38	1.32
8	h	103	THR	N-CA	-5.44	1.39	1.46
32	M	358	ALA	CA-C	-5.44	1.45	1.52
12	l	111	GLU	CA-CB	5.44	1.59	1.53
9	2	92	ILE	C-N	5.44	1.41	1.34
21	N	188	TYR	CA-CB	5.44	1.62	1.53
24	Q	334	HIS	CA-C	-5.44	1.45	1.52
4	D	87	GLU	CA-CB	5.44	1.61	1.53
7	G	102	LEU	N-CA	-5.44	1.39	1.46
8	1	38	ARG	CA-CB	5.44	1.62	1.53
10	3	63	LEU	CA-C	-5.44	1.45	1.52
3	C	229	ILE	CA-CB	5.44	1.60	1.54
10	3	144	ASP	N-CA	-5.44	1.39	1.46
25	R	207	ARG	CD-NE	5.44	1.53	1.46
26	U	262	GLN	CD-NE2	5.44	1.44	1.33
1	a	39	ASN	C-N	5.44	1.41	1.33
7	g	219	CYS	C-O	-5.44	1.17	1.23
4	D	149	GLN	N-CA	-5.44	1.39	1.45
8	1	47	HIS	N-CA	-5.44	1.40	1.46
10	3	112	ILE	CA-C	-5.44	1.46	1.52
16	V	67	ASP	C-O	5.44	1.30	1.23
25	R	238	PHE	C-N	5.44	1.40	1.33
28	H	214	CYS	CA-CB	5.44	1.60	1.53
21	N	894	ARG	CZ-NH2	5.44	1.40	1.33
1	a	113	PRO	N-CD	-5.43	1.40	1.47
13	m	116	HIS	CG-CD2	5.43	1.41	1.35
9	2	41	VAL	CA-CB	-5.43	1.47	1.54
21	N	327	LEU	C-N	5.43	1.41	1.34
21	N	607	GLN	C-O	-5.43	1.17	1.24
8	h	45	ARG	C-N	5.43	1.39	1.33
9	i	232	TYR	N-CA	-5.43	1.39	1.46
3	C	207	THR	CA-C	-5.43	1.46	1.52
13	6	106	TYR	C-N	5.43	1.40	1.33
14	7	97	GLU	C-N	5.43	1.41	1.33
21	N	551	GLY	C-N	5.43	1.41	1.33
24	Q	205	ALA	C-N	5.43	1.40	1.33
7	G	149	TYR	CA-C	-5.43	1.46	1.52
12	5	243	ASP	N-CA	-5.43	1.38	1.45
23	P	348	HIS	C-N	5.43	1.41	1.33
25	R	372	ILE	N-CA	-5.43	1.40	1.46
33	J	26	LYS	CA-CB	5.43	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ARG	CD-NE	5.43	1.53	1.46
14	7	35	GLN	C-N	5.43	1.41	1.33
21	N	398	ARG	CZ-NH2	5.43	1.40	1.33
21	N	604	ARG	NE-CZ	5.43	1.39	1.33
22	S	134	ILE	C-N	5.43	1.40	1.33
4	d	71	VAL	CA-CB	-5.42	1.47	1.54
5	E	93	ARG	CA-CB	5.42	1.61	1.53
27	O	223	LEU	CA-C	-5.42	1.44	1.52
23	P	202	LYS	N-CA	5.42	1.52	1.46
30	K	64	GLN	CA-CB	5.42	1.62	1.53
2	B	162	THR	CA-CB	5.42	1.62	1.53
3	C	190	ILE	N-CA	-5.42	1.40	1.46
8	1	38	ARG	CZ-NH1	5.42	1.40	1.32
30	K	202	GLY	C-N	5.42	1.40	1.33
2	B	46	ALA	C-N	5.42	1.40	1.33
7	G	237	GLN	N-CA	-5.42	1.39	1.46
16	V	288	LEU	CA-C	-5.42	1.46	1.52
21	N	476	THR	N-CA	5.42	1.52	1.45
21	N	822	GLY	N-CA	5.42	1.49	1.44
28	H	362	ASP	N-CA	-5.42	1.38	1.45
4	D	169	LYS	CA-CB	-5.42	1.44	1.53
14	7	93	MET	CA-C	-5.42	1.45	1.52
21	N	378	ASN	CA-C	-5.42	1.47	1.53
24	Q	210	CYS	C-N	5.42	1.40	1.33
26	U	169	ILE	C-O	-5.42	1.17	1.24
30	K	167	PRO	CA-CB	-5.42	1.46	1.53
18	X	94	ASN	CA-CB	5.42	1.62	1.53
25	R	62	TYR	CA-C	5.42	1.60	1.52
32	M	148	VAL	CA-C	-5.42	1.46	1.52
32	M	247	ALA	N-CA	-5.42	1.39	1.46
22	S	381	VAL	C-N	5.42	1.41	1.33
11	k	95	ARG	C-N	5.41	1.42	1.33
3	C	8	SER	N-CA	-5.41	1.42	1.46
21	N	417	ARG	CA-CB	5.41	1.61	1.53
21	N	492	THR	CA-C	5.41	1.59	1.52
29	I	413	ALA	N-CA	-5.41	1.39	1.46
32	M	78	LEU	N-CA	5.41	1.52	1.45
33	J	268	VAL	C-O	-5.41	1.17	1.24
8	h	131	LEU	CA-C	-5.41	1.47	1.52
21	N	772	GLN	CA-C	-5.41	1.46	1.52
28	H	49	LEU	C-N	5.41	1.41	1.33
29	I	408	ARG	CZ-NH1	5.41	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	90	LYS	C-N	5.41	1.41	1.33
1	a	15	HIS	CD2-NE2	5.41	1.43	1.37
2	b	246	ARG	CA-C	-5.41	1.45	1.52
6	f	155	GLU	CA-C	-5.41	1.46	1.52
6	f	214	ALA	CA-C	-5.41	1.46	1.52
14	7	182	HIS	ND1-CE1	5.41	1.38	1.32
17	T	12	SER	N-CA	-5.41	1.39	1.46
23	P	336	HIS	CD2-NE2	5.41	1.43	1.37
5	e	41	ALA	CA-C	-5.41	1.45	1.52
14	n	182	HIS	C-O	-5.41	1.17	1.24
11	4	187	ASP	N-CA	-5.41	1.40	1.46
12	5	205	GLY	C-O	-5.41	1.18	1.24
1	a	90	ALA	CA-CB	5.41	1.61	1.53
6	F	39	ARG	NE-CZ	5.41	1.39	1.33
13	6	109	ARG	NE-CZ	5.41	1.39	1.33
21	N	566	SER	N-CA	-5.41	1.39	1.46
31	L	77	ARG	NE-CZ	5.41	1.39	1.33
1	A	205	PHE	C-O	-5.40	1.17	1.24
16	V	51	GLY	N-CA	-5.40	1.38	1.45
16	V	214	MET	N-CA	-5.40	1.39	1.46
22	S	252	ASP	CA-C	-5.40	1.45	1.52
14	n	144	TRP	CA-CB	5.40	1.60	1.52
14	n	219	TYR	N-CA	-5.40	1.40	1.46
23	P	279	ASP	CA-CB	5.40	1.62	1.53
25	R	196	SER	C-N	5.40	1.42	1.33
29	I	426	ASN	CA-CB	5.40	1.61	1.53
3	C	93	ILE	CA-C	-5.40	1.45	1.52
13	6	124	GLU	C-N	5.40	1.41	1.33
8	h	32	GLY	N-CA	-5.40	1.37	1.45
3	C	104	GLU	CA-C	-5.40	1.45	1.52
13	6	18	GLY	C-N	5.40	1.40	1.33
21	N	180	SER	CA-CB	5.40	1.61	1.53
29	I	239	GLN	N-CA	-5.40	1.40	1.46
30	K	255	ARG	CZ-NH1	5.40	1.40	1.32
26	U	65	VAL	N-CA	-5.40	1.39	1.46
9	i	246	ILE	CA-CB	-5.39	1.47	1.54
13	m	44	ASN	N-CA	-5.39	1.39	1.46
21	N	334	VAL	CA-CB	-5.39	1.47	1.54
22	S	423	VAL	N-CA	-5.39	1.39	1.46
33	J	176	SER	N-CA	5.39	1.52	1.46
24	Q	44	ALA	C-N	5.39	1.41	1.33
1	A	115	ASP	CA-C	-5.39	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	59	ALA	C-N	5.39	1.41	1.33
10	3	148	GLY	CA-C	-5.39	1.46	1.52
26	U	82	LYS	CA-CB	5.39	1.61	1.53
8	1	146	TYR	CA-CB	5.39	1.62	1.53
17	T	47	GLN	CA-CB	5.39	1.61	1.53
17	T	266	TYR	CA-C	-5.39	1.45	1.52
18	X	76	VAL	N-CA	-5.39	1.41	1.46
21	N	382	GLY	CA-C	-5.39	1.44	1.51
31	L	67	HIS	ND1-CE1	5.39	1.38	1.32
2	b	225	THR	N-CA	-5.39	1.39	1.45
11	4	174	MET	CA-C	-5.39	1.45	1.52
25	R	263	ARG	CD-NE	5.39	1.53	1.46
7	g	120	VAL	C-N	5.39	1.41	1.33
13	m	212	ILE	N-CA	-5.39	1.39	1.46
21	N	349	ILE	N-CA	5.39	1.52	1.46
22	S	280	ASN	CA-C	-5.39	1.46	1.52
25	R	391	ASN	CA-C	-5.39	1.46	1.52
7	G	232	LYS	CA-C	-5.38	1.46	1.52
10	3	104	PHE	N-CA	-5.38	1.39	1.46
11	4	112	ASN	CA-C	-5.38	1.46	1.53
32	M	288	THR	CA-C	-5.38	1.46	1.52
8	h	98	ASN	CA-CB	5.38	1.59	1.52
5	e	177	GLU	N-CA	-5.38	1.39	1.46
12	l	214	VAL	CA-CB	-5.38	1.47	1.54
13	m	84	HIS	C-N	5.38	1.41	1.33
6	F	223	THR	C-N	5.38	1.40	1.33
16	V	195	HIS	CA-CB	5.38	1.62	1.53
21	N	35	LEU	C-N	5.38	1.41	1.33
32	M	397	GLU	C-N	5.38	1.41	1.34
4	d	72	VAL	CA-C	5.38	1.59	1.52
13	m	162	VAL	N-CA	5.38	1.53	1.46
29	I	145	CYS	C-N	5.38	1.41	1.33
31	L	247	PRO	C-N	5.38	1.41	1.33
11	k	171	ARG	CZ-NH1	5.38	1.40	1.32
23	P	86	HIS	CE1-NE2	5.38	1.38	1.32
23	P	211	PRO	CA-C	5.38	1.58	1.52
25	R	339	ALA	C-N	5.38	1.41	1.33
26	U	219	LEU	C-N	5.38	1.40	1.33
28	H	128	ASN	C-N	5.38	1.41	1.33
9	i	65	ARG	CA-C	-5.38	1.46	1.52
3	C	51	LYS	N-CA	-5.38	1.39	1.46
17	T	54	ASP	CA-C	5.38	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	94	ASN	CA-C	5.38	1.59	1.52
21	N	57	ASP	CA-CB	5.38	1.60	1.53
13	6	145	ARG	N-CA	-5.38	1.39	1.46
21	N	566	SER	C-N	5.38	1.41	1.33
2	b	100	ILE	CA-CB	-5.37	1.47	1.54
9	i	170	HIS	CA-C	-5.37	1.45	1.52
4	D	153	SER	N-CA	-5.37	1.39	1.46
21	N	681	ASN	CA-C	-5.37	1.45	1.52
5	e	72	ARG	CD-NE	5.37	1.53	1.46
3	C	125	HIS	N-CA	5.37	1.52	1.45
16	V	267	LYS	CA-C	-5.37	1.45	1.52
23	P	146	ILE	CA-CB	-5.37	1.47	1.54
27	O	166	ARG	N-CA	-5.37	1.39	1.46
33	J	83	LYS	CA-C	-5.37	1.46	1.52
12	5	106	VAL	CA-C	-5.37	1.45	1.52
21	N	577	SER	C-N	5.37	1.41	1.33
9	i	132	VAL	CA-C	-5.37	1.46	1.52
3	C	48	ALA	CA-CB	5.37	1.64	1.54
5	E	191	LEU	C-N	5.37	1.40	1.33
12	5	154	ALA	N-CA	-5.37	1.39	1.46
23	P	344	ARG	CZ-NH2	5.37	1.40	1.33
24	Q	30	LEU	C-N	5.37	1.40	1.33
25	R	206	ARG	CZ-NH1	5.37	1.40	1.32
11	4	144	LEU	CA-CB	5.37	1.61	1.53
12	5	138	CYS	C-N	5.37	1.41	1.33
24	Q	39	SER	C-N	5.37	1.41	1.33
12	l	81	PHE	N-CA	-5.37	1.39	1.46
13	m	169	GLU	C-N	5.37	1.40	1.33
4	D	92	GLU	N-CA	-5.37	1.39	1.46
21	N	584	ARG	CA-C	-5.37	1.46	1.52
16	V	156	PHE	C-N	5.36	1.40	1.33
19	Y	10	ALA	CA-CB	5.36	1.61	1.53
21	N	660	LEU	CA-C	-5.36	1.45	1.52
11	k	159	ASP	CA-C	-5.36	1.45	1.52
21	N	258	ALA	CA-C	5.36	1.59	1.52
4	d	89	ALA	CA-CB	5.36	1.61	1.53
10	3	64	ASN	N-CA	-5.36	1.40	1.46
21	N	764	SER	CA-C	-5.36	1.45	1.52
25	R	281	SER	C-N	5.36	1.41	1.33
28	H	220	LYS	C-N	5.36	1.41	1.33
9	i	102	GLU	CA-C	-5.36	1.46	1.52
4	D	147	LEU	CA-C	-5.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	231	LEU	C-N	5.36	1.41	1.33
9	i	144	ALA	CA-C	-5.36	1.46	1.52
4	D	46	CYS	CA-C	-5.36	1.46	1.52
17	T	253	GLU	CA-CB	5.36	1.61	1.53
26	U	223	HIS	CG-CD2	-5.36	1.29	1.35
32	M	169	ALA	CA-CB	5.36	1.62	1.53
32	M	378	GLU	CA-CB	5.36	1.61	1.53
6	F	76	GLY	C-N	5.36	1.40	1.33
31	L	308	LEU	N-CA	-5.36	1.39	1.46
32	M	100	THR	C-N	5.36	1.40	1.33
3	C	33	GLY	C-N	5.35	1.40	1.33
23	P	428	THR	C-N	5.35	1.40	1.33
24	Q	27	TYR	CA-CB	5.35	1.61	1.53
31	L	340	PRO	N-CA	-5.35	1.41	1.46
23	P	280	LEU	CA-CB	5.35	1.62	1.53
29	I	365	HIS	CG-ND1	-5.35	1.32	1.38
17	T	60	ARG	NE-CZ	5.35	1.39	1.33
31	L	345	ARG	CZ-NH1	5.35	1.40	1.32
2	b	247	LEU	N-CA	-5.35	1.39	1.46
4	d	156	TYR	C-N	5.35	1.40	1.33
23	P	364	ARG	C-O	-5.35	1.17	1.24
1	a	96	ARG	NE-CZ	5.35	1.39	1.33
6	f	230	VAL	CA-CB	-5.35	1.49	1.54
14	7	37	PRO	CA-CB	-5.35	1.46	1.53
21	N	773	MET	CA-C	-5.35	1.46	1.52
27	O	57	LEU	C-N	5.35	1.40	1.33
18	X	75	TRP	NE1-CE2	5.35	1.43	1.37
27	O	324	VAL	C-N	5.35	1.41	1.33
14	n	135	GLN	C-O	-5.34	1.17	1.24
14	n	184	ALA	CA-C	-5.34	1.45	1.52
1	A	204	GLU	C-O	5.34	1.30	1.24
10	3	166	THR	C-N	5.34	1.40	1.33
18	X	105	ASN	CA-CB	5.34	1.62	1.53
21	N	103	SER	CA-CB	5.34	1.61	1.53
27	O	56	PRO	N-CA	-5.34	1.41	1.47
27	O	307	MET	CA-C	5.34	1.59	1.52
30	K	403	LEU	CA-CB	5.34	1.61	1.53
7	G	130	ARG	NE-CZ	5.34	1.39	1.33
28	H	175	GLY	CA-C	-5.34	1.48	1.52
9	i	50	THR	CB-OG1	-5.34	1.35	1.43
29	I	138	LYS	N-CA	-5.34	1.39	1.46
29	I	365	HIS	CA-CB	5.34	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	195	GLU	N-CA	-5.34	1.39	1.46
1	A	31	ALA	C-O	-5.34	1.17	1.24
1	A	117	LEU	CA-CB	5.34	1.61	1.53
1	A	130	GLN	C-N	5.34	1.41	1.33
3	C	117	ASP	C-N	-5.34	1.27	1.33
13	6	75	ARG	NE-CZ	5.34	1.39	1.33
15	W	136	ASN	C-N	5.34	1.40	1.33
2	b	159	TRP	CZ2-CH2	5.34	1.47	1.37
7	G	109	ILE	CA-CB	-5.34	1.50	1.53
14	7	256	LYS	C-N	5.34	1.40	1.33
21	N	23	TYR	N-CA	-5.34	1.39	1.46
21	N	471	TYR	CA-CB	5.34	1.62	1.53
21	N	893	VAL	CA-CB	-5.34	1.48	1.54
27	O	110	ASP	C-N	5.34	1.41	1.33
30	K	413	THR	CA-CB	-5.34	1.46	1.53
23	P	188	ILE	C-N	5.33	1.41	1.33
2	b	235	PHE	C-N	5.33	1.41	1.33
2	B	113	GLU	C-O	-5.33	1.17	1.24
14	7	198	ILE	C-O	-5.33	1.20	1.24
16	V	20	ARG	N-CA	-5.33	1.39	1.46
24	Q	380	MET	CA-C	-5.33	1.45	1.52
7	g	73	HIS	CD2-NE2	5.33	1.43	1.37
5	e	239	LEU	CA-CB	5.33	1.62	1.53
11	k	41	HIS	N-CA	-5.33	1.41	1.46
11	k	108	ASP	CA-CB	5.33	1.61	1.53
13	6	179	PRO	C-N	5.33	1.40	1.33
17	T	271	GLU	CA-C	-5.33	1.45	1.52
31	L	278	ILE	CA-CB	-5.33	1.47	1.54
11	k	132	ALA	C-N	5.33	1.41	1.33
9	2	211	LYS	CA-C	-5.33	1.46	1.52
14	7	244	ASN	CG-ND2	5.33	1.44	1.33
23	P	359	ARG	CZ-NH2	5.33	1.40	1.33
27	O	27	GLU	C-O	-5.33	1.17	1.24
29	I	85	PHE	CA-C	-5.33	1.46	1.53
29	I	300	ARG	CD-NE	5.33	1.53	1.46
16	V	225	LEU	C-N	5.33	1.40	1.33
26	U	38	LEU	CA-C	-5.33	1.46	1.52
6	f	45	VAL	N-CA	5.32	1.52	1.46
22	S	480	ARG	NE-CZ	5.32	1.39	1.33
24	Q	309	ARG	NE-CZ	5.32	1.39	1.33
30	K	396	ARG	CD-NE	5.32	1.53	1.46
5	e	88	MET	C-N	5.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	142	PHE	CG-CD1	5.32	1.50	1.38
10	j	129	CYS	C-N	5.32	1.38	1.33
5	E	76	CYS	N-CA	-5.32	1.39	1.46
33	J	403	LEU	N-CA	-5.32	1.40	1.46
4	D	45	GLY	C-N	5.32	1.40	1.33
7	G	165	THR	N-CA	-5.32	1.40	1.46
8	1	170	GLN	N-CA	5.32	1.53	1.46
10	3	157	ASN	C-N	5.32	1.41	1.33
27	O	277	ILE	C-N	5.32	1.38	1.33
28	H	266	ARG	NE-CZ	5.32	1.39	1.33
28	H	338	THR	N-CA	-5.32	1.39	1.46
4	d	179	TYR	CA-CB	5.32	1.62	1.53
11	k	149	ARG	CZ-NH2	5.32	1.40	1.33
24	Q	380	MET	C-N	5.32	1.40	1.33
32	M	119	VAL	C-O	-5.32	1.18	1.24
4	D	6	ARG	CZ-NH2	5.32	1.40	1.33
28	H	461	SER	CA-C	-5.32	1.44	1.53
30	K	313	LYS	CA-CB	5.32	1.62	1.53
4	d	185	PRO	N-CD	-5.32	1.40	1.47
6	f	222	PHE	CA-C	-5.32	1.46	1.52
18	X	8	ILE	CA-CB	5.32	1.60	1.54
21	N	698	GLY	CA-C	-5.32	1.46	1.52
27	O	365	LYS	CA-C	-5.32	1.45	1.52
9	i	201	ASN	N-CA	-5.31	1.39	1.45
19	Y	36	GLU	C-N	5.31	1.41	1.33
23	P	386	GLN	C-N	5.31	1.41	1.33
31	L	109	MET	CA-CB	-5.31	1.44	1.53
3	c	93	ILE	N-CA	-5.31	1.40	1.46
11	k	22	THR	N-CA	-5.31	1.40	1.46
4	D	197	ARG	CA-CB	5.31	1.62	1.53
24	Q	408	THR	N-CA	-5.31	1.39	1.46
30	K	216	GLY	C-N	5.31	1.41	1.33
33	J	136	LEU	C-N	5.31	1.41	1.34
7	g	87	HIS	CB-CG	5.31	1.57	1.50
13	m	54	CYS	CA-CB	5.31	1.61	1.54
3	C	220	ALA	CA-CB	5.31	1.60	1.52
23	P	301	LYS	C-N	5.31	1.40	1.33
27	O	392	TRP	NE1-CE2	5.31	1.43	1.37
29	I	340	ARG	CZ-NH1	5.31	1.40	1.32
6	F	178	THR	CA-CB	-5.31	1.44	1.53
22	S	405	ARG	CA-C	-5.31	1.45	1.52
5	e	10	ARG	CA-C	-5.31	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	323	THR	CA-C	-5.31	1.46	1.52
7	g	141	VAL	C-N	5.30	1.38	1.33
8	h	36	ALA	C-N	5.30	1.40	1.33
22	S	456	ASP	C-N	5.30	1.40	1.34
24	Q	209	TYR	N-CA	-5.30	1.40	1.46
29	I	151	HIS	ND1-CE1	5.30	1.37	1.32
31	L	404	ARG	C-O	-5.30	1.18	1.24
22	S	475	TYR	N-CA	-5.30	1.40	1.46
30	K	243	VAL	N-CA	-5.30	1.39	1.46
9	i	143	HIS	ND1-CE1	5.30	1.37	1.32
11	4	86	GLN	N-CA	-5.30	1.40	1.46
21	N	816	LYS	CA-CB	5.30	1.61	1.53
1	a	40	ILE	CA-C	-5.30	1.46	1.52
11	k	173	PRO	N-CA	-5.30	1.40	1.47
12	5	250	VAL	CA-C	-5.30	1.45	1.52
16	V	135	ARG	CD-NE	5.30	1.53	1.46
13	6	36	ARG	CZ-NH2	5.30	1.40	1.33
22	S	359	LYS	CA-C	-5.30	1.46	1.52
13	m	194	ASP	CA-C	-5.30	1.45	1.52
22	S	302	HIS	C-N	5.30	1.41	1.33
22	S	384	ARG	CZ-NH2	5.30	1.40	1.33
14	n	220	ARG	CD-NE	5.29	1.53	1.46
6	F	22	VAL	CA-C	-5.29	1.45	1.52
16	V	219	GLU	CA-CB	5.29	1.60	1.53
3	c	173	GLN	CA-C	-5.29	1.45	1.52
5	E	157	HIS	CB-CG	5.29	1.57	1.50
24	Q	375	GLY	CA-C	-5.29	1.46	1.52
32	M	279	PHE	CA-CB	5.29	1.59	1.53
32	M	299	ARG	CD-NE	5.29	1.53	1.46
33	J	32	LEU	C-N	5.29	1.40	1.33
1	a	74	CYS	CA-CB	5.29	1.60	1.53
2	b	109	LEU	N-CA	-5.29	1.40	1.46
12	5	164	GLN	C-O	-5.29	1.18	1.24
21	N	294	PRO	N-CA	-5.29	1.40	1.47
22	S	229	THR	N-CA	-5.29	1.39	1.46
25	R	116	LYS	N-CA	-5.29	1.40	1.46
25	R	166	ALA	CA-CB	5.29	1.61	1.53
3	c	146	TYR	C-N	5.29	1.41	1.33
25	R	71	LEU	C-N	5.29	1.40	1.33
25	R	110	ILE	N-CA	-5.29	1.40	1.46
2	b	95	THR	C-N	5.29	1.42	1.33
23	P	397	ALA	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	220	SER	N-CA	-5.29	1.40	1.46
33	J	12	LEU	CA-C	-5.29	1.45	1.52
1	a	142	THR	CA-C	-5.29	1.46	1.52
7	g	146	ALA	C-N	5.29	1.40	1.33
2	B	208	THR	CA-C	5.29	1.59	1.52
28	H	307	PHE	CA-C	-5.29	1.46	1.53
33	J	319	PRO	C-N	5.29	1.41	1.33
4	d	55	GLN	C-N	5.29	1.40	1.33
10	j	3	ASP	C-N	5.29	1.40	1.33
11	k	95	ARG	NE-CZ	5.29	1.38	1.33
31	L	414	ASP	CA-C	-5.29	1.46	1.52
1	a	42	SER	CA-C	-5.28	1.46	1.52
9	2	217	ARG	CZ-NH1	5.28	1.40	1.32
12	5	222	ASP	CA-C	-5.28	1.46	1.52
12	5	267	ASP	C-N	5.28	1.40	1.33
21	N	468	GLU	CA-C	-5.28	1.45	1.52
29	I	224	ALA	CA-C	5.28	1.60	1.53
32	M	317	SER	CA-C	-5.28	1.45	1.52
33	J	61	GLU	CA-CB	5.28	1.62	1.53
33	J	178	GLY	CA-C	5.28	1.59	1.51
4	d	6	ARG	NE-CZ	5.28	1.38	1.33
14	7	227	ASN	C-N	5.28	1.40	1.33
17	T	224	ARG	CD-NE	5.28	1.53	1.46
23	P	396	PRO	C-N	5.28	1.41	1.33
1	a	14	ARG	CD-NE	5.28	1.53	1.46
2	B	60	THR	CA-CB	-5.28	1.46	1.54
11	4	147	HIS	N-CA	-5.28	1.38	1.46
27	O	67	SER	C-N	5.28	1.41	1.33
31	L	49	GLU	C-N	5.28	1.40	1.33
21	N	283	ASP	CA-CB	5.28	1.61	1.53
9	2	106	VAL	C-N	5.28	1.40	1.33
28	H	451	ILE	CA-C	-5.28	1.46	1.52
30	K	214	PRO	C-N	5.28	1.39	1.33
32	M	235	CYS	N-CA	5.28	1.53	1.46
7	G	123	HIS	ND1-CE1	5.28	1.37	1.32
12	5	285	VAL	CA-C	-5.28	1.46	1.52
23	P	120	GLU	N-CA	5.28	1.52	1.46
23	P	143	LEU	N-CA	5.28	1.52	1.46
32	M	187	ASP	N-CA	-5.28	1.40	1.46
7	g	175	GLU	CA-C	-5.27	1.46	1.52
6	F	187	ASP	C-N	5.27	1.41	1.33
24	Q	251	THR	CA-C	-5.27	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	136	ALA	CA-CB	5.27	1.61	1.53
7	G	182	HIS	C-N	5.27	1.39	1.33
21	N	9	LEU	CA-C	-5.27	1.45	1.52
21	N	568	VAL	N-CA	5.27	1.52	1.46
21	N	689	LYS	N-CA	-5.27	1.40	1.46
23	P	173	MET	CA-C	5.27	1.59	1.52
23	P	203	ILE	CA-C	-5.27	1.46	1.52
24	Q	273	ASN	N-CA	-5.27	1.39	1.46
30	K	102	PRO	N-CA	-5.27	1.41	1.46
11	k	22	THR	C-N	5.27	1.40	1.33
11	k	190	ARG	CA-CB	5.27	1.63	1.53
4	D	132	SER	CA-C	-5.27	1.46	1.52
15	W	80	GLN	N-CA	-5.27	1.39	1.46
5	E	122	ARG	NE-CZ	5.27	1.38	1.33
14	7	107	ASN	CA-C	-5.27	1.46	1.52
21	N	633	GLY	N-CA	-5.27	1.39	1.45
23	P	26	SER	C-N	5.27	1.41	1.33
24	Q	27	TYR	C-N	5.27	1.40	1.33
28	H	140	ASP	CA-C	-5.27	1.46	1.52
30	K	372	ILE	CA-CB	5.27	1.61	1.54
31	L	184	GLY	N-CA	5.27	1.50	1.44
32	M	93	ASP	N-CA	5.27	1.52	1.46
32	M	197	ILE	C-O	5.27	1.29	1.23
7	g	116	LEU	CA-C	-5.27	1.46	1.52
13	6	218	ASP	C-N	5.27	1.39	1.33
29	I	117	HIS	ND1-CE1	5.27	1.37	1.32
24	Q	199	THR	N-CA	-5.26	1.40	1.46
5	e	90	GLU	N-CA	5.26	1.52	1.46
11	k	152	MET	CA-C	-5.26	1.46	1.52
6	f	171	TYR	CA-CB	5.26	1.61	1.53
7	g	81	LEU	N-CA	-5.26	1.39	1.46
12	5	192	SER	CA-C	5.26	1.60	1.52
16	V	192	LEU	CA-C	-5.26	1.46	1.52
21	N	387	ALA	C-O	-5.26	1.19	1.24
27	O	277	ILE	CA-CB	-5.26	1.50	1.54
13	m	98	ALA	N-CA	-5.26	1.40	1.46
1	A	231	ASP	CA-C	-5.26	1.45	1.52
4	D	175	LEU	CA-C	-5.26	1.46	1.52
21	N	703	GLN	CA-CB	5.26	1.61	1.53
22	S	160	ARG	CZ-NH2	5.26	1.40	1.33
27	O	98	TYR	CA-C	-5.26	1.46	1.52
12	5	129	PHE	C-N	5.26	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	289	ARG	CZ-NH1	5.26	1.40	1.32
3	c	57	LEU	C-O	-5.26	1.17	1.23
4	d	172	ARG	CD-NE	5.26	1.53	1.46
7	g	65	VAL	N-CA	-5.26	1.40	1.46
13	6	214	ILE	CB-CG1	5.26	1.64	1.53
21	N	584	ARG	NE-CZ	5.26	1.38	1.33
25	R	294	ILE	N-CA	-5.26	1.40	1.46
2	B	107	THR	C-O	-5.25	1.18	1.24
8	1	35	ILE	CA-CB	-5.25	1.47	1.53
8	1	45	ARG	C-N	5.25	1.38	1.33
11	4	104	ILE	CA-C	-5.25	1.45	1.52
26	U	105	LYS	C-N	5.25	1.40	1.33
28	H	442	ASP	CA-CB	5.25	1.62	1.53
30	K	255	ARG	N-CA	-5.25	1.39	1.46
32	M	53	HIS	ND1-CE1	5.25	1.37	1.32
32	M	54	GLU	CA-C	-5.25	1.46	1.52
4	d	168	SER	CA-CB	5.25	1.61	1.53
2	B	210	GLU	N-CA	-5.25	1.39	1.46
7	G	228	HIS	CA-C	-5.25	1.46	1.52
14	7	84	VAL	CA-CB	-5.25	1.47	1.54
21	N	131	PRO	N-CA	-5.25	1.40	1.47
21	N	456	GLY	N-CA	-5.25	1.37	1.45
24	Q	25	GLN	CA-C	-5.25	1.46	1.52
26	U	302	GLN	C-N	5.25	1.40	1.33
31	L	327	THR	N-CA	-5.25	1.39	1.45
31	L	392	ARG	NE-CZ	5.25	1.38	1.33
4	d	98	LEU	C-N	5.25	1.40	1.33
5	e	87	SER	N-CA	-5.25	1.40	1.46
9	i	102	GLU	CA-CB	5.25	1.61	1.53
10	3	58	THR	CA-C	5.25	1.59	1.52
31	L	297	ALA	CA-C	5.25	1.59	1.52
12	l	255	VAL	CA-CB	5.25	1.60	1.54
2	B	64	VAL	CA-C	-5.25	1.46	1.52
4	D	3	GLY	N-CA	5.25	1.53	1.45
7	G	150	MET	N-CA	-5.25	1.39	1.46
15	W	19	GLY	C-N	5.25	1.41	1.33
17	T	41	ILE	N-CA	-5.25	1.40	1.46
17	T	59	LYS	C-N	5.25	1.40	1.33
25	R	314	ASN	CA-C	-5.25	1.45	1.52
30	K	209	VAL	C-O	5.25	1.29	1.24
12	5	107	LYS	CA-C	-5.25	1.46	1.52
13	6	144	CYS	CA-C	-5.25	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	593	PHE	CA-CB	5.25	1.61	1.53
23	P	257	TRP	NE1-CE2	5.25	1.43	1.37
6	f	41	ASN	N-CA	-5.24	1.39	1.46
10	3	203	ARG	NE-CZ	5.24	1.38	1.33
14	7	248	GLU	CA-C	-5.24	1.46	1.52
22	S	407	ILE	C-N	5.24	1.40	1.33
30	K	262	ARG	CZ-NH1	5.24	1.40	1.32
6	F	174	ARG	NE-CZ	5.24	1.38	1.33
21	N	776	TYR	CA-C	-5.24	1.46	1.52
23	P	403	GLU	N-CA	-5.24	1.39	1.46
6	f	126	ARG	CZ-NH2	5.24	1.40	1.33
17	T	268	ILE	CA-C	-5.24	1.44	1.52
23	P	395	ARG	CD-NE	5.24	1.53	1.46
29	I	192	GLN	N-CA	-5.24	1.40	1.46
32	M	101	THR	N-CA	5.24	1.52	1.45
2	b	63	LYS	CA-CB	5.24	1.62	1.53
6	f	122	SER	CA-C	-5.24	1.46	1.53
12	l	249	SER	CA-C	-5.24	1.46	1.52
13	m	141	ARG	N-CA	-5.24	1.39	1.46
11	4	121	TYR	CA-CB	5.24	1.61	1.53
20	Z	255	LEU	CG-CD2	-5.24	1.35	1.52
24	Q	428	GLU	C-N	5.24	1.40	1.33
28	H	223	GLU	C-N	5.24	1.38	1.33
31	L	109	MET	C-N	5.24	1.41	1.33
9	i	223	ASN	CA-CB	5.24	1.61	1.53
11	k	187	ASP	CA-CB	5.24	1.61	1.53
7	G	72	ARG	CD-NE	5.24	1.53	1.46
21	N	687	THR	C-N	5.24	1.40	1.33
24	Q	161	LEU	CA-CB	5.24	1.61	1.53
7	g	67	ILE	C-N	5.23	1.40	1.33
26	U	213	LYS	C-O	-5.23	1.18	1.24
30	K	255	ARG	CZ-NH2	5.23	1.40	1.33
30	K	369	ASP	N-CA	-5.23	1.39	1.46
9	2	115	HIS	CA-C	5.23	1.59	1.52
13	6	79	SER	CA-CB	5.23	1.61	1.53
17	T	33	GLU	N-CA	-5.23	1.39	1.46
22	S	236	LEU	N-CA	-5.23	1.40	1.46
24	Q	426	LEU	CA-CB	5.23	1.61	1.53
25	R	25	GLU	N-CA	5.23	1.52	1.46
26	U	48	VAL	N-CA	-5.23	1.39	1.46
27	O	154	GLU	N-CA	-5.23	1.40	1.46
25	R	162	ILE	C-N	5.23	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	154	PHE	C-N	5.23	1.40	1.33
13	6	199	ALA	C-N	5.23	1.41	1.33
22	S	55	ARG	CA-C	-5.23	1.45	1.52
30	K	207	ARG	CD-NE	5.23	1.53	1.46
32	M	213	ARG	CZ-NH2	5.23	1.40	1.33
13	m	46	ARG	N-CA	-5.23	1.39	1.46
4	D	29	ARG	CA-CB	5.23	1.61	1.53
15	W	60	ARG	NE-CZ	5.23	1.38	1.33
29	I	388	SER	CA-CB	5.23	1.61	1.53
32	M	347	ILE	CA-C	-5.23	1.46	1.52
1	a	217	GLU	N-CA	-5.23	1.38	1.45
8	h	11	SER	CA-C	-5.23	1.46	1.52
12	l	255	VAL	CA-C	5.23	1.59	1.52
31	L	364	HIS	ND1-CE1	5.23	1.37	1.32
7	g	130	ARG	CZ-NH1	5.22	1.40	1.32
5	E	16	SER	C-N	5.22	1.39	1.34
9	2	233	LYS	C-N	5.22	1.39	1.32
10	3	9	GLY	CA-C	-5.22	1.44	1.52
13	6	92	LEU	CA-CB	5.22	1.60	1.53
18	X	97	TYR	CA-C	-5.22	1.46	1.52
24	Q	315	ASN	CA-CB	5.22	1.61	1.53
25	R	244	THR	C-N	5.22	1.40	1.33
28	H	97	LEU	C-N	5.22	1.41	1.33
31	L	164	ASP	N-CA	5.22	1.52	1.45
9	i	60	CYS	CA-C	-5.22	1.45	1.52
5	E	164	PHE	N-CA	5.22	1.52	1.46
22	S	319	CYS	C-N	5.22	1.40	1.33
23	P	138	ARG	CZ-NH2	5.22	1.40	1.33
24	Q	154	SER	CA-C	-5.22	1.46	1.52
24	Q	255	TYR	CA-CB	5.22	1.61	1.53
29	I	428	VAL	CA-C	5.22	1.59	1.52
30	K	322	ASP	CA-C	-5.22	1.45	1.52
30	K	374	ARG	NE-CZ	5.22	1.38	1.33
33	J	374	ARG	CZ-NH1	5.22	1.40	1.32
24	Q	16	ASN	CA-C	5.22	1.59	1.52
31	L	264	ARG	CD-NE	5.22	1.53	1.46
7	G	174	ALA	CA-C	-5.22	1.46	1.52
15	W	141	ILE	CA-CB	-5.22	1.47	1.53
17	T	69	SER	CA-C	-5.22	1.46	1.52
24	Q	93	THR	N-CA	5.22	1.52	1.46
24	Q	202	ARG	CZ-NH1	5.22	1.40	1.32
25	R	265	ASP	CA-CB	5.22	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	281	GLN	C-N	5.22	1.41	1.33
17	T	52	LEU	N-CA	-5.22	1.40	1.46
22	S	30	GLN	C-N	5.22	1.40	1.33
12	l	230	TYR	CG-CD1	5.22	1.50	1.39
3	C	134	SER	C-N	5.22	1.40	1.33
10	3	68	ARG	CZ-NH1	5.22	1.40	1.32
14	7	201	THR	CA-C	-5.22	1.46	1.52
15	W	60	ARG	CD-NE	5.22	1.53	1.46
23	P	41	VAL	C-O	-5.22	1.18	1.24
27	O	344	VAL	C-N	5.22	1.41	1.33
31	L	110	LYS	CA-C	-5.22	1.45	1.52
3	C	120	GLN	CA-C	-5.21	1.46	1.52
21	N	123	PHE	C-N	5.21	1.41	1.33
22	S	298	ARG	CZ-NH1	5.21	1.40	1.32
30	K	176	GLY	C-N	5.21	1.40	1.33
31	L	234	ALA	C-N	5.21	1.40	1.34
4	d	249	LYS	C-N	5.21	1.40	1.33
10	j	124	PHE	N-CA	5.21	1.52	1.46
13	6	168	TYR	CA-C	-5.21	1.45	1.52
21	N	608	LEU	CA-CB	5.21	1.61	1.53
29	I	148	LEU	CA-CB	5.21	1.60	1.53
5	e	10	ARG	NE-CZ	5.21	1.38	1.33
30	K	240	SER	CA-C	-5.21	1.46	1.53
32	M	180	TYR	C-N	5.21	1.41	1.34
5	E	20	ARG	N-CA	-5.21	1.39	1.46
9	2	86	GLN	C-N	5.21	1.40	1.33
21	N	103	SER	N-CA	-5.21	1.40	1.46
32	M	62	ILE	CA-CB	5.21	1.61	1.54
2	b	226	GLY	C-N	5.21	1.39	1.33
4	d	182	LYS	N-CA	-5.21	1.39	1.46
8	h	181	VAL	CA-CB	-5.21	1.46	1.54
14	n	86	ILE	CA-C	-5.21	1.46	1.52
10	3	197	LYS	C-O	-5.21	1.17	1.24
13	6	90	LYS	CA-CB	5.21	1.61	1.53
22	S	51	ARG	CD-NE	5.21	1.53	1.46
25	R	336	LYS	CA-C	-5.21	1.46	1.52
29	I	427	LYS	CA-CB	5.21	1.61	1.53
3	C	242	THR	CA-C	-5.21	1.45	1.52
12	5	270	GLU	CA-C	-5.21	1.46	1.52
22	S	447	GLU	CA-C	5.21	1.59	1.52
25	R	419	ALA	N-CA	-5.21	1.40	1.46
32	M	302	GLN	CA-C	-5.21	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	70	ASN	CA-C	-5.21	1.45	1.52
10	3	6	SER	CA-CB	5.21	1.62	1.53
14	7	62	SER	N-CA	-5.21	1.39	1.45
17	T	264	MET	CA-C	-5.21	1.46	1.52
25	R	222	ARG	N-CA	-5.21	1.39	1.46
26	U	44	SER	C-O	-5.21	1.18	1.24
14	n	85	GLY	CA-C	-5.20	1.48	1.52
3	C	68	LYS	C-N	5.20	1.41	1.33
21	N	122	GLN	CA-C	-5.20	1.46	1.52
24	Q	339	TYR	C-O	-5.20	1.18	1.24
27	O	318	HIS	ND1-CE1	5.20	1.37	1.32
6	f	87	TYR	C-O	-5.20	1.18	1.24
7	g	218	TRP	CZ2-CH2	5.20	1.47	1.37
8	1	80	GLY	N-CA	-5.20	1.38	1.45
9	i	225	ARG	C-N	5.20	1.40	1.33
13	m	117	THR	CA-CB	5.20	1.61	1.53
13	m	222	LYS	N-CA	-5.20	1.39	1.46
16	V	131	GLN	C-N	5.20	1.41	1.33
24	Q	410	ASP	CA-C	5.20	1.59	1.52
32	M	56	ASN	CA-C	-5.20	1.46	1.52
12	l	237	LEU	CA-C	-5.20	1.46	1.52
17	T	51	TYR	C-N	5.20	1.41	1.33
21	N	269	LEU	C-O	-5.20	1.18	1.24
28	H	291	VAL	C-N	5.20	1.40	1.33
33	J	112	ARG	NE-CZ	5.20	1.38	1.33
2	b	34	SER	N-CA	-5.20	1.39	1.45
1	A	186	PHE	CA-CB	5.20	1.61	1.53
3	C	125	HIS	CA-C	-5.20	1.46	1.52
23	P	117	SER	CA-CB	5.20	1.61	1.53
4	d	85	LEU	N-CA	5.20	1.52	1.46
12	l	142	GLU	N-CA	-5.20	1.39	1.46
21	N	504	TYR	CA-C	-5.20	1.45	1.52
27	O	329	MET	C-O	-5.20	1.18	1.24
11	k	30	ASP	CA-CB	5.19	1.61	1.53
8	1	98	ASN	CA-C	-5.19	1.44	1.52
3	c	177	GLN	N-CA	-5.19	1.39	1.46
12	l	198	LYS	CA-C	-5.19	1.46	1.52
12	l	242	ARG	CZ-NH2	5.19	1.40	1.33
5	E	135	SER	N-CA	-5.19	1.39	1.46
6	F	59	TYR	CZ-OH	5.19	1.49	1.38
8	1	148	ASP	CA-C	-5.19	1.46	1.52
32	M	339	ARG	CZ-NH1	5.19	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	415	PHE	CA-C	5.19	1.59	1.52
4	D	63	LYS	CA-CB	5.19	1.62	1.53
16	V	229	ASP	CA-C	-5.19	1.45	1.52
18	X	41	GLU	CA-CB	5.19	1.61	1.53
21	N	313	LEU	C-N	5.19	1.40	1.33
29	I	73	GLU	CA-CB	5.19	1.61	1.53
1	a	143	PHE	N-CA	5.19	1.52	1.46
6	f	66	CYS	N-CA	-5.19	1.39	1.46
10	j	122	ALA	CA-CB	5.19	1.62	1.53
3	C	175	LEU	C-N	5.19	1.40	1.33
7	G	156	SER	N-CA	-5.19	1.39	1.46
21	N	283	ASP	N-CA	-5.19	1.39	1.45
29	I	331	ILE	CA-CB	-5.19	1.47	1.54
33	J	309	ARG	NE-CZ	5.19	1.38	1.33
33	J	311	ASP	C-N	5.19	1.40	1.33
22	S	203	SER	C-N	5.19	1.40	1.33
2	B	166	LYS	CA-CB	5.18	1.61	1.53
2	B	209	ILE	CA-CB	-5.18	1.48	1.54
3	C	109	GLU	C-N	5.18	1.40	1.33
29	I	283	GLU	CA-C	-5.18	1.48	1.53
32	M	51	LEU	C-O	-5.18	1.17	1.24
3	c	30	SER	C-N	5.18	1.40	1.33
23	P	227	ILE	C-O	-5.18	1.18	1.24
25	R	347	THR	C-O	-5.18	1.17	1.23
29	I	119	ILE	C-O	-5.18	1.18	1.24
2	B	21	ILE	N-CA	-5.18	1.40	1.46
4	D	17	ILE	N-CA	-5.18	1.41	1.46
11	4	180	ILE	N-CA	-5.18	1.40	1.46
4	d	34	VAL	C-N	5.18	1.40	1.32
11	k	10	GLN	N-CA	5.18	1.52	1.46
4	D	23	ALA	N-CA	-5.18	1.40	1.46
7	G	173	LYS	C-N	5.18	1.41	1.33
23	P	83	SER	CA-CB	5.18	1.61	1.53
21	N	140	MET	CA-CB	5.18	1.61	1.53
22	S	281	ALA	N-CA	-5.18	1.40	1.46
22	S	393	ARG	N-CA	-5.18	1.39	1.46
4	d	4	TYR	N-CA	-5.18	1.41	1.46
12	l	193	ASP	C-N	5.18	1.39	1.33
14	7	162	TYR	C-N	5.18	1.40	1.33
23	P	334	ASN	CG-ND2	5.18	1.44	1.33
6	f	202	ARG	NE-CZ	5.17	1.38	1.33
9	i	221	THR	CA-CB	-5.17	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	201	ASN	CA-C	-5.17	1.46	1.53
24	Q	336	ASN	CG-ND2	5.17	1.44	1.33
28	H	275	ILE	N-CA	-5.17	1.40	1.46
5	e	202	LYS	CA-CB	5.17	1.61	1.53
7	g	212	PHE	CA-C	-5.17	1.46	1.52
6	F	57	SER	C-N	5.17	1.41	1.33
21	N	640	VAL	N-CA	-5.17	1.39	1.46
6	f	106	GLU	C-N	5.17	1.40	1.33
7	g	167	LYS	CA-C	5.17	1.59	1.52
22	S	482	PRO	C-N	5.17	1.40	1.33
33	J	200	ARG	NE-CZ	5.17	1.38	1.33
13	6	25	GLY	CA-C	-5.17	1.44	1.51
13	6	188	VAL	N-CA	-5.17	1.40	1.46
14	7	226	ARG	C-O	-5.17	1.17	1.24
21	N	64	ILE	CA-C	-5.17	1.46	1.52
10	j	160	PRO	N-CD	-5.17	1.40	1.47
3	C	10	THR	N-CA	-5.17	1.39	1.46
21	N	588	VAL	C-N	5.17	1.40	1.33
22	S	384	ARG	NE-CZ	5.17	1.38	1.33
26	U	302	GLN	N-CA	-5.17	1.39	1.46
27	O	265	LYS	CA-C	-5.17	1.46	1.52
3	c	163	ILE	C-N	5.17	1.41	1.33
27	O	62	TYR	N-CA	5.17	1.52	1.46
3	c	106	ILE	CA-CB	-5.16	1.47	1.54
7	g	184	PRO	C-N	5.16	1.41	1.33
5	E	140	VAL	CA-CB	5.16	1.62	1.54
6	F	31	GLN	N-CA	-5.16	1.39	1.46
13	6	110	PHE	CA-CB	5.16	1.61	1.54
29	I	325	ILE	N-CA	-5.16	1.40	1.46
28	H	106	ILE	N-CA	-5.16	1.39	1.46
30	K	199	GLU	CA-C	-5.16	1.45	1.52
14	n	219	TYR	C-N	-5.16	1.26	1.33
5	E	37	ALA	CA-C	-5.16	1.46	1.52
8	1	94	LEU	CA-C	-5.16	1.46	1.52
16	V	301	ASN	CA-C	-5.16	1.46	1.52
23	P	136	ARG	CA-C	-5.16	1.46	1.52
23	P	321	VAL	N-CA	-5.16	1.39	1.46
25	R	420	ALA	C-N	5.16	1.40	1.33
26	U	83	ILE	CB-CG1	5.16	1.63	1.53
30	K	236	ARG	CZ-NH2	5.16	1.40	1.33
4	d	138	PHE	CA-C	-5.16	1.46	1.52
6	f	44	ALA	C-N	5.16	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	67	ILE	N-CA	-5.16	1.40	1.46
6	F	110	HIS	C-N	5.16	1.41	1.34
22	S	302	HIS	ND1-CE1	5.16	1.37	1.32
24	Q	66	VAL	C-N	5.16	1.41	1.33
24	Q	108	PRO	CA-C	5.16	1.58	1.52
32	M	178	GLU	CA-CB	-5.16	1.45	1.53
30	K	367	ASP	CA-C	-5.16	1.46	1.52
33	J	118	ASP	CA-CB	5.16	1.62	1.53
24	Q	155	LEU	CA-CB	5.16	1.61	1.53
33	J	373	ARG	CD-NE	5.16	1.53	1.46
3	c	90	THR	C-N	5.15	1.40	1.33
13	m	183	LEU	C-N	5.15	1.40	1.33
26	U	197	LEU	CA-C	-5.15	1.46	1.52
32	M	195	GLU	CA-C	-5.15	1.46	1.52
3	C	125	HIS	ND1-CE1	5.15	1.37	1.32
9	2	238	THR	C-N	5.15	1.40	1.33
32	M	41	ILE	C-N	5.15	1.41	1.34
33	J	172	GLU	C-N	5.15	1.40	1.33
3	c	85	GLU	N-CA	-5.15	1.40	1.46
4	d	111	ARG	CD-NE	5.15	1.53	1.46
7	g	49	ALA	N-CA	-5.15	1.39	1.45
14	n	194	ARG	CA-C	-5.15	1.46	1.52
23	P	342	GLN	CD-NE2	5.15	1.44	1.33
28	H	454	TYR	CA-CB	5.15	1.61	1.53
13	m	94	ILE	CA-C	-5.15	1.46	1.52
5	E	237	ALA	CA-C	-5.15	1.45	1.52
27	O	272	VAL	CA-CB	5.15	1.60	1.54
29	I	100	ARG	CD-NE	5.15	1.53	1.46
29	I	417	LYS	C-N	5.15	1.40	1.33
30	K	288	SER	C-N	5.15	1.41	1.33
33	J	349	LYS	CA-C	-5.15	1.46	1.52
6	f	114	ASP	CA-CB	5.15	1.61	1.53
8	h	50	ILE	CA-CB	5.15	1.61	1.54
14	7	129	LEU	C-N	5.15	1.40	1.33
23	P	285	GLN	CA-C	-5.15	1.46	1.52
24	Q	411	SER	CA-CB	5.15	1.62	1.53
31	L	209	ARG	CD-NE	5.15	1.53	1.46
6	f	123	TYR	CA-CB	5.15	1.60	1.53
9	i	191	GLY	CA-C	-5.15	1.43	1.51
12	l	125	ALA	CA-CB	-5.15	1.45	1.53
14	7	89	ASP	C-N	5.15	1.39	1.33
25	R	180	PHE	CA-CB	5.15	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	368	VAL	CA-C	-5.15	1.46	1.52
10	3	31	SER	CA-C	-5.14	1.48	1.53
27	O	372	GLU	CA-C	-5.14	1.46	1.52
30	K	84	GLU	CA-C	-5.14	1.46	1.52
30	K	339	GLU	C-N	5.14	1.38	1.33
5	e	121	LEU	C-N	5.14	1.40	1.33
12	l	144	ARG	NE-CZ	5.14	1.38	1.33
12	l	218	ASN	CA-C	-5.14	1.46	1.53
24	Q	317	ALA	N-CA	5.14	1.52	1.46
16	V	26	THR	CA-C	-5.14	1.46	1.52
24	Q	201	ALA	N-CA	-5.14	1.40	1.46
28	H	433	ALA	C-N	5.14	1.41	1.33
10	3	45	HIS	ND1-CE1	5.14	1.37	1.32
19	Y	13	LYS	C-N	5.14	1.40	1.33
23	P	131	PHE	C-N	5.14	1.40	1.33
33	J	28	GLN	N-CA	-5.14	1.39	1.46
10	3	85	GLU	C-N	5.14	1.41	1.34
13	6	114	TYR	CA-C	-5.14	1.45	1.52
17	T	145	PRO	CA-CB	5.14	1.61	1.53
17	T	265	ASP	N-CA	5.14	1.52	1.46
25	R	211	LYS	N-CA	-5.14	1.40	1.46
28	H	437	VAL	CA-C	-5.14	1.48	1.52
11	k	194	ASP	CA-CB	5.13	1.62	1.53
14	n	232	ILE	CA-CB	5.13	1.60	1.54
5	E	209	GLU	CA-CB	5.13	1.61	1.54
7	G	172	ALA	C-O	-5.13	1.18	1.24
14	7	44	VAL	CA-CB	-5.13	1.46	1.55
17	T	183	SER	CA-C	-5.13	1.46	1.52
5	e	9	ASP	CA-CB	5.13	1.61	1.53
5	E	163	THR	C-N	5.13	1.40	1.33
5	E	201	LEU	C-N	5.13	1.40	1.33
12	5	78	THR	N-CA	-5.13	1.39	1.45
14	7	245	LEU	C-N	5.13	1.40	1.33
33	J	344	ARG	NE-CZ	5.13	1.38	1.33
4	d	12	SER	C-N	5.13	1.39	1.34
5	e	73	HIS	CB-CG	-5.13	1.43	1.50
6	f	4	ASN	CA-CB	5.13	1.63	1.53
8	h	160	THR	C-N	5.13	1.40	1.33
14	n	263	THR	C-N	5.13	1.40	1.33
32	M	415	PHE	CG-CD1	5.13	1.49	1.38
12	l	223	LEU	N-CA	-5.13	1.40	1.46
16	V	211	LYS	CA-CB	5.13	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	90	ASP	CA-CB	5.13	1.62	1.53
1	a	217	GLU	CA-CB	5.13	1.61	1.53
4	d	141	ARG	CD-NE	5.13	1.53	1.46
14	n	113	LEU	C-N	5.13	1.40	1.33
21	N	293	LEU	C-O	-5.13	1.19	1.24
22	S	39	ASN	CA-C	-5.13	1.46	1.52
24	Q	196	ALA	C-N	5.13	1.41	1.33
27	O	203	THR	CA-C	-5.13	1.46	1.52
29	I	149	LEU	N-CA	-5.13	1.39	1.45
29	I	215	PRO	CA-CB	-5.13	1.47	1.54
13	m	49	PRO	CA-CB	5.13	1.60	1.53
1	A	114	CYS	CA-C	5.13	1.59	1.52
7	G	53	LEU	CA-C	-5.13	1.46	1.52
7	G	152	GLU	C-N	-5.13	1.28	1.34
24	Q	61	LEU	N-CA	-5.13	1.39	1.46
29	I	436	TYR	CA-CB	5.13	1.61	1.53
32	M	345	ARG	CZ-NH1	5.13	1.40	1.32
33	J	71	TYR	CG-CD1	5.13	1.50	1.39
13	m	36	ARG	N-CA	-5.12	1.39	1.46
12	5	266	HIS	CA-C	-5.12	1.46	1.52
2	b	106	PRO	N-CA	5.12	1.53	1.47
13	m	61	SER	N-CA	-5.12	1.39	1.46
13	6	27	ASP	CA-C	-5.12	1.46	1.52
14	7	108	ALA	CA-CB	5.12	1.62	1.53
19	Y	69	VAL	C-N	5.12	1.40	1.33
3	c	151	SER	CA-C	-5.12	1.46	1.52
16	V	236	SER	CA-C	-5.12	1.46	1.52
26	U	152	LYS	CA-C	5.12	1.59	1.52
28	H	121	ASN	CA-C	-5.12	1.45	1.52
31	L	368	VAL	N-CA	-5.12	1.40	1.46
32	M	111	THR	C-N	5.12	1.40	1.33
11	k	70	ARG	CA-C	5.12	1.59	1.52
27	O	347	LEU	C-O	-5.12	1.17	1.23
4	d	91	VAL	CA-C	-5.12	1.46	1.52
7	g	79	SER	N-CA	-5.12	1.39	1.45
11	k	47	ALA	C-O	-5.12	1.17	1.23
1	A	214	LEU	CB-CG	5.12	1.63	1.53
3	C	70	ASN	N-CA	-5.12	1.39	1.46
24	Q	242	SER	CA-C	-5.12	1.45	1.52
25	R	158	LEU	C-N	5.12	1.40	1.33
31	L	63	LYS	C-N	5.12	1.40	1.33
5	E	34	GLY	CA-C	5.12	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	765	ASP	CG-OD2	5.12	1.35	1.25
9	2	104	ARG	NE-CZ	5.12	1.38	1.33
31	L	277	ILE	CA-C	-5.12	1.46	1.52
33	J	74	GLU	CA-C	-5.12	1.46	1.52
9	i	174	ASP	CA-C	-5.11	1.47	1.53
1	A	33	LYS	C-N	5.11	1.40	1.33
7	G	110	PRO	N-CA	5.11	1.54	1.47
12	5	119	THR	N-CA	-5.11	1.39	1.46
24	Q	230	LYS	CA-C	-5.11	1.46	1.52
28	H	149	LEU	C-N	5.11	1.40	1.33
3	C	62	SER	CA-CB	5.11	1.62	1.53
30	K	113	THR	C-N	5.11	1.41	1.33
14	n	46	SER	C-N	5.11	1.39	1.33
28	H	69	VAL	C-N	5.11	1.40	1.33
28	H	247	LEU	C-N	5.11	1.40	1.33
29	I	123	PRO	N-CD	5.11	1.54	1.47
6	f	97	LEU	CA-C	-5.11	1.46	1.52
23	P	120	GLU	CA-CB	5.11	1.61	1.53
33	J	204	HIS	CG-ND1	5.11	1.43	1.38
4	D	16	HIS	CA-CB	-5.11	1.46	1.53
13	6	111	PHE	CA-CB	5.11	1.61	1.53
16	V	259	LYS	CA-CB	5.11	1.62	1.53
17	T	216	GLU	N-CA	-5.11	1.39	1.46
24	Q	371	GLN	C-O	-5.11	1.18	1.24
30	K	333	ARG	NE-CZ	5.11	1.38	1.33
31	L	222	GLY	CA-C	-5.11	1.44	1.51
10	j	51	LEU	N-CA	5.11	1.52	1.46
23	P	34	SER	CA-C	-5.11	1.46	1.52
28	H	274	VAL	CA-CB	-5.11	1.47	1.54
5	e	83	ALA	C-O	-5.10	1.18	1.24
23	P	265	VAL	N-CA	-5.10	1.40	1.46
4	d	248	LYS	CA-C	-5.10	1.46	1.52
14	n	189	ARG	NE-CZ	5.10	1.38	1.33
2	B	240	SER	CA-CB	5.10	1.61	1.53
2	B	242	GLU	CA-C	-5.10	1.46	1.52
4	D	122	GLN	CA-C	-5.10	1.45	1.52
11	4	74	GLU	N-CA	-5.10	1.39	1.46
13	6	173	ASN	CA-C	5.10	1.59	1.53
15	W	133	LYS	C-N	5.10	1.40	1.33
21	N	415	PHE	CA-C	-5.10	1.46	1.52
28	H	137	ASP	CA-CB	5.10	1.62	1.53
30	K	382	VAL	CA-C	-5.10	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	72	TYR	C-N	5.10	1.40	1.33
30	K	288	SER	CA-C	5.10	1.59	1.52
33	J	73	GLY	N-CA	-5.10	1.40	1.44
5	e	42	THR	CA-C	-5.10	1.46	1.52
8	h	26	ASP	C-N	5.10	1.40	1.33
7	G	104	LYS	CA-C	-5.10	1.46	1.53
15	W	33	VAL	CA-CB	-5.10	1.48	1.54
33	J	54	LYS	N-CA	-5.10	1.40	1.46
5	e	112	LEU	C-N	5.10	1.40	1.33
7	g	231	VAL	CA-C	-5.10	1.46	1.52
11	4	56	PHE	CA-CB	5.10	1.61	1.53
26	U	37	ILE	CA-CB	5.10	1.60	1.54
33	J	121	MET	CA-CB	5.10	1.60	1.53
21	N	438	ASP	CA-C	-5.10	1.46	1.52
28	H	456	LYS	C-N	5.10	1.40	1.33
14	n	43	SER	CA-C	-5.09	1.46	1.52
3	C	8	SER	CA-CB	5.09	1.61	1.53
15	W	36	ILE	N-CA	5.09	1.52	1.46
15	W	193	GLU	CA-CB	5.09	1.61	1.53
23	P	282	HIS	N-CA	-5.09	1.39	1.46
25	R	89	ASN	N-CA	-5.09	1.39	1.46
32	M	18	LEU	CA-C	-5.09	1.46	1.52
14	n	106	GLU	CA-C	-5.09	1.46	1.52
11	4	141	PHE	CA-CB	5.09	1.61	1.53
12	5	144	ARG	CA-C	-5.09	1.46	1.52
14	7	247	VAL	C-O	-5.09	1.19	1.24
21	N	159	GLU	CA-C	-5.09	1.46	1.52
32	M	183	VAL	C-N	5.09	1.38	1.33
24	Q	113	ASP	CA-C	-5.09	1.46	1.52
26	U	143	VAL	C-N	5.09	1.40	1.33
29	I	351	GLU	C-O	-5.09	1.17	1.23
1	a	45	VAL	CA-C	-5.09	1.46	1.52
10	3	21	VAL	N-CA	-5.09	1.40	1.46
19	Y	13	LYS	CA-C	5.09	1.58	1.52
29	I	177	PRO	CA-CB	5.09	1.60	1.53
30	K	189	GLU	N-CA	-5.09	1.40	1.46
10	3	132	GLU	C-N	5.08	1.40	1.33
23	P	282	HIS	C-N	5.08	1.40	1.33
24	Q	343	LEU	CA-CB	5.08	1.61	1.53
32	M	259	GLY	C-N	5.08	1.41	1.33
4	d	91	VAL	CA-CB	-5.08	1.47	1.54
1	A	81	MET	C-N	5.08	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	207	MET	C-N	5.08	1.40	1.33
13	6	141	ARG	N-CA	-5.08	1.39	1.46
21	N	661	SER	N-CA	-5.08	1.39	1.46
24	Q	399	VAL	CA-CB	-5.08	1.47	1.53
30	K	306	PHE	N-CA	-5.08	1.40	1.46
30	K	308	GLN	CA-CB	5.08	1.61	1.53
31	L	124	GLY	N-CA	5.08	1.51	1.44
31	L	365	THR	CB-OG1	-5.08	1.35	1.43
7	G	227	LEU	CA-CB	5.08	1.62	1.53
20	Z	738	TYR	CE1-CZ	5.08	1.50	1.38
24	Q	190	ASN	N-CA	-5.08	1.39	1.46
27	O	344	VAL	N-CA	-5.08	1.39	1.46
28	H	250	GLY	CA-C	5.08	1.59	1.51
6	f	186	PRO	N-CD	5.08	1.54	1.47
32	M	212	ILE	CA-C	-5.08	1.46	1.52
33	J	147	TYR	CA-CB	5.08	1.61	1.53
6	f	207	THR	CA-C	-5.08	1.46	1.52
2	B	109	LEU	N-CA	-5.08	1.40	1.46
9	2	35	VAL	C-N	5.08	1.40	1.33
9	2	97	LEU	C-O	-5.08	1.18	1.24
28	H	156	VAL	CA-CB	5.08	1.60	1.54
30	K	143	SER	CA-C	5.08	1.59	1.52
5	e	174	SER	CA-CB	5.08	1.61	1.53
10	j	108	VAL	N-CA	-5.08	1.40	1.46
3	C	20	TYR	CA-CB	5.08	1.61	1.53
17	T	266	TYR	CG-CD1	5.08	1.50	1.39
29	I	334	LEU	C-O	-5.08	1.17	1.23
1	a	209	HIS	ND1-CE1	5.08	1.37	1.32
3	c	155	GLY	C-N	5.08	1.40	1.33
11	k	50	ALA	C-N	5.08	1.40	1.33
14	n	167	GLY	C-N	5.08	1.39	1.33
17	T	53	ASN	CA-CB	5.08	1.61	1.53
31	L	404	ARG	CZ-NH1	5.08	1.39	1.32
32	M	15	ASP	CA-C	-5.08	1.46	1.52
9	2	189	GLN	CA-CB	5.07	1.61	1.53
16	V	281	SER	CA-C	-5.07	1.46	1.52
21	N	736	PHE	C-N	5.07	1.41	1.33
24	Q	65	TYR	N-CA	-5.07	1.40	1.46
15	W	122	ARG	CZ-NH2	5.07	1.40	1.33
26	U	89	LEU	N-CA	-5.07	1.39	1.46
30	K	349	ARG	C-N	5.07	1.40	1.33
6	f	164	ARG	NE-CZ	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	161	GLU	C-N	5.07	1.41	1.33
13	6	149	ALA	C-N	5.07	1.41	1.33
25	R	334	ARG	NE-CZ	5.07	1.38	1.33
30	K	344	ARG	NE-CZ	5.07	1.38	1.33
2	B	222	LEU	CA-CB	5.07	1.61	1.53
23	P	26	SER	CA-C	-5.07	1.46	1.52
23	P	33	ASN	C-N	5.07	1.40	1.33
24	Q	384	LYS	CA-CB	5.07	1.60	1.53
28	H	420	ARG	CZ-NH1	5.07	1.39	1.32
30	K	346	ARG	NE-CZ	5.07	1.38	1.33
33	J	204	HIS	CA-CB	5.07	1.61	1.53
10	j	196	VAL	CA-CB	-5.07	1.48	1.54
11	4	109	LYS	N-CA	-5.07	1.39	1.46
12	5	273	TRP	N-CA	-5.07	1.40	1.46
13	6	16	ASN	CA-C	-5.07	1.46	1.53
28	H	176	VAL	CA-C	-5.07	1.46	1.52
28	H	261	ARG	NE-CZ	5.07	1.38	1.33
28	H	390	ARG	CD-NE	5.07	1.53	1.46
30	K	377	SER	N-CA	5.07	1.51	1.46
31	L	388	GLY	C-N	5.07	1.41	1.33
6	f	122	SER	CA-CB	5.06	1.61	1.53
21	N	180	SER	N-CA	-5.06	1.40	1.46
3	c	206	LEU	CA-C	-5.06	1.46	1.52
6	f	18	ARG	NE-CZ	5.06	1.38	1.33
12	l	81	PHE	C-N	5.06	1.40	1.33
5	E	226	ASP	CA-CB	5.06	1.62	1.53
22	S	315	LYS	CA-C	-5.06	1.46	1.52
27	O	355	PRO	CA-C	-5.06	1.46	1.52
13	m	19	THR	N-CA	-5.06	1.39	1.46
22	S	135	ASN	CA-C	-5.06	1.46	1.52
24	Q	286	TYR	CA-C	5.06	1.59	1.52
5	e	65	GLU	N-CA	-5.06	1.39	1.46
8	h	135	ILE	CB-CG1	5.06	1.63	1.53
3	C	229	ILE	C-N	5.06	1.40	1.33
13	6	221	ARG	CZ-NH2	5.06	1.40	1.33
21	N	124	TYR	CA-C	-5.06	1.45	1.52
29	I	233	ALA	CA-CB	5.06	1.61	1.53
4	D	97	ARG	CD-NE	5.06	1.53	1.46
18	X	34	GLU	CA-CB	5.06	1.61	1.53
32	M	425	ARG	CD-NE	5.06	1.53	1.46
14	n	45	ILE	C-N	5.06	1.39	1.33
24	Q	220	LEU	N-CA	-5.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	246	ARG	NE-CZ	5.06	1.38	1.33
2	b	150	VAL	CA-CB	-5.05	1.47	1.54
3	c	134	SER	CA-C	-5.05	1.46	1.52
5	e	17	PRO	N-CA	-5.05	1.40	1.47
12	5	159	SER	N-CA	5.05	1.52	1.46
26	U	3	LEU	C-N	5.05	1.40	1.33
30	K	388	GLN	CA-CB	5.05	1.61	1.53
14	n	229	SER	N-CA	-5.05	1.39	1.45
1	a	62	LYS	CA-CB	5.05	1.62	1.53
14	n	246	GLN	CA-C	-5.05	1.46	1.52
13	6	187	GLU	N-CA	-5.05	1.40	1.46
21	N	219	ASN	C-N	5.05	1.40	1.33
28	H	168	ILE	CA-C	-5.05	1.46	1.52
3	c	228	LYS	C-N	5.05	1.39	1.33
15	W	124	GLU	CA-C	-5.05	1.46	1.52
30	K	117	SER	CA-CB	5.05	1.60	1.53
30	K	251	PRO	C-N	5.05	1.41	1.34
31	L	344	ASP	CA-C	-5.05	1.46	1.52
13	m	160	ASN	N-CA	-5.05	1.39	1.46
22	S	438	HIS	CG-ND1	5.05	1.43	1.38
33	J	16	GLU	C-N	5.05	1.40	1.33
13	m	104	LEU	N-CA	-5.05	1.40	1.46
4	D	120	TYR	CA-CB	5.05	1.61	1.53
7	G	40	ILE	C-N	5.05	1.40	1.33
17	T	257	THR	N-CA	5.05	1.52	1.46
24	Q	339	TYR	CE2-CZ	5.05	1.50	1.38
25	R	401	HIS	ND1-CE1	5.05	1.37	1.32
33	J	259	GLU	N-CA	-5.05	1.40	1.46
3	C	231	LYS	N-CA	-5.04	1.38	1.45
2	b	178	ARG	NE-CZ	5.04	1.38	1.33
6	f	144	LEU	C-N	5.04	1.40	1.33
10	j	16	THR	C-N	5.04	1.40	1.33
14	n	161	ARG	CZ-NH1	5.04	1.39	1.32
1	A	18	ILE	CA-CB	5.04	1.59	1.54
11	4	95	ARG	CD-NE	5.04	1.53	1.46
12	5	215	LEU	CA-CB	5.04	1.61	1.53
26	U	242	PRO	CA-C	5.04	1.61	1.52
28	H	373	ARG	C-N	5.04	1.40	1.33
30	K	235	ILE	CB-CG1	5.04	1.63	1.53
4	d	151	GLU	CA-CB	-5.04	1.47	1.54
3	C	196	THR	CA-CB	5.04	1.61	1.53
11	4	41	HIS	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	416	LYS	C-N	5.04	1.40	1.33
26	U	32	ARG	CZ-NH2	5.04	1.40	1.33
26	U	33	CYS	C-N	5.04	1.40	1.33
27	O	306	ARG	C-O	-5.04	1.18	1.24
28	H	225	VAL	CA-C	-5.04	1.46	1.52
30	K	95	VAL	C-N	5.04	1.40	1.33
32	M	158	THR	C-N	5.04	1.39	1.32
10	3	49	VAL	CA-C	-5.04	1.46	1.52
21	N	651	PHE	C-N	5.04	1.40	1.33
24	Q	211	PRO	N-CD	-5.04	1.40	1.47
27	O	24	PRO	C-N	5.04	1.40	1.33
2	b	8	SER	CA-CB	5.04	1.61	1.53
3	c	188	ASP	N-CA	-5.04	1.39	1.46
7	g	196	ALA	C-O	-5.04	1.17	1.24
5	E	239	LEU	N-CA	-5.04	1.39	1.46
19	Y	6	ALA	N-CA	-5.04	1.40	1.46
22	S	406	ASP	C-N	-5.04	1.27	1.33
7	G	185	GLU	C-N	5.04	1.40	1.33
17	T	51	TYR	CE1-CZ	5.04	1.50	1.38
26	U	219	LEU	CA-C	-5.04	1.46	1.53
3	C	212	GLU	C-N	5.04	1.39	1.33
5	E	130	GLU	N-CA	-5.04	1.39	1.45
6	F	56	LEU	N-CA	-5.04	1.39	1.46
9	2	187	ALA	CA-C	-5.04	1.46	1.52
14	7	213	ALA	N-CA	-5.04	1.39	1.46
16	V	216	LEU	C-N	5.04	1.39	1.33
21	N	365	PHE	CA-CB	5.04	1.61	1.53
27	O	302	VAL	CA-CB	-5.04	1.47	1.54
4	d	213	THR	C-N	5.03	1.40	1.33
10	j	135	ASP	CA-C	-5.03	1.46	1.52
1	A	200	GLU	CA-CB	5.03	1.61	1.53
3	C	90	THR	CB-OG1	-5.03	1.35	1.43
8	1	30	THR	CA-C	-5.03	1.46	1.52
21	N	40	SER	N-CA	-5.03	1.39	1.46
21	N	236	GLY	C-N	5.03	1.40	1.33
1	a	83	VAL	C-N	5.03	1.40	1.33
28	H	184	GLU	N-CA	-5.03	1.40	1.46
33	J	362	CYS	C-N	5.03	1.40	1.33
5	e	107	ILE	N-CA	-5.03	1.40	1.46
3	C	18	ARG	CZ-NH1	5.03	1.39	1.32
12	5	134	LEU	CA-C	-5.03	1.46	1.52
27	O	272	VAL	N-CA	-5.03	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	194	SER	CA-C	-5.03	1.46	1.52
29	I	204	HIS	ND1-CE1	5.03	1.37	1.32
30	K	185	ARG	NE-CZ	5.03	1.38	1.33
4	d	74	SER	N-CA	5.03	1.51	1.45
3	C	60	ASP	N-CA	-5.03	1.39	1.45
6	F	176	LEU	CA-CB	5.03	1.61	1.53
17	T	267	ALA	C-N	-5.03	1.28	1.34
31	L	280	MET	C-N	5.03	1.40	1.33
3	c	119	LYS	CA-CB	5.03	1.61	1.53
1	A	233	PHE	CA-C	-5.03	1.46	1.52
7	G	82	ILE	CA-C	5.03	1.57	1.52
11	4	14	ILE	N-CA	-5.03	1.40	1.46
20	Z	255	LEU	CA-CB	-5.03	1.45	1.53
21	N	109	TYR	N-CA	-5.03	1.40	1.46
21	N	741	TYR	C-N	5.03	1.40	1.33
21	N	754	THR	CA-C	-5.03	1.47	1.53
25	R	23	ASN	C-O	-5.03	1.18	1.24
31	L	262	ILE	C-N	5.03	1.40	1.33
7	g	107	ILE	N-CA	-5.03	1.40	1.46
11	k	107	TYR	N-CA	-5.03	1.40	1.46
5	E	139	GLY	C-N	-5.03	1.27	1.33
16	V	228	TYR	CA-C	-5.03	1.46	1.52
19	Y	69	VAL	N-CA	-5.03	1.40	1.46
6	f	206	LEU	CA-CB	5.02	1.61	1.53
10	j	102	PRO	CA-C	-5.02	1.46	1.52
5	E	9	ASP	N-CA	-5.02	1.39	1.46
5	E	41	ALA	N-CA	-5.02	1.39	1.46
6	F	42	THR	CA-CB	5.02	1.61	1.53
14	7	200	LYS	C-N	5.02	1.40	1.33
21	N	612	SER	C-N	5.02	1.40	1.33
24	Q	41	ALA	C-O	5.02	1.30	1.24
27	O	33	TYR	N-CA	5.02	1.52	1.46
27	O	124	ASP	CA-CB	5.02	1.61	1.53
32	M	27	THR	CA-C	-5.02	1.46	1.52
32	M	97	SER	C-N	5.02	1.40	1.33
9	i	246	ILE	N-CA	5.02	1.52	1.46
13	m	28	PHE	C-N	5.02	1.39	1.33
1	A	212	ASP	CA-C	-5.02	1.46	1.52
3	C	92	ARG	N-CA	-5.02	1.39	1.46
25	R	28	GLU	N-CA	-5.02	1.40	1.46
26	U	126	LYS	CA-C	-5.02	1.46	1.52
30	K	121	ARG	NE-CZ	5.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	111	GLN	CA-CB	5.02	1.60	1.53
4	d	29	ARG	CD-NE	5.02	1.53	1.46
4	d	71	VAL	N-CA	5.02	1.51	1.46
2	B	214	ILE	C-N	5.02	1.40	1.33
3	C	213	PHE	N-CA	-5.02	1.39	1.45
6	F	161	ILE	N-CA	-5.02	1.40	1.46
10	3	58	THR	N-CA	-5.02	1.40	1.46
19	Y	60	TRP	N-CA	5.02	1.51	1.45
30	K	338	ILE	CA-C	-5.02	1.47	1.52
30	K	417	THR	N-CA	-5.02	1.39	1.46
12	l	150	SER	C-N	5.02	1.40	1.33
4	D	229	ILE	C-N	5.02	1.40	1.33
17	T	94	HIS	ND1-CE1	5.02	1.37	1.32
24	Q	208	ILE	CA-C	-5.02	1.46	1.52
25	R	156	LYS	N-CA	-5.02	1.39	1.46
12	5	114	PRO	C-N	5.01	1.41	1.33
15	W	173	THR	CA-C	-5.01	1.46	1.52
30	K	136	SER	C-N	5.01	1.38	1.33
13	m	28	PHE	CA-CB	5.01	1.62	1.53
6	F	196	ALA	C-N	5.01	1.39	1.33
13	6	197	THR	C-N	5.01	1.40	1.34
3	C	53	THR	N-CA	-5.01	1.39	1.46
9	2	213	ALA	CA-C	-5.01	1.46	1.52
21	N	16	ASN	C-N	5.01	1.40	1.33
22	S	53	ILE	C-N	5.01	1.40	1.33
25	R	71	LEU	CA-CB	5.01	1.61	1.53
33	J	280	ASP	CA-C	-5.01	1.46	1.52
2	b	30	GLN	CA-CB	5.01	1.61	1.53
13	m	57	ASN	CG-ND2	5.01	1.43	1.33
5	E	204	LEU	N-CA	-5.01	1.40	1.46
21	N	448	LEU	CA-C	-5.01	1.46	1.52
22	S	100	HIS	CE1-NE2	-5.01	1.27	1.32
14	n	103	LEU	CA-C	5.01	1.59	1.52
16	V	196	TYR	CA-CB	5.01	1.61	1.53
21	N	273	LEU	C-N	5.01	1.40	1.33
3	c	178	MET	N-CA	-5.01	1.40	1.46
23	P	252	SER	C-O	5.00	1.30	1.24
33	J	112	ARG	CD-NE	5.00	1.53	1.46
33	J	117	SER	CA-CB	5.00	1.59	1.52
6	F	99	PHE	C-N	5.00	1.40	1.33
8	1	110	GLY	CA-C	-5.00	1.46	1.51
18	X	87	PHE	CA-C	-5.00	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	120	GLU	N-CA	-5.00	1.40	1.46
25	R	210	TYR	CA-CB	5.00	1.61	1.53
27	O	172	TYR	CZ-OH	5.00	1.48	1.38
9	i	224	VAL	CA-C	5.00	1.59	1.52
23	P	233	GLU	CA-C	-5.00	1.46	1.52
23	P	259	PRO	N-CA	-5.00	1.41	1.47
27	O	162	SER	C-N	5.00	1.39	1.33
33	J	56	ARG	CZ-NH1	5.00	1.39	1.32

All (7309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	748	LEU	CB-CA-C	32.94	173.91	110.67
28	H	272	ILE	O-C-N	-29.48	91.97	122.92
20	Z	747	ALA	CA-C-O	-29.37	89.98	120.82
20	Z	748	LEU	N-CA-CB	-26.93	68.54	110.28
29	I	315	GLY	O-C-N	-16.81	107.63	122.92
7	g	81	LEU	CA-C-N	16.55	130.67	120.24
7	g	81	LEU	C-N-CA	16.55	130.67	120.24
29	I	316	PHE	N-CA-CB	15.32	132.22	110.01
20	Z	747	ALA	CA-C-N	14.85	142.88	120.31
20	Z	747	ALA	C-N-CA	14.85	142.88	120.31
3	c	182	ASP	CA-CB-CG	-14.72	97.88	112.60
19	Y	36	GLU	N-CA-C	-14.35	96.33	114.56
3	C	244	ILE	N-CA-C	-13.98	100.58	111.90
20	Z	728	LYS	CB-CG-CD	13.42	142.16	111.30
20	Z	728	LYS	CA-CB-CG	13.23	140.56	114.10
29	I	316	PHE	CB-CA-C	-13.05	90.39	110.88
33	J	301	ASP	CA-C-N	12.41	132.22	119.56
33	J	301	ASP	C-N-CA	12.41	132.22	119.56
21	N	841	THR	CA-C-O	12.24	127.02	119.55
29	I	151	HIS	N-CA-C	11.94	123.85	111.07
22	S	399	TYR	CA-C-N	11.93	136.40	120.65
22	S	399	TYR	C-N-CA	11.93	136.40	120.65
20	Z	728	LYS	CB-CA-C	11.69	133.69	110.42
31	L	233	LYS	N-CA-C	-11.69	99.12	113.50
27	O	229	ASN	N-CA-C	-11.66	99.39	112.57
31	L	246	SER	CA-C-N	11.65	131.79	119.90
31	L	246	SER	C-N-CA	11.65	131.79	119.90
14	7	121	GLU	N-CA-C	-11.50	90.62	108.55
1	A	86	PRO	CA-C-N	11.41	129.45	120.33
1	A	86	PRO	C-N-CA	11.41	129.45	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	154	GLN	OE1-CD-NE2	11.37	133.97	122.60
8	1	138	SER	N-CA-C	-11.16	99.79	113.41
23	P	319	GLU	CA-C-O	-10.99	108.24	118.79
14	7	197	ASP	CA-C-N	10.96	129.10	120.33
14	7	197	ASP	C-N-CA	10.96	129.10	120.33
27	O	326	HIS	CA-CB-CG	-10.94	102.86	113.80
28	H	272	ILE	CA-C-N	-10.94	100.65	121.54
28	H	272	ILE	C-N-CA	-10.94	100.65	121.54
1	A	38	THR	N-CA-C	-10.91	100.23	114.31
10	j	29	LEU	CA-C-N	10.88	129.05	121.65
10	j	29	LEU	C-N-CA	10.88	129.05	121.65
1	A	218	PHE	CA-CB-CG	-10.87	102.93	113.80
7	g	130	ARG	CA-C-N	10.81	130.59	120.21
7	g	130	ARG	C-N-CA	10.81	130.59	120.21
10	j	100	PHE	CA-CB-CG	-10.68	103.12	113.80
13	6	109	ARG	N-CA-C	-10.67	98.42	114.64
5	E	163	THR	CA-C-N	10.61	136.22	121.05
5	E	163	THR	C-N-CA	10.61	136.22	121.05
14	7	182	HIS	N-CA-C	-10.61	100.47	113.41
3	C	81	THR	N-CA-C	-10.59	100.09	113.23
7	g	105	THR	O-C-N	-10.59	114.44	121.85
23	P	130	ILE	N-CA-C	10.59	121.42	110.62
20	Z	748	LEU	O-C-N	-10.57	109.27	122.27
10	j	33	SER	N-CA-C	-10.45	101.29	114.56
5	E	148	ASP	N-CA-C	-10.44	93.96	110.14
2	B	10	THR	N-CA-C	-10.42	99.32	113.18
21	N	61	ALA	CA-C-N	10.37	133.92	120.44
21	N	61	ALA	C-N-CA	10.37	133.92	120.44
32	M	394	VAL	N-CA-C	-10.37	100.59	111.58
21	N	416	GLY	CA-C-N	10.35	134.15	120.28
21	N	416	GLY	C-N-CA	10.35	134.15	120.28
2	b	51	SER	CA-C-N	10.31	141.22	121.54
2	b	51	SER	C-N-CA	10.31	141.22	121.54
7	G	111	ALA	CA-C-O	10.30	131.64	120.82
5	E	15	PHE	CA-CB-CG	-10.28	103.52	113.80
30	K	277	ILE	N-CA-C	-10.23	100.73	111.58
13	6	95	ASN	O-C-N	-10.22	109.70	122.27
13	m	160	ASN	CA-CB-CG	-10.21	102.39	112.60
29	I	165	ASP	CA-CB-CG	-10.20	102.40	112.60
13	6	125	ASP	CA-CB-CG	-10.18	102.42	112.60
22	S	70	ASN	N-CA-C	-10.18	103.02	114.62
2	b	10	THR	N-CA-C	-10.14	101.46	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	408	SER	N-CA-C	-10.14	97.58	111.87
8	1	98	ASN	CA-CB-CG	-10.12	102.47	112.60
15	W	116	SER	CA-C-O	-10.12	109.07	119.49
24	Q	370	THR	CA-C-N	10.11	133.83	120.28
24	Q	370	THR	C-N-CA	10.11	133.83	120.28
13	6	203	HIS	CA-CB-CG	10.11	123.91	113.80
33	J	131	ASP	CA-CB-CG	-10.11	102.49	112.60
7	G	16	SER	N-CA-CB	10.10	120.91	109.49
13	6	125	ASP	N-CA-C	-10.06	100.64	113.72
2	b	100	ILE	N-CA-C	-10.03	102.90	112.83
24	Q	254	SER	CA-C-N	10.04	134.54	120.29
24	Q	254	SER	C-N-CA	10.04	134.54	120.29
29	I	259	ASP	CA-CB-CG	10.01	122.61	112.60
27	O	64	ASN	CA-CB-CG	-10.00	102.60	112.60
25	R	115	GLU	CA-C-N	9.98	133.42	120.44
25	R	115	GLU	C-N-CA	9.98	133.42	120.44
8	h	116	LYS	CA-C-N	9.96	129.81	120.34
8	h	116	LYS	C-N-CA	9.96	129.81	120.34
21	N	510	HIS	CA-C-N	9.96	130.95	120.00
21	N	510	HIS	C-N-CA	9.96	130.95	120.00
23	P	286	ASN	CA-C-N	9.96	134.85	120.71
23	P	286	ASN	C-N-CA	9.96	134.85	120.71
22	S	207	ASN	CA-CB-CG	9.94	122.53	112.60
12	l	222	ASP	N-CA-CB	9.93	126.00	110.21
20	Z	747	ALA	N-CA-C	9.89	121.65	111.07
14	n	219	TYR	N-CA-C	9.86	121.62	111.07
20	Z	245	VAL	N-CA-C	9.86	119.89	110.42
25	R	383	ARG	NE-CZ-NH1	9.85	131.35	121.50
26	U	283	ARG	CA-C-N	9.82	133.20	120.44
26	U	283	ARG	C-N-CA	9.82	133.20	120.44
6	f	5	ASN	N-CA-C	-9.80	98.91	114.09
6	F	188	GLU	CA-C-O	-9.78	110.06	120.42
12	l	150	SER	CA-C-N	9.75	133.81	120.46
12	l	150	SER	C-N-CA	9.75	133.81	120.46
4	D	207	ALA	N-CA-C	-9.74	98.99	114.09
30	K	130	LEU	N-CA-C	-9.73	102.49	114.75
21	N	654	GLN	OE1-CD-NE2	9.71	132.31	122.60
21	N	534	ASP	CA-C-N	9.70	134.06	120.29
21	N	534	ASP	C-N-CA	9.70	134.06	120.29
24	Q	48	ASP	CA-CB-CG	-9.70	102.90	112.60
16	V	291	ASN	CA-CB-CG	-9.68	102.92	112.60
4	d	63	LYS	N-CA-C	-9.67	101.17	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	274	GLN	N-CA-CB	9.66	125.18	114.17
17	T	7	LEU	CA-C-N	9.65	132.98	120.44
17	T	7	LEU	C-N-CA	9.65	132.98	120.44
3	c	7	ASP	N-CA-C	-9.62	101.70	113.15
4	d	128	PRO	CA-C-N	9.60	134.93	120.82
4	d	128	PRO	C-N-CA	9.60	134.93	120.82
2	B	12	PHE	CA-CB-CG	-9.59	104.21	113.80
25	R	310	GLU	CA-C-N	9.57	133.10	120.28
25	R	310	GLU	C-N-CA	9.57	133.10	120.28
2	b	25	LEU	CA-C-N	9.56	133.09	120.28
2	b	25	LEU	C-N-CA	9.56	133.09	120.28
8	h	156	SER	CA-C-N	9.55	133.08	120.28
8	h	156	SER	C-N-CA	9.55	133.08	120.28
22	S	279	ILE	CA-C-N	9.55	132.86	120.44
22	S	279	ILE	C-N-CA	9.55	132.86	120.44
13	m	152	SER	CA-C-N	9.54	132.85	120.44
13	m	152	SER	C-N-CA	9.54	132.85	120.44
21	N	822	GLY	O-C-N	-9.54	117.64	121.07
32	M	366	ARG	N-CA-CB	-9.54	99.39	110.35
28	H	48	LYS	CA-C-N	9.52	133.80	120.29
28	H	48	LYS	C-N-CA	9.52	133.80	120.29
9	2	59	ASN	CA-CB-CG	-9.50	103.10	112.60
23	P	275	ASN	CA-C-N	9.49	133.00	120.28
23	P	275	ASN	C-N-CA	9.49	133.00	120.28
22	S	483	GLU	CA-C-N	9.49	133.76	120.29
22	S	483	GLU	C-N-CA	9.49	133.76	120.29
20	Z	738	TYR	CE1-CZ-CE2	-9.48	101.33	120.30
3	C	136	ILE	N-CA-C	-9.48	94.15	107.99
2	b	21	ILE	N-CA-C	-9.44	101.66	110.82
25	R	27	SER	CA-C-N	9.44	132.93	120.28
25	R	27	SER	C-N-CA	9.44	132.93	120.28
31	L	128	ILE	N-CA-C	-9.43	94.97	108.17
7	G	82	ILE	N-CA-CB	9.43	117.80	110.45
2	b	133	SER	CA-C-O	-9.43	110.18	120.36
4	D	142	ASP	CA-CB-CG	-9.40	103.20	112.60
20	Z	206	ASP	CA-CB-CG	-9.40	103.20	112.60
1	A	186	PHE	CA-CB-CG	-9.39	104.41	113.80
28	H	129	SER	N-CA-C	-9.38	101.84	113.38
27	O	235	HIS	CB-CG-CD2	-9.35	119.04	131.20
18	X	72	GLU	N-CA-C	-9.35	102.45	114.04
14	n	76	ILE	N-CA-C	-9.34	97.08	107.73
16	V	205	LYS	CA-C-O	-9.33	110.62	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	241	GLU	N-CA-C	-9.30	101.19	114.12
32	M	173	ASP	CA-CB-CG	9.29	121.89	112.60
29	I	403	ALA	CA-C-N	9.29	133.65	120.28
29	I	403	ALA	C-N-CA	9.29	133.65	120.28
33	J	163	VAL	CA-C-N	-9.26	113.73	123.08
33	J	163	VAL	C-N-CA	-9.26	113.73	123.08
17	T	124	SER	CA-C-N	9.24	133.41	120.29
17	T	124	SER	C-N-CA	9.24	133.41	120.29
6	f	182	ILE	N-CA-CB	9.22	121.05	110.82
25	R	214	TYR	CA-C-N	9.22	130.41	119.99
25	R	214	TYR	C-N-CA	9.22	130.41	119.99
7	G	15	PHE	CA-CB-CG	-9.21	104.59	113.80
25	R	187	VAL	CA-C-N	9.21	133.59	120.79
25	R	187	VAL	C-N-CA	9.21	133.59	120.79
23	P	70	ASN	CA-CB-CG	9.20	121.80	112.60
8	1	34	TYR	N-CA-C	-9.17	94.23	109.46
31	L	54	ASN	OD1-CG-ND2	9.16	131.76	122.60
19	Y	10	ALA	N-CA-C	9.14	121.32	111.36
1	A	231	ASP	CA-CB-CG	-9.11	103.49	112.60
9	2	190	ALA	CA-C-N	9.11	130.28	119.99
9	2	190	ALA	C-N-CA	9.11	130.28	119.99
15	W	100	HIS	ND1-CE1-NE2	9.10	117.50	108.40
12	5	200	ASP	N-CA-C	-9.10	103.01	114.56
6	F	153	VAL	N-CA-C	-9.09	95.03	108.12
33	J	391	ASN	CA-C-N	9.09	132.46	120.28
33	J	391	ASN	C-N-CA	9.09	132.46	120.28
9	i	200	SER	CB-CA-C	-9.09	104.87	117.23
19	Y	65	ASP	CA-CB-CG	-9.09	103.51	112.60
23	P	385	ASN	OD1-CG-ND2	-9.09	113.52	122.60
24	Q	334	HIS	CA-CB-CG	-9.08	104.72	113.80
13	6	166	ASN	OD1-CG-ND2	9.08	131.68	122.60
2	b	105	PRO	CB-CA-C	-9.07	102.64	111.17
21	N	880	ARG	NE-CZ-NH2	-9.06	111.04	119.20
12	l	201	ILE	CA-C-O	-9.05	110.53	120.67
29	I	95	GLN	CA-C-N	9.05	132.75	120.54
29	I	95	GLN	C-N-CA	9.05	132.75	120.54
22	S	145	PHE	CA-CB-CG	-9.04	104.76	113.80
24	Q	212	THR	CA-C-O	9.03	130.38	120.63
28	H	343	PHE	CA-CB-CG	-9.03	104.77	113.80
1	a	77	ARG	CA-C-O	-9.03	111.40	120.70
2	B	70	ASP	N-CA-C	-9.03	102.40	113.50
24	Q	190	ASN	CA-CB-CG	9.02	121.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	37	ASN	OD1-CG-ND2	9.02	131.62	122.60
13	m	56	ASP	CA-CB-CG	-9.01	103.59	112.60
7	g	62	GLN	O-C-N	9.01	132.85	122.67
33	J	284	THR	N-CA-CB	8.99	125.68	110.49
15	W	78	ASP	CA-CB-CG	-8.99	103.61	112.60
2	B	187	ASP	CA-CB-CG	-8.98	103.62	112.60
14	7	198	ILE	O-C-N	-8.97	114.68	120.42
29	I	316	PHE	O-C-N	8.97	131.31	122.07
22	S	259	TYR	O-C-N	-8.96	113.32	121.30
7	g	182	HIS	ND1-CE1-NE2	8.96	117.36	108.40
8	h	92	LYS	CA-C-O	-8.96	111.31	120.90
31	L	71	ASP	CA-CB-CG	8.94	121.54	112.60
25	R	315	VAL	N-CA-CB	8.94	118.97	111.64
20	Z	250	VAL	N-CA-C	8.93	119.74	110.72
27	O	23	HIS	CE1-NE2-CD2	-8.93	100.07	109.00
23	P	190	LYS	CA-C-O	8.92	130.18	120.10
28	H	212	GLY	CA-C-N	8.92	135.19	121.45
28	H	212	GLY	C-N-CA	8.92	135.19	121.45
1	a	61	ASP	CA-CB-CG	-8.91	103.69	112.60
21	N	340	HIS	ND1-CE1-NE2	8.91	117.31	108.40
22	S	437	ASN	CA-CB-CG	-8.89	103.71	112.60
30	K	101	GLU	N-CA-CB	8.89	119.63	111.27
15	W	153	LEU	N-CA-C	-8.89	101.51	111.82
21	N	138	GLU	CA-C-O	-8.89	111.13	120.55
5	e	133	LEU	N-CA-C	-8.89	103.02	114.04
14	7	197	ASP	CA-CB-CG	-8.88	103.72	112.60
1	A	193	HIS	CG-CD2-NE2	8.88	116.08	107.20
2	B	239	THR	CA-C-N	8.88	132.18	120.28
2	B	239	THR	C-N-CA	8.88	132.18	120.28
3	c	60	ASP	CA-CB-CG	-8.87	103.73	112.60
21	N	546	LEU	CA-C-N	8.87	132.88	120.29
21	N	546	LEU	C-N-CA	8.87	132.88	120.29
30	K	148	ASP	CA-CB-CG	8.86	121.46	112.60
13	6	227	LEU	CA-C-N	8.86	133.72	121.05
13	6	227	LEU	C-N-CA	8.86	133.72	121.05
21	N	84	ALA	CA-C-N	8.86	132.87	120.29
21	N	84	ALA	C-N-CA	8.86	132.87	120.29
21	N	728	LYS	CA-C-N	8.86	132.49	120.44
21	N	728	LYS	C-N-CA	8.86	132.49	120.44
6	F	220	THR	CA-C-N	8.82	130.87	119.84
6	F	220	THR	C-N-CA	8.82	130.87	119.84
6	f	87	TYR	N-CA-C	-8.81	101.75	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	205	SER	CA-C-N	8.80	133.24	120.82
6	f	205	SER	C-N-CA	8.80	133.24	120.82
25	R	417	TYR	N-CA-C	-8.80	101.77	111.36
29	I	232	LEU	N-CA-CB	8.79	123.05	110.12
21	N	681	ASN	CA-C-O	8.79	129.87	120.55
21	N	324	LYS	N-CA-C	-8.79	102.58	113.38
27	O	246	SER	CA-C-N	8.77	132.03	120.28
27	O	246	SER	C-N-CA	8.77	132.03	120.28
13	6	115	VAL	CA-C-O	8.75	130.26	120.90
21	N	653	ARG	NE-CZ-NH2	-8.75	111.32	119.20
26	U	211	LEU	CA-C-N	8.75	131.81	120.44
26	U	211	LEU	C-N-CA	8.75	131.81	120.44
21	N	326	SER	CA-C-N	8.75	132.71	120.29
5	e	52	LYS	CA-C-O	-8.75	111.36	121.68
3	C	10	THR	N-CA-C	8.75	123.25	112.23
21	N	326	SER	C-N-CA	8.75	132.71	120.29
13	m	143	GLN	N-CA-C	-8.74	103.13	113.88
27	O	286	PHE	N-CA-C	8.74	120.81	111.28
11	4	172	MET	O-C-N	-8.73	113.62	121.39
22	S	244	ASN	CA-CB-CG	-8.73	103.87	112.60
32	M	233	ARG	CA-C-N	8.73	132.69	120.29
32	M	233	ARG	C-N-CA	8.73	132.69	120.29
17	T	81	TYR	CA-C-N	8.72	131.97	120.28
17	T	81	TYR	C-N-CA	8.72	131.97	120.28
32	M	245	LYS	CA-C-O	8.72	129.56	120.40
4	d	66	LYS	CA-C-N	8.72	131.55	120.56
4	d	66	LYS	C-N-CA	8.72	131.55	120.56
7	g	84	ASP	N-CA-C	-8.71	101.86	111.36
16	V	225	LEU	N-CA-C	-8.71	100.34	112.45
18	X	36	LYS	O-C-N	-8.71	116.14	121.71
10	j	44	PHE	CA-CB-CG	-8.71	105.09	113.80
7	g	142	ASP	N-CA-CB	8.70	126.44	110.86
4	D	106	VAL	CA-C-N	8.70	132.65	120.29
4	D	106	VAL	C-N-CA	8.70	132.65	120.29
5	E	223	THR	O-C-N	-8.69	113.14	123.31
26	U	117	ASN	N-CA-C	-8.69	98.86	109.72
17	T	240	LYS	CA-C-N	8.68	131.91	120.28
17	T	240	LYS	C-N-CA	8.68	131.91	120.28
11	4	64	ILE	CA-C-N	8.68	131.91	120.28
11	4	64	ILE	C-N-CA	8.68	131.91	120.28
23	P	58	VAL	N-CA-C	-8.68	102.37	110.53
23	P	263	HIS	CE1-NE2-CD2	-8.68	100.32	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	232	VAL	CA-C-N	8.65	133.47	120.31
25	R	232	VAL	C-N-CA	8.65	133.47	120.31
10	j	3	ASP	CA-CB-CG	-8.65	103.95	112.60
16	V	79	SER	CA-C-N	8.64	134.13	120.47
16	V	79	SER	C-N-CA	8.64	134.13	120.47
28	H	431	ILE	N-CA-CB	8.63	120.65	110.55
10	3	59	ASP	CA-CB-CG	-8.62	103.98	112.60
23	P	263	HIS	ND1-CE1-NE2	8.62	117.02	108.40
23	P	413	ASN	OD1-CG-ND2	8.62	131.22	122.60
22	S	79	ASN	OD1-CG-ND2	-8.61	113.99	122.60
29	I	150	HIS	CA-CB-CG	8.61	122.41	113.80
21	N	448	LEU	CA-C-N	8.61	129.32	119.94
21	N	448	LEU	C-N-CA	8.61	129.32	119.94
20	Z	253	VAL	N-CA-CB	8.60	117.16	110.45
1	a	84	ASN	N-CA-C	-8.60	95.38	109.40
1	a	113	PRO	N-CA-C	8.59	124.77	111.11
23	P	230	HIS	CE1-NE2-CD2	-8.59	100.41	109.00
21	N	849	THR	N-CA-C	-8.59	95.51	108.99
17	T	137	GLU	N-CA-C	-8.58	101.80	113.30
16	V	109	HIS	CA-CB-CG	8.58	122.38	113.80
7	G	50	VAL	CA-C-N	8.55	133.96	122.84
7	G	50	VAL	C-N-CA	8.55	133.96	122.84
28	H	111	GLU	N-CA-C	-8.54	103.45	114.04
13	6	218	ASP	N-CA-C	-8.54	102.41	113.17
22	S	261	HIS	CB-CG-CD2	-8.54	120.10	131.20
9	i	106	VAL	CA-C-N	8.54	132.41	120.29
9	i	106	VAL	C-N-CA	8.54	132.41	120.29
13	m	204	ILE	O-C-N	-8.53	113.87	122.14
28	H	339	GLN	OE1-CD-NE2	8.53	131.13	122.60
9	2	238	THR	N-CA-C	-8.52	102.88	113.28
1	a	188	LYS	N-CA-C	8.51	120.64	111.36
9	i	105	VAL	CA-C-N	8.51	132.50	120.42
9	i	105	VAL	C-N-CA	8.51	132.50	120.42
2	B	53	SER	O-C-N	-8.51	112.17	121.53
32	M	378	GLU	CA-C-N	8.50	132.53	120.28
32	M	378	GLU	C-N-CA	8.50	132.53	120.28
7	g	10	LEU	N-CA-CB	8.50	124.85	110.49
13	6	129	ALA	N-CA-C	-8.50	95.33	108.76
1	a	114	CYS	CA-C-N	8.49	131.47	120.44
1	a	114	CYS	C-N-CA	8.49	131.47	120.44
16	V	265	GLU	N-CA-C	8.49	120.53	111.28
7	g	22	PHE	N-CA-C	8.48	120.22	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	630	LYS	CA-C-N	8.48	129.53	120.03
20	Z	630	LYS	C-N-CA	8.48	129.53	120.03
1	A	61	ASP	CA-CB-CG	-8.48	104.12	112.60
21	N	582	ASP	N-CA-C	-8.48	102.04	111.28
24	Q	216	ALA	CA-C-N	8.48	131.97	120.44
24	Q	216	ALA	C-N-CA	8.48	131.97	120.44
28	H	210	ASP	CA-CB-CG	8.48	121.08	112.60
4	d	43	VAL	N-CA-C	-8.47	96.25	108.11
7	g	84	ASP	CA-CB-CG	-8.47	104.13	112.60
4	D	50	SER	CA-C-N	8.47	132.32	120.29
4	D	50	SER	C-N-CA	8.47	132.32	120.29
8	h	95	CYS	N-CA-CB	8.47	122.56	110.12
11	k	64	ILE	O-C-N	8.47	130.21	121.91
6	F	173	GLU	CA-C-N	8.46	131.62	120.28
6	F	173	GLU	C-N-CA	8.46	131.62	120.28
11	4	138	PHE	N-CA-C	-8.46	102.75	113.23
23	P	343	LYS	CA-C-O	-8.45	111.59	120.55
1	a	212	ASP	CA-CB-CG	-8.45	104.15	112.60
9	2	246	ILE	N-CA-C	-8.45	96.31	108.48
14	n	172	SER	CA-C-N	8.45	128.43	119.05
14	n	172	SER	C-N-CA	8.45	128.43	119.05
23	P	30	ASN	CA-C-O	-8.45	111.47	120.42
30	K	262	ARG	CD-NE-CZ	-8.45	112.58	124.40
5	e	205	LYS	CA-C-N	8.44	131.58	120.28
5	e	205	LYS	C-N-CA	8.44	131.58	120.28
26	U	69	ASP	CA-C-N	8.44	131.91	120.44
26	U	69	ASP	C-N-CA	8.44	131.91	120.44
33	J	79	VAL	N-CA-C	-8.44	96.33	108.48
17	T	187	ASP	CA-C-N	8.43	131.39	120.44
17	T	187	ASP	C-N-CA	8.43	131.39	120.44
2	b	105	PRO	N-CA-C	8.42	119.59	110.58
24	Q	212	THR	CA-C-N	8.42	131.39	120.44
24	Q	212	THR	C-N-CA	8.42	131.39	120.44
11	4	151	ASP	CA-CB-CG	-8.42	104.18	112.60
25	R	89	ASN	CA-C-O	-8.41	111.74	121.16
7	G	204	HIS	CG-CD2-NE2	8.41	115.61	107.20
20	Z	253	VAL	CB-CA-C	-8.41	102.98	114.00
11	4	176	PHE	N-CA-C	-8.40	104.16	114.75
10	3	159	GLU	CA-C-O	-8.40	111.19	120.69
29	I	71	LEU	N-CA-CB	8.40	122.25	110.07
26	U	155	LEU	CA-C-O	8.39	129.61	120.71
3	c	42	ASP	CA-CB-CG	-8.39	104.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	192	THR	N-CA-C	-8.39	96.97	109.81
1	a	84	ASN	CA-CB-CG	-8.39	104.21	112.60
13	m	148	GLY	CA-C-N	8.38	131.52	120.28
13	m	148	GLY	C-N-CA	8.38	131.52	120.28
28	H	134	THR	N-CA-CB	8.38	122.57	110.16
13	6	203	HIS	ND1-CE1-NE2	8.38	116.78	108.40
4	d	79	ASN	CA-CB-CG	8.37	120.97	112.60
21	N	638	ILE	CB-CA-C	-8.36	101.18	111.88
1	a	86	PRO	CA-C-N	8.36	127.01	120.33
1	a	86	PRO	C-N-CA	8.36	127.01	120.33
6	F	77	LEU	CA-C-O	8.35	130.41	120.81
25	R	342	LEU	CA-C-N	8.35	131.29	120.44
25	R	342	LEU	C-N-CA	8.35	131.29	120.44
13	m	52	PHE	CA-CB-CG	-8.34	105.46	113.80
31	L	355	ALA	N-CA-C	-8.34	94.99	108.41
2	B	228	PRO	N-CA-C	-8.33	102.60	114.18
28	H	361	LEU	CA-C-N	8.33	131.97	120.39
28	H	361	LEU	C-N-CA	8.33	131.97	120.39
27	O	221	ALA	CA-C-N	8.32	132.11	120.29
27	O	221	ALA	C-N-CA	8.32	132.11	120.29
33	J	219	VAL	N-CA-C	-8.32	104.77	112.43
23	P	87	GLY	N-CA-C	-8.32	104.29	115.36
21	N	163	LEU	N-CA-C	-8.31	103.27	113.41
27	O	343	GLN	N-CA-C	-8.31	103.28	113.50
8	h	61	THR	CA-C-N	8.31	131.24	120.44
8	h	61	THR	C-N-CA	8.31	131.24	120.44
27	O	156	THR	CA-C-N	8.31	131.24	120.44
27	O	156	THR	C-N-CA	8.31	131.24	120.44
7	g	224	THR	N-CA-C	-8.31	101.22	114.09
13	6	209	GLY	O-C-N	-8.30	116.04	123.76
4	d	104	VAL	CA-C-O	-8.30	113.04	121.59
13	6	11	ASN	N-CA-C	-8.29	95.30	109.15
11	4	133	HIS	CE1-NE2-CD2	-8.29	100.71	109.00
25	R	68	GLU	CA-C-O	-8.29	111.76	120.55
31	L	415	LEU	N-CA-C	8.29	119.94	111.07
33	J	168	VAL	CA-C-N	8.28	131.21	120.44
33	J	168	VAL	C-N-CA	8.28	131.21	120.44
8	1	127	SER	N-CA-CB	8.28	117.96	109.51
1	a	212	ASP	N-CA-C	8.28	120.08	111.14
3	C	227	GLN	CB-CA-C	8.28	123.60	110.19
13	m	50	LYS	N-CA-C	-8.28	102.96	113.72
12	5	259	GLY	N-CA-C	-8.28	102.11	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	243	LYS	CA-C-N	8.28	134.84	122.68
14	7	243	LYS	C-N-CA	8.28	134.84	122.68
21	N	373	VAL	CA-C-N	8.28	130.99	120.56
21	N	373	VAL	C-N-CA	8.28	130.99	120.56
32	M	42	ARG	CA-C-N	8.27	132.17	120.42
32	M	42	ARG	C-N-CA	8.27	132.17	120.42
29	I	260	GLY	O-C-N	-8.27	113.50	121.77
6	f	187	ASP	CA-CB-CG	-8.27	104.33	112.60
23	P	94	GLN	CA-C-N	8.27	132.03	120.29
23	P	94	GLN	C-N-CA	8.27	132.03	120.29
21	N	708	ALA	CA-C-O	-8.27	112.06	121.15
4	D	33	ALA	N-CA-C	-8.26	96.02	108.99
32	M	276	THR	N-CA-C	-8.26	96.02	108.99
1	A	87	ILE	CA-C-O	-8.25	113.16	118.69
7	G	40	ILE	N-CA-C	-8.24	95.72	107.75
25	R	270	VAL	CA-C-O	-8.24	111.90	120.14
24	Q	81	SER	N-CA-C	-8.23	103.22	113.18
3	c	143	ARG	NE-CZ-NH1	8.22	129.72	121.50
4	d	118	GLN	OE1-CD-NE2	-8.22	114.38	122.60
3	C	179	ASP	CA-CB-CG	-8.22	104.38	112.60
4	D	94	GLN	CA-C-N	8.22	132.12	120.28
4	D	94	GLN	C-N-CA	8.22	132.12	120.28
24	Q	266	LEU	CA-C-N	8.22	131.30	120.28
24	Q	266	LEU	C-N-CA	8.22	131.30	120.28
23	P	404	LYS	CB-CA-C	8.22	118.31	110.17
10	3	80	ARG	N-CA-CB	8.22	124.37	110.49
6	F	38	LEU	O-C-N	-8.21	114.64	123.26
17	T	188	GLU	CA-C-N	8.21	131.70	120.46
17	T	188	GLU	C-N-CA	8.21	131.70	120.46
24	Q	252	HIS	CA-CB-CG	8.20	122.00	113.80
11	k	167	GLU	CA-C-O	8.20	129.24	120.55
8	h	47	HIS	CA-CB-CG	8.20	122.00	113.80
21	N	686	ILE	O-C-N	8.20	130.28	121.83
28	H	241	ASP	N-CA-C	-8.20	96.85	109.64
10	3	99	ARG	NE-CZ-NH2	8.20	126.58	119.20
15	W	29	GLN	N-CA-C	-8.19	102.54	112.54
18	X	18	ASN	N-CA-C	8.18	121.15	110.43
4	d	184	PRO	N-CA-CB	8.18	107.77	103.19
23	P	104	LEU	CB-CA-C	-8.18	97.22	110.79
11	k	4	ILE	N-CA-C	-8.17	97.56	108.35
1	A	57	LYS	N-CA-C	-8.17	94.94	108.34
18	X	41	GLU	N-CA-C	8.17	122.77	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	63	ASN	CA-CB-CG	-8.16	104.44	112.60
5	E	187	TRP	N-CA-C	-8.15	96.69	108.60
9	i	194	ASN	CA-CB-CG	-8.15	104.45	112.60
4	D	114	ALA	CA-C-N	8.15	128.82	119.94
4	D	114	ALA	C-N-CA	8.15	128.82	119.94
12	5	209	THR	O-C-N	8.15	131.44	122.15
21	N	672	ASN	CA-CB-CG	-8.15	104.45	112.60
5	e	95	ALA	N-CA-C	8.13	120.15	111.28
15	W	99	LYS	N-CA-C	-8.14	103.44	112.72
13	m	70	ASP	CA-CB-CG	-8.13	104.47	112.60
15	W	163	ASN	CA-CB-CG	8.13	120.73	112.60
17	T	230	ASN	CA-CB-CG	8.13	120.73	112.60
14	n	185	ASN	CA-C-N	8.13	128.90	119.47
14	n	185	ASN	C-N-CA	8.13	128.90	119.47
10	3	19	ASP	N-CA-CB	8.13	124.23	110.49
32	M	358	ALA	CA-C-N	8.12	131.00	120.44
32	M	358	ALA	C-N-CA	8.12	131.00	120.44
19	Y	60	TRP	N-CA-C	-8.11	97.85	110.42
12	l	122	GLY	N-CA-C	-8.10	99.17	111.24
22	S	52	TYR	CA-C-N	8.10	130.77	120.56
22	S	52	TYR	C-N-CA	8.10	130.77	120.56
23	P	226	LYS	CA-C-N	8.10	130.93	120.56
23	P	226	LYS	C-N-CA	8.10	130.93	120.56
25	R	355	SER	O-C-N	8.10	131.38	122.15
18	X	25	THR	CA-C-N	8.10	128.59	119.93
18	X	25	THR	C-N-CA	8.10	128.59	119.93
3	C	50	ARG	N-CA-CB	8.09	122.27	110.06
4	D	209	ASN	CA-CB-CG	-8.09	104.51	112.60
27	O	380	LEU	N-CA-C	-8.09	102.54	111.36
31	L	204	PRO	N-CA-C	-8.09	101.00	114.75
21	N	515	ARG	CA-C-N	8.09	128.89	120.00
21	N	515	ARG	C-N-CA	8.09	128.89	120.00
21	N	182	ASN	CA-C-N	8.08	133.56	120.30
21	N	182	ASN	C-N-CA	8.08	133.56	120.30
8	h	151	PHE	CA-C-O	8.08	129.77	120.80
13	m	11	ASN	CA-C-O	-8.08	111.45	119.69
1	A	199	TRP	CG-CD2-CE3	-8.08	125.82	133.90
22	S	188	TYR	O-C-N	-8.08	113.75	122.07
16	V	186	GLN	CA-C-N	8.07	131.90	120.28
16	V	186	GLN	C-N-CA	8.07	131.90	120.28
22	S	280	ASN	CA-C-N	8.07	131.09	120.28
22	S	280	ASN	C-N-CA	8.07	131.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	190	PRO	N-CA-C	-8.07	102.72	110.47
25	R	170	VAL	CA-C-O	-8.07	112.30	120.85
5	E	72	ARG	NE-CZ-NH1	-8.06	113.44	121.50
27	O	23	HIS	ND1-CE1-NE2	8.06	116.47	108.40
31	L	81	ILE	N-CA-CB	8.06	122.67	110.58
24	Q	277	ASP	CA-CB-CG	-8.06	104.54	112.60
3	c	204	SER	O-C-N	8.06	130.79	122.09
10	j	72	ASN	CA-CB-CG	-8.06	104.54	112.60
10	3	87	PHE	CA-CB-CG	-8.05	105.75	113.80
10	j	62	THR	O-C-N	8.05	131.33	122.15
6	f	119	ASN	CA-CB-CG	-8.05	104.55	112.60
30	K	135	MET	CA-C-N	8.05	132.91	120.75
30	K	135	MET	C-N-CA	8.05	132.91	120.75
6	F	85	SER	CA-C-N	8.05	131.06	120.28
6	F	85	SER	C-N-CA	8.05	131.06	120.28
22	S	161	LYS	N-CA-C	8.05	119.68	111.07
32	M	136	ASP	CA-CB-CG	-8.05	104.55	112.60
19	Y	25	ASN	O-C-N	-8.04	113.59	122.12
3	c	170	SER	CA-C-N	8.03	130.88	120.44
3	c	170	SER	C-N-CA	8.03	130.88	120.44
13	6	172	THR	N-CA-C	-8.03	103.61	113.41
1	a	175	GLN	CA-C-O	-8.02	111.97	120.63
24	Q	336	ASN	CA-CB-CG	-8.02	104.58	112.60
29	I	435	LEU	CA-C-N	8.02	131.34	120.44
29	I	435	LEU	C-N-CA	8.02	131.34	120.44
30	K	367	ASP	CA-CB-CG	-8.01	104.59	112.60
21	N	229	VAL	CB-CA-C	-8.01	101.72	111.97
28	H	103	THR	N-CA-C	-8.01	104.11	114.04
4	d	26	ALA	CA-C-N	8.01	131.43	120.46
4	d	26	ALA	C-N-CA	8.01	131.43	120.46
21	N	906	ARG	NE-CZ-NH1	8.01	129.50	121.50
29	I	68	HIS	CA-C-N	8.00	131.00	120.28
29	I	68	HIS	C-N-CA	8.00	131.00	120.28
7	g	71	ASP	CA-CB-CG	-8.00	104.60	112.60
20	Z	745	LEU	CA-C-N	8.00	133.42	120.30
20	Z	745	LEU	C-N-CA	8.00	133.42	120.30
22	S	226	ASP	CA-C-N	8.00	131.65	120.29
22	S	226	ASP	C-N-CA	8.00	131.65	120.29
1	A	199	TRP	CE2-CD2-CE3	7.99	126.79	118.80
10	3	147	PHE	CA-CB-CG	-7.99	105.81	113.80
24	Q	93	THR	CA-C-N	7.99	130.63	120.56
24	Q	93	THR	C-N-CA	7.99	130.63	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	228	PHE	CA-CB-CG	-7.99	105.81	113.80
13	6	12	PRO	N-CA-C	-7.98	101.18	114.75
8	h	81	THR	CA-C-N	7.98	129.81	119.84
8	h	81	THR	C-N-CA	7.98	129.81	119.84
13	m	37	ASN	N-CA-C	-7.97	95.92	109.24
10	3	50	PHE	CA-CB-CG	-7.97	105.83	113.80
24	Q	50	ARG	NE-CZ-NH2	7.97	126.37	119.20
13	6	166	ASN	CA-CB-CG	-7.97	104.63	112.60
33	J	298	ASP	O-C-N	7.97	130.57	122.12
11	k	162	LYS	CA-C-N	7.96	130.95	120.28
11	k	162	LYS	C-N-CA	7.96	130.95	120.28
12	5	81	PHE	CA-CB-CG	-7.96	105.84	113.80
14	7	143	LEU	N-CA-C	-7.96	95.75	108.73
3	C	105	ASP	CA-CB-CG	-7.96	104.64	112.60
7	G	247	ILE	CA-C-O	-7.96	111.88	120.47
21	N	607	GLN	CA-C-O	7.95	129.09	120.10
11	k	127	GLU	CA-C-O	-7.95	111.56	120.54
1	a	65	ASP	N-CA-C	-7.94	94.40	108.69
17	T	259	ILE	CA-C-N	7.94	130.56	120.56
17	T	259	ILE	C-N-CA	7.94	130.56	120.56
33	J	388	LYS	N-CA-C	-7.94	102.56	112.72
4	D	134	LEU	N-CA-C	-7.93	95.97	108.90
20	Z	207	ILE	CA-C-N	7.93	126.68	120.33
20	Z	207	ILE	C-N-CA	7.93	126.68	120.33
18	X	76	VAL	N-CA-C	-7.93	98.17	107.61
27	O	184	ASP	CA-CB-CG	-7.93	104.67	112.60
21	N	683	LEU	CA-C-N	7.92	131.54	120.29
21	N	683	LEU	C-N-CA	7.92	131.54	120.29
33	J	345	LYS	CA-C-N	7.92	131.70	120.53
33	J	345	LYS	C-N-CA	7.92	131.70	120.53
10	j	104	PHE	CA-CB-CG	-7.92	105.88	113.80
4	d	247	ASP	CA-C-N	7.92	130.89	120.28
4	d	247	ASP	C-N-CA	7.92	130.89	120.28
11	4	79	ALA	CA-C-N	7.91	131.30	120.46
11	4	79	ALA	C-N-CA	7.91	131.30	120.46
6	f	216	VAL	N-CA-C	-7.91	97.11	108.42
17	T	23	CYS	CA-C-N	7.91	131.53	120.29
17	T	23	CYS	C-N-CA	7.91	131.53	120.29
11	4	120	ASP	CA-C-N	7.91	130.88	120.28
11	4	120	ASP	C-N-CA	7.91	130.88	120.28
5	e	216	ASN	N-CA-C	-7.90	100.60	112.54
18	X	111	LEU	CA-C-O	-7.90	112.41	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	185	ASP	CA-CB-CG	7.90	120.50	112.60
16	V	182	LYS	N-CA-C	-7.90	97.41	109.41
5	e	51	GLU	N-CA-C	-7.89	96.54	109.40
17	T	132	HIS	CG-CD2-NE2	7.89	115.09	107.20
27	O	263	PHE	CA-CB-CG	-7.89	105.91	113.80
6	f	26	LEU	CA-C-N	7.89	131.49	120.29
6	f	26	LEU	C-N-CA	7.89	131.49	120.29
23	P	195	GLN	O-C-N	7.89	130.48	122.12
7	g	176	LEU	CA-C-N	7.88	130.84	120.28
7	g	176	LEU	C-N-CA	7.88	130.84	120.28
24	Q	278	VAL	CB-CA-C	-7.88	101.34	112.22
13	m	76	PHE	CA-C-O	7.88	128.77	120.42
21	N	477	SER	CA-C-N	7.88	128.67	120.00
21	N	477	SER	C-N-CA	7.88	128.67	120.00
15	W	158	ILE	N-CA-C	-7.88	102.76	110.72
26	U	167	GLU	CA-C-N	7.88	130.84	120.28
26	U	167	GLU	C-N-CA	7.88	130.84	120.28
28	H	167	ASP	CA-C-O	-7.88	112.20	120.55
2	b	122	THR	N-CA-C	-7.87	104.28	114.04
27	O	318	HIS	ND1-CE1-NE2	7.87	116.27	108.40
24	Q	394	ASN	OD1-CG-ND2	7.87	130.47	122.60
4	d	67	ILE	N-CA-CB	7.86	119.75	110.55
29	I	316	PHE	CA-CB-CG	7.86	121.66	113.80
5	E	218	GLN	OE1-CD-NE2	-7.86	114.74	122.60
16	V	200	ASN	CA-CB-CG	-7.86	104.74	112.60
2	B	207	ASP	CA-CB-CG	-7.86	104.74	112.60
14	n	181	ALA	N-CA-CB	7.86	121.79	110.16
31	L	207	PHE	CA-CB-CG	-7.86	105.94	113.80
3	C	218	LYS	N-CA-C	-7.85	103.00	114.39
16	V	218	LYS	N-CA-C	-7.85	103.01	112.59
31	L	390	ASP	CA-CB-CG	7.85	120.45	112.60
4	D	14	ASP	N-CA-C	-7.85	103.73	113.38
21	N	262	VAL	CA-C-N	7.84	131.11	120.44
21	N	262	VAL	C-N-CA	7.84	131.11	120.44
22	S	55	ARG	NE-CZ-NH2	7.84	126.26	119.20
33	J	317	PRO	CB-CA-C	-7.84	101.35	110.92
27	O	318	HIS	CE1-NE2-CD2	-7.84	101.16	109.00
21	N	810	ALA	CA-C-N	7.84	131.12	120.38
21	N	810	ALA	C-N-CA	7.84	131.12	120.38
30	K	141	ARG	NE-CZ-NH2	-7.84	112.14	119.20
7	g	54	ILE	N-CA-C	-7.84	96.44	107.80
25	R	339	ALA	CB-CA-C	-7.83	97.78	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	209	SER	N-CA-C	-7.83	103.74	113.38
1	a	152	PRO	CA-C-O	-7.83	112.85	121.23
27	O	20	PRO	CA-C-N	7.83	130.62	120.44
27	O	20	PRO	C-N-CA	7.83	130.62	120.44
31	L	175	GLN	OE1-CD-NE2	7.83	130.43	122.60
32	M	384	ASP	N-CA-C	-7.83	95.50	108.34
12	l	119	THR	N-CA-C	-7.81	97.44	109.24
25	R	129	GLU	N-CA-C	7.81	119.79	111.28
23	P	373	GLU	CA-C-O	7.80	128.82	120.55
7	G	123	HIS	CB-CG-CD2	-7.80	121.06	131.20
26	U	135	ASP	N-CA-C	-7.80	97.53	109.85
21	N	93	GLU	N-CA-C	-7.80	104.25	114.31
27	O	59	LEU	CA-C-N	7.79	130.57	120.44
27	O	59	LEU	C-N-CA	7.79	130.57	120.44
7	g	182	HIS	CE1-NE2-CD2	-7.79	101.21	109.00
13	6	52	PHE	CA-CB-CG	-7.79	106.01	113.80
22	S	82	TYR	CB-CA-C	7.79	119.94	109.42
2	b	245	ASP	CA-CB-CG	7.79	120.39	112.60
24	Q	237	SER	O-C-N	7.79	131.03	122.15
7	g	224	THR	CA-C-N	7.78	133.72	122.35
7	g	224	THR	C-N-CA	7.78	133.72	122.35
28	H	90	ARG	NE-CZ-NH1	7.78	129.28	121.50
29	I	79	SER	O-C-N	7.78	130.49	122.09
16	V	263	GLU	CA-C-N	7.77	130.70	120.28
16	V	263	GLU	C-N-CA	7.77	130.70	120.28
21	N	437	GLU	CA-C-N	7.77	130.69	120.28
21	N	437	GLU	C-N-CA	7.77	130.69	120.28
28	H	133	SER	O-C-N	-7.77	113.01	122.34
31	L	53	HIS	CA-CB-CG	7.77	121.57	113.80
7	g	24	VAL	CA-C-O	7.77	128.64	120.25
21	N	835	LYS	CA-C-N	7.77	133.78	122.36
21	N	835	LYS	C-N-CA	7.77	133.78	122.36
2	B	77	GLY	CA-C-N	7.77	131.77	120.82
2	B	77	GLY	C-N-CA	7.77	131.77	120.82
27	O	262	ASP	CA-CB-CG	7.77	120.37	112.60
6	F	183	ASP	CA-CB-CG	-7.76	104.84	112.60
2	B	99	ARG	N-CA-C	-7.76	103.63	113.72
16	V	127	LYS	CA-C-N	7.76	130.68	120.28
16	V	127	LYS	C-N-CA	7.76	130.68	120.28
24	Q	334	HIS	ND1-CE1-NE2	7.76	116.16	108.40
4	d	174	PHE	CA-C-N	7.76	130.67	120.28
4	d	174	PHE	C-N-CA	7.76	130.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	110	LEU	CA-C-N	7.76	131.00	120.38
23	P	110	LEU	C-N-CA	7.76	131.00	120.38
33	J	108	LYS	CA-C-O	-7.76	112.95	121.33
33	J	308	GLY	CA-C-O	-7.76	109.67	119.13
26	U	238	ASN	CA-CB-CG	-7.75	104.84	112.60
13	m	40	ASP	CA-CB-CG	-7.75	104.85	112.60
33	J	200	ARG	N-CA-C	7.75	119.51	111.14
33	J	269	GLN	N-CA-C	7.75	120.62	111.71
3	c	31	HIS	CE1-NE2-CD2	-7.75	101.25	109.00
6	f	99	PHE	N-CA-C	-7.75	103.35	114.12
1	A	219	SER	N-CA-C	-7.75	98.05	108.74
22	S	72	GLU	CA-C-N	7.75	130.66	120.28
22	S	72	GLU	C-N-CA	7.75	130.66	120.28
27	O	129	ILE	N-CA-C	7.75	117.86	110.42
27	O	286	PHE	CA-C-N	7.75	131.29	120.29
27	O	286	PHE	C-N-CA	7.75	131.29	120.29
7	G	108	PRO	CA-C-N	7.74	125.12	120.24
7	G	108	PRO	C-N-CA	7.74	125.12	120.24
8	1	204	GLN	N-CA-C	-7.74	103.84	113.28
22	S	78	VAL	CA-C-N	7.73	130.64	120.28
22	S	78	VAL	C-N-CA	7.73	130.64	120.28
31	L	54	ASN	CA-C-N	7.73	131.27	120.29
31	L	54	ASN	C-N-CA	7.73	131.27	120.29
22	S	275	TYR	CB-CA-C	-7.73	97.96	110.79
30	K	101	GLU	N-CA-C	-7.72	101.18	108.13
5	e	106	ASP	CA-C-O	-7.72	112.52	121.16
31	L	153	LEU	N-CA-CB	7.72	124.91	111.40
27	O	235	HIS	CA-CB-CG	-7.71	106.09	113.80
30	K	359	LYS	N-CA-CB	7.71	121.52	110.88
14	7	76	ILE	CA-C-O	-7.70	115.94	119.94
9	i	138	HIS	ND1-CE1-NE2	7.70	116.10	108.40
23	P	11	LYS	CA-C-N	7.70	130.45	120.44
23	P	11	LYS	C-N-CA	7.70	130.45	120.44
14	n	64	GLY	CA-C-N	7.70	130.45	120.44
14	n	64	GLY	C-N-CA	7.70	130.45	120.44
4	d	70	HIS	CE1-NE2-CD2	-7.69	101.31	109.00
7	g	183	HIS	CA-CB-CG	-7.69	106.11	113.80
28	H	59	ILE	N-CA-C	7.69	118.47	110.62
3	c	22	VAL	CB-CA-C	-7.69	101.61	112.22
16	V	209	GLU	CA-C-N	7.69	130.59	120.28
16	V	209	GLU	C-N-CA	7.69	130.59	120.28
17	T	174	PHE	CA-C-N	7.69	133.57	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	174	PHE	C-N-CA	7.69	133.57	120.72
23	P	60	ALA	CA-C-N	7.69	131.21	120.29
23	P	60	ALA	C-N-CA	7.69	131.21	120.29
6	f	108	ALA	CA-C-N	7.69	129.99	120.22
6	f	108	ALA	C-N-CA	7.69	129.99	120.22
18	X	127	GLY	CA-C-N	7.69	131.34	120.42
18	X	127	GLY	C-N-CA	7.69	131.34	120.42
29	I	238	ASN	N-CA-C	-7.69	102.84	111.14
28	H	239	GLY	N-CA-C	-7.69	104.43	115.27
21	N	29	ASN	OD1-CG-ND2	7.68	130.28	122.60
27	O	283	HIS	ND1-CE1-NE2	7.68	116.08	108.40
7	g	102	LEU	CB-CA-C	-7.67	97.81	110.85
33	J	51	LEU	CA-C-N	7.67	130.56	120.28
33	J	51	LEU	C-N-CA	7.67	130.56	120.28
23	P	230	HIS	ND1-CE1-NE2	7.67	116.07	108.40
5	E	60	GLU	N-CA-CB	7.67	121.78	110.35
11	4	192	VAL	N-CA-C	-7.67	97.44	108.48
23	P	57	GLU	CA-C-N	7.66	130.37	120.56
23	P	57	GLU	C-N-CA	7.66	130.37	120.56
33	J	376	HIS	CA-CB-CG	-7.66	106.14	113.80
11	4	90	LYS	CA-C-N	7.65	131.30	120.28
11	4	90	LYS	C-N-CA	7.65	131.30	120.28
20	Z	726	GLU	CA-C-N	7.65	131.58	120.71
20	Z	726	GLU	C-N-CA	7.65	131.58	120.71
2	b	159	TRP	CE2-CD2-CE3	7.65	126.45	118.80
5	E	173	GLY	CA-C-N	7.65	130.53	120.28
5	E	173	GLY	C-N-CA	7.65	130.53	120.28
2	b	26	THR	CA-C-N	7.65	130.53	120.28
2	b	26	THR	C-N-CA	7.65	130.53	120.28
11	4	181	VAL	CA-C-O	7.64	128.71	120.53
13	6	137	GLY	O-C-N	7.64	130.14	122.65
7	G	84	ASP	CA-CB-CG	-7.64	104.96	112.60
1	a	63	LEU	N-CA-C	-7.64	103.98	113.38
33	J	384	LEU	CA-C-O	-7.64	112.32	120.42
8	h	90	VAL	N-CA-CB	7.63	119.48	110.55
10	3	62	THR	CA-C-O	-7.63	112.46	120.55
9	i	107	SER	N-CA-C	-7.63	103.04	111.36
19	Y	25	ASN	CA-CB-CG	-7.63	104.97	112.60
29	I	305	THR	CA-C-N	7.62	131.12	120.29
29	I	305	THR	C-N-CA	7.62	131.12	120.29
12	5	212	TYR	CA-C-N	7.62	128.60	119.99
12	5	212	TYR	C-N-CA	7.62	128.60	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	13	SER	CA-C-O	-7.62	113.34	121.27
31	L	53	HIS	CA-C-N	7.62	130.35	120.44
31	L	53	HIS	C-N-CA	7.62	130.35	120.44
13	6	77	LYS	CB-CA-C	-7.62	98.15	110.79
4	d	91	VAL	CA-C-N	7.61	131.10	120.29
4	d	91	VAL	C-N-CA	7.61	131.10	120.29
6	f	70	MET	CA-C-O	7.61	130.00	121.40
25	R	300	ASP	N-CA-C	-7.61	95.90	108.76
3	C	221	ASN	N-CA-CB	7.61	123.35	110.49
29	I	147	VAL	CA-C-N	7.61	133.70	123.05
29	I	147	VAL	C-N-CA	7.61	133.70	123.05
1	a	175	GLN	O-C-N	7.61	130.18	122.12
25	R	82	ASP	CA-CB-CG	7.60	120.20	112.60
3	C	8	SER	N-CA-C	7.60	115.01	108.78
27	O	337	LEU	O-C-N	-7.60	113.89	123.24
7	g	121	GLN	O-C-N	-7.60	112.15	122.33
19	Y	23	GLU	CA-C-N	7.60	130.87	120.46
19	Y	23	GLU	C-N-CA	7.60	130.87	120.46
12	5	138	CYS	CA-C-N	7.59	130.46	120.28
12	5	138	CYS	C-N-CA	7.59	130.46	120.28
21	N	258	ALA	CA-C-N	7.59	131.07	120.29
21	N	258	ALA	C-N-CA	7.59	131.07	120.29
25	R	351	LYS	CA-C-N	7.59	130.46	120.28
25	R	351	LYS	C-N-CA	7.59	130.46	120.28
1	A	152	PRO	CA-C-O	-7.59	113.04	121.32
33	J	123	HIS	CE1-NE2-CD2	-7.59	101.41	109.00
22	S	481	TYR	CA-C-O	-7.59	109.76	120.16
21	N	262	VAL	CB-CA-C	-7.59	101.90	112.14
4	d	192	VAL	CA-C-O	-7.58	113.13	121.17
17	T	149	ASP	CA-CB-CG	-7.58	105.02	112.60
2	B	209	ILE	N-CA-C	-7.58	97.50	108.11
21	N	151	LYS	CA-C-N	7.58	131.06	120.29
21	N	151	LYS	C-N-CA	7.58	131.06	120.29
33	J	171	PRO	CA-C-N	7.58	131.06	120.29
33	J	171	PRO	C-N-CA	7.58	131.06	120.29
7	G	193	VAL	CA-C-N	7.58	131.05	120.29
7	G	193	VAL	C-N-CA	7.58	131.05	120.29
19	Y	39	PRO	CA-C-N	7.58	130.11	120.56
19	Y	39	PRO	C-N-CA	7.58	130.11	120.56
32	M	349	PHE	CA-CB-CG	-7.58	106.22	113.80
23	P	284	ILE	CA-C-N	7.58	130.44	120.28
23	P	284	ILE	C-N-CA	7.58	130.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	156	HIS	CE1-NE2-CD2	-7.58	101.42	109.00
7	G	231	VAL	N-CA-C	-7.57	97.53	108.36
8	1	46	VAL	N-CA-C	-7.57	105.82	113.47
23	P	140	THR	CA-C-N	7.57	131.19	120.28
23	P	140	THR	C-N-CA	7.57	131.19	120.28
4	D	90	ARG	N-CA-C	7.57	119.53	111.28
30	K	414	GLN	O-C-N	7.57	131.22	122.67
1	a	74	CYS	N-CA-C	-7.56	96.94	108.96
2	B	23	TYR	N-CA-C	7.56	120.41	111.71
24	Q	405	GLN	OE1-CD-NE2	-7.56	115.04	122.60
29	I	298	GLY	CA-C-N	7.56	130.41	120.28
29	I	298	GLY	C-N-CA	7.56	130.41	120.28
6	F	32	GLY	O-C-N	7.56	129.31	122.81
14	7	152	VAL	N-CA-C	-7.56	97.60	108.48
24	Q	121	SER	CA-C-N	7.55	130.81	120.46
24	Q	121	SER	C-N-CA	7.55	130.81	120.46
15	W	103	ASN	CA-CB-CG	-7.55	105.05	112.60
30	K	196	ASP	CA-CB-CG	-7.55	105.05	112.60
5	e	93	ARG	CA-C-N	7.55	130.25	120.44
5	e	93	ARG	C-N-CA	7.55	130.25	120.44
7	g	178	LYS	CB-CA-C	-7.55	98.02	110.85
28	H	387	ASN	CA-CB-CG	-7.55	105.05	112.60
8	h	105	GLY	N-CA-C	-7.54	99.17	110.71
28	H	440	GLU	N-CA-C	-7.54	103.69	113.12
6	f	166	GLN	N-CA-C	-7.54	102.73	112.23
21	N	550	GLY	CA-C-N	7.54	128.51	119.99
21	N	550	GLY	C-N-CA	7.54	128.51	119.99
29	I	285	ASP	N-CA-C	-7.54	103.34	112.54
8	h	198	TYR	CA-C-O	-7.54	113.81	120.60
32	M	406	GLY	O-C-N	7.53	130.99	122.55
7	g	207	ASN	N-CA-C	-7.53	101.52	110.41
21	N	389	TYR	N-CA-C	-7.53	103.93	113.72
13	6	18	GLY	N-CA-C	-7.53	103.22	112.33
16	V	268	THR	CA-C-N	7.53	130.37	120.28
16	V	268	THR	C-N-CA	7.53	130.37	120.28
17	T	120	THR	N-CA-C	7.53	119.12	111.07
21	N	340	HIS	CE1-NE2-CD2	-7.53	101.47	109.00
31	L	241	ALA	O-C-N	7.53	131.12	121.79
17	T	132	HIS	CE1-NE2-CD2	-7.53	101.47	109.00
1	A	58	LYS	N-CA-C	-7.52	96.16	108.41
1	A	105	ARG	CA-C-O	-7.52	112.93	120.82
33	J	349	LYS	CA-C-O	7.52	128.39	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	104	LEU	N-CA-CB	7.51	121.16	110.12
21	N	866	TYR	CA-C-O	-7.51	112.58	120.99
21	N	593	PHE	CA-C-N	7.51	130.02	120.56
21	N	593	PHE	C-N-CA	7.51	130.02	120.56
7	G	23	GLN	CA-C-N	7.50	132.61	120.30
7	G	23	GLN	C-N-CA	7.50	132.61	120.30
10	3	20	CYS	CA-C-O	-7.50	112.59	120.99
12	l	276	LYS	O-C-N	7.50	129.79	122.07
24	Q	375	GLY	CA-C-N	7.50	130.94	120.29
24	Q	375	GLY	C-N-CA	7.50	130.94	120.29
3	C	26	LEU	O-C-N	7.50	130.07	122.12
24	Q	20	TYR	CA-C-N	7.50	130.32	120.28
24	Q	20	TYR	C-N-CA	7.50	130.32	120.28
7	G	81	LEU	CA-C-N	7.50	126.33	120.33
7	G	81	LEU	C-N-CA	7.50	126.33	120.33
33	J	404	PHE	CA-CB-CG	7.50	121.30	113.80
25	R	383	ARG	NE-CZ-NH2	-7.49	112.46	119.20
26	U	88	LYS	CA-C-N	7.49	131.39	120.82
26	U	88	LYS	C-N-CA	7.49	131.39	120.82
26	U	101	ALA	N-CA-C	-7.49	103.73	113.17
24	Q	208	ILE	CA-C-O	-7.49	112.42	120.59
24	Q	67	THR	CA-C-N	7.49	135.18	121.70
24	Q	67	THR	C-N-CA	7.49	135.18	121.70
19	Y	6	ALA	CA-C-O	-7.49	112.96	120.82
27	O	174	THR	CA-C-N	7.48	130.17	120.44
27	O	174	THR	C-N-CA	7.48	130.17	120.44
14	7	254	PHE	CA-CB-CG	7.48	121.28	113.80
2	b	59	GLU	N-CA-C	-7.48	103.75	113.17
9	i	39	ASN	O-C-N	-7.48	113.14	122.19
21	N	837	LYS	N-CA-C	-7.48	103.09	114.16
32	M	209	ASP	CA-CB-CG	7.48	120.08	112.60
33	J	349	LYS	N-CA-C	7.48	119.51	111.36
1	a	151	GLY	CA-C-N	7.48	127.91	119.83
1	a	151	GLY	C-N-CA	7.48	127.91	119.83
21	N	205	SER	CA-C-N	7.47	131.03	120.42
21	N	205	SER	C-N-CA	7.47	131.03	120.42
32	M	147	GLY	N-CA-C	-7.47	102.50	112.82
12	l	115	PHE	CA-CB-CG	-7.47	106.33	113.80
14	n	81	ASN	CB-CA-C	-7.47	97.54	110.17
28	H	115	THR	CA-C-N	7.47	130.63	120.54
28	H	115	THR	C-N-CA	7.47	130.63	120.54
30	K	406	ASP	CA-C-N	7.47	130.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	406	ASP	C-N-CA	7.47	130.29	120.28
30	K	273	GLU	N-CA-C	-7.47	97.26	108.99
11	4	110	LYS	N-CA-C	-7.47	104.78	114.04
20	Z	209	PRO	CB-CA-C	-7.46	101.22	112.11
21	N	698	GLY	CA-C-N	7.46	130.28	120.28
21	N	698	GLY	C-N-CA	7.46	130.28	120.28
29	I	166	PRO	CA-C-N	7.46	130.28	120.28
29	I	166	PRO	C-N-CA	7.46	130.28	120.28
13	m	212	ILE	N-CA-C	-7.46	97.73	108.17
7	G	151	LEU	N-CA-C	-7.46	97.07	109.07
4	d	42	VAL	N-CA-C	-7.45	97.36	108.46
15	W	100	HIS	CE1-NE2-CD2	-7.45	101.55	109.00
30	K	375	ASN	OD1-CG-ND2	-7.45	115.15	122.60
21	N	556	ALA	CB-CA-C	-7.45	99.19	110.88
21	N	211	PHE	N-CA-C	-7.45	103.16	111.28
17	T	91	SER	CA-C-O	-7.44	112.58	121.66
7	g	109	ILE	N-CA-CB	7.44	115.19	110.50
13	m	109	ARG	N-CA-C	-7.44	104.05	113.72
14	7	249	ASN	OD1-CG-ND2	-7.44	115.16	122.60
25	R	315	VAL	CB-CA-C	-7.44	104.43	111.05
12	l	243	ASP	CA-CB-CG	-7.44	105.16	112.60
6	f	233	TYR	N-CA-C	-7.44	101.94	113.02
5	e	12	VAL	CB-CA-C	-7.43	99.10	111.29
7	g	14	VAL	CB-CA-C	7.43	121.17	110.98
1	A	47	GLY	CA-C-O	-7.43	113.77	121.28
6	F	99	PHE	CA-CB-CG	-7.43	106.37	113.80
30	K	223	VAL	N-CA-C	-7.43	102.90	111.00
6	f	97	LEU	CA-C-O	-7.43	113.05	120.70
28	H	433	ALA	CA-C-N	7.43	133.20	122.35
28	H	433	ALA	C-N-CA	7.43	133.20	122.35
4	d	96	HIS	CA-C-N	7.43	131.60	120.31
4	d	96	HIS	C-N-CA	7.43	131.60	120.31
2	B	160	LYS	N-CA-CB	7.43	121.78	110.42
33	J	195	LYS	N-CA-C	7.43	119.38	111.28
4	d	17	ILE	N-CA-C	-7.43	97.43	108.12
11	4	135	TYR	N-CA-C	-7.43	103.79	112.92
30	K	150	LEU	CA-C-N	7.42	128.02	120.38
30	K	150	LEU	C-N-CA	7.42	128.02	120.38
30	K	246	TYR	N-CA-C	-7.42	97.79	109.07
4	D	223	ALA	N-CA-CB	7.42	122.22	110.57
29	I	159	VAL	N-CA-C	-7.42	97.47	108.45
33	J	23	PHE	CA-CB-CG	-7.42	106.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	141	LYS	O-C-N	-7.42	116.66	121.85
26	U	123	VAL	CA-C-N	7.41	131.92	121.24
26	U	123	VAL	C-N-CA	7.41	131.92	121.24
33	J	258	VAL	CA-C-N	7.41	130.22	120.28
33	J	258	VAL	C-N-CA	7.41	130.22	120.28
2	b	105	PRO	CA-C-O	-7.41	114.88	120.73
6	f	114	ASP	CA-C-N	7.41	130.55	120.54
6	f	114	ASP	C-N-CA	7.41	130.55	120.54
4	D	201	GLU	CB-CG-CD	-7.41	100.00	112.60
9	2	102	GLU	CA-C-O	-7.41	112.32	120.69
8	h	47	HIS	CA-C-N	7.41	130.21	120.28
8	h	47	HIS	C-N-CA	7.41	130.21	120.28
29	I	165	ASP	CA-C-N	7.41	127.04	119.56
29	I	165	ASP	C-N-CA	7.41	127.04	119.56
9	2	115	HIS	CA-C-N	7.41	130.20	120.28
9	2	115	HIS	C-N-CA	7.41	130.20	120.28
27	O	47	LYS	CA-C-N	7.40	130.51	120.44
27	O	47	LYS	C-N-CA	7.40	130.51	120.44
21	N	747	HIS	CE1-NE2-CD2	-7.40	101.60	109.00
21	N	549	TYR	N-CA-C	-7.40	103.15	111.07
9	2	88	ILE	N-CA-C	-7.40	102.94	111.00
21	N	99	GLU	CA-C-N	7.40	130.06	120.44
21	N	99	GLU	C-N-CA	7.40	130.06	120.44
7	G	193	VAL	N-CA-C	-7.40	103.65	110.82
18	X	131	ASN	N-CA-CB	7.39	120.81	110.17
30	K	74	HIS	CA-CB-CG	-7.39	106.41	113.80
4	d	42	VAL	CA-C-O	7.39	128.94	120.67
14	n	188	LEU	O-C-N	-7.39	112.53	122.43
1	A	158	ASP	CA-CB-CG	-7.39	105.21	112.60
21	N	180	SER	N-CA-C	-7.39	103.31	111.36
14	n	130	ALA	CA-C-N	7.38	130.17	120.28
14	n	130	ALA	C-N-CA	7.38	130.17	120.28
12	l	171	SER	N-CA-C	-7.38	97.91	109.72
22	S	54	TRP	CB-CG-CD2	-7.38	116.46	126.80
26	U	209	GLU	N-CA-CB	7.38	121.67	110.30
22	S	166	ASN	OD1-CG-ND2	7.38	129.98	122.60
2	b	117	ILE	O-C-N	-7.38	114.23	121.90
11	k	130	TYR	N-CA-CB	7.38	123.26	110.65
13	6	110	PHE	N-CA-C	-7.37	103.87	114.12
21	N	363	ALA	CA-C-N	7.37	131.52	120.31
21	N	363	ALA	C-N-CA	7.37	131.52	120.31
33	J	237	ALA	N-CA-C	-7.37	102.94	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	39	ASN	CA-CB-CG	-7.37	105.23	112.60
2	B	159	TRP	CZ3-CH2-CZ2	-7.37	111.92	121.50
11	k	88	LEU	CA-C-N	7.37	130.75	120.29
11	k	88	LEU	C-N-CA	7.37	130.75	120.29
26	U	5	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	205	PHE	CA-C-N	7.36	130.75	120.29
1	A	205	PHE	C-N-CA	7.36	130.75	120.29
21	N	638	ILE	CA-C-O	-7.36	113.61	121.27
26	U	124	ASP	N-CA-C	-7.36	98.77	109.59
4	d	48	ARG	NE-CZ-NH1	-7.36	114.14	121.50
5	e	164	PHE	CA-CB-CG	7.36	121.16	113.80
10	3	3	ASP	CA-C-O	-7.36	112.40	119.91
3	c	168	ASN	CA-C-N	7.36	130.00	120.44
3	c	168	ASN	C-N-CA	7.36	130.00	120.44
21	N	756	THR	O-C-N	7.36	132.06	123.30
24	Q	237	SER	CA-C-O	-7.36	112.62	120.42
25	R	91	TRP	N-CA-C	-7.36	103.44	113.30
30	K	212	TYR	CA-C-O	-7.36	112.53	121.06
20	Z	918	ASP	CB-CA-C	-7.36	99.21	110.83
25	R	88	LEU	N-CA-C	-7.36	104.33	113.38
31	L	161	ARG	N-CA-CB	-7.36	99.84	110.36
12	5	225	VAL	O-C-N	7.35	129.41	121.83
8	h	118	GLU	O-C-N	7.35	131.63	123.25
9	i	122	HIS	CE1-NE2-CD2	-7.35	101.65	109.00
27	O	244	ASN	OD1-CG-ND2	-7.35	115.25	122.60
28	H	251	PRO	N-CA-C	7.35	119.66	110.70
27	O	239	MET	N-CA-C	-7.34	104.85	113.88
6	f	149	PRO	CA-C-N	7.34	130.42	120.44
6	f	149	PRO	C-N-CA	7.34	130.42	120.44
6	F	104	ALA	CA-C-N	7.34	130.52	120.46
6	F	104	ALA	C-N-CA	7.34	130.52	120.46
26	U	288	PHE	CA-C-N	7.34	130.71	120.29
26	U	288	PHE	C-N-CA	7.34	130.71	120.29
4	d	147	LEU	CA-C-O	7.33	129.30	120.28
19	Y	39	PRO	CA-C-O	-7.33	108.41	119.55
1	A	185	HIS	ND1-CE1-NE2	7.33	115.73	108.40
2	b	239	THR	CA-C-N	7.33	130.09	120.28
2	b	239	THR	C-N-CA	7.33	130.09	120.28
4	d	251	LYS	CA-C-O	-7.33	112.66	120.42
29	I	316	PHE	N-CA-C	-7.33	103.23	111.07
13	m	136	VAL	N-CA-C	-7.32	104.85	113.42
23	P	431	HIS	CA-CB-CG	-7.32	106.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	130	ALA	O-C-N	-7.32	114.91	123.25
4	d	57	THR	N-CA-C	-7.32	103.95	114.12
13	6	39	THR	N-CA-C	-7.32	95.14	107.80
9	i	67	SER	N-CA-C	-7.32	101.64	108.22
25	R	65	TYR	CA-C-N	7.32	130.08	120.28
25	R	65	TYR	C-N-CA	7.32	130.08	120.28
27	O	212	GLN	OE1-CD-NE2	7.32	129.91	122.60
29	I	316	PHE	CB-CG-CD2	7.32	133.13	120.70
32	M	251	LEU	N-CA-C	-7.31	103.34	111.82
2	b	159	TRP	CG-CD2-CE3	-7.31	126.59	133.90
1	A	194	ILE	N-CA-C	-7.30	97.96	108.48
26	U	264	ALA	CA-C-O	7.30	128.29	120.55
2	B	27	ALA	N-CA-C	7.30	119.24	111.28
5	E	122	ARG	N-CA-CB	7.30	121.27	109.95
28	H	115	THR	N-CA-C	-7.30	105.29	114.56
28	H	216	ASP	CA-CB-CG	7.30	119.90	112.60
2	b	140	ASP	CA-CB-CG	-7.30	105.30	112.60
7	g	91	ARG	CA-C-N	7.29	128.20	120.03
7	g	91	ARG	C-N-CA	7.29	128.20	120.03
12	5	137	GLN	CA-C-O	-7.29	112.69	120.42
31	L	339	ARG	CA-C-N	7.29	127.46	120.31
31	L	339	ARG	C-N-CA	7.29	127.46	120.31
2	B	207	ASP	N-CA-C	-7.29	104.41	113.38
29	I	412	THR	CA-C-N	7.29	130.78	120.28
29	I	412	THR	C-N-CA	7.29	130.78	120.28
33	J	130	ALA	N-CA-C	-7.29	96.67	109.06
12	l	86	GLY	N-CA-C	-7.29	100.74	110.58
17	T	89	TYR	CB-CG-CD2	-7.29	109.87	120.80
26	U	212	ASP	CA-C-O	-7.29	113.17	120.82
27	O	108	GLU	CA-C-N	7.29	130.04	120.28
27	O	108	GLU	C-N-CA	7.29	130.04	120.28
32	M	318	ASP	CA-CB-CG	7.29	119.89	112.60
8	1	126	GLY	CA-C-N	7.28	132.68	120.81
8	1	126	GLY	C-N-CA	7.28	132.68	120.81
24	Q	390	LEU	CA-C-O	-7.28	112.31	120.32
28	H	216	ASP	CA-C-N	7.28	130.04	120.28
28	H	216	ASP	C-N-CA	7.28	130.04	120.28
6	F	26	LEU	N-CA-CB	7.28	121.56	110.28
26	U	43	SER	CA-C-N	7.28	130.34	120.44
26	U	43	SER	C-N-CA	7.28	130.34	120.44
4	D	23	ALA	N-CA-CB	7.28	120.82	110.12
28	H	65	GLU	CA-C-N	7.28	133.03	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	65	GLU	C-N-CA	7.28	133.03	120.58
33	J	331	HIS	CE1-NE2-CD2	-7.28	101.72	109.00
5	e	82	THR	CA-C-N	7.28	129.90	120.44
5	e	82	THR	C-N-CA	7.28	129.90	120.44
10	j	45	HIS	CE1-NE2-CD2	-7.28	101.72	109.00
22	S	461	PHE	CA-CB-CG	7.27	121.07	113.80
13	m	200	THR	O-C-N	7.27	129.83	122.12
23	P	425	HIS	N-CA-CB	7.27	120.92	110.16
30	K	44	ASN	CB-CA-C	-7.27	98.31	110.68
31	L	139	LYS	N-CA-C	-7.27	102.69	112.94
10	j	152	SER	N-CA-C	7.27	119.21	111.28
3	C	70	ASN	N-CA-CB	7.27	122.31	110.97
21	N	16	ASN	CA-C-N	7.27	131.12	120.95
21	N	16	ASN	C-N-CA	7.27	131.12	120.95
10	j	53	ILE	N-CA-C	-7.26	97.56	108.17
5	E	63	SER	N-CA-C	-7.26	104.45	113.38
8	h	113	ASP	N-CA-C	-7.26	104.45	113.38
4	d	216	LYS	O-C-N	-7.26	115.89	121.55
8	h	142	PHE	CA-CB-CG	-7.26	106.54	113.80
1	A	36	ASN	CA-CB-CG	-7.26	105.34	112.60
18	X	51	ARG	O-C-N	-7.26	114.32	121.94
27	O	151	ASP	CA-CB-CG	-7.26	105.34	112.60
26	U	20	ASP	O-C-N	-7.26	114.43	122.12
7	G	123	HIS	CB-CG-ND1	7.26	133.58	122.70
10	3	45	HIS	ND1-CE1-NE2	7.25	115.66	108.40
30	K	269	ILE	N-CA-CB	7.25	119.70	110.99
31	L	286	ILE	O-C-N	7.25	128.62	122.09
32	M	362	GLN	OE1-CD-NE2	7.25	129.85	122.60
4	d	222	VAL	N-CA-CB	7.25	125.34	111.93
9	2	143	HIS	CA-C-N	7.25	130.00	120.28
9	2	143	HIS	C-N-CA	7.25	130.00	120.28
17	T	255	GLN	CA-C-N	7.25	129.87	120.44
17	T	255	GLN	C-N-CA	7.25	129.87	120.44
24	Q	254	SER	N-CA-C	-7.25	104.24	113.23
27	O	185	PHE	CA-C-O	7.25	128.31	120.55
15	W	103	ASN	N-CA-C	-7.25	98.00	109.23
19	Y	83	ARG	O-C-N	-7.25	114.44	122.12
27	O	300	VAL	O-C-N	7.25	129.01	121.91
32	M	330	VAL	N-CA-C	-7.25	105.53	113.43
23	P	182	GLU	O-C-N	-7.25	114.44	122.12
30	K	308	GLN	CA-C-O	7.25	129.27	120.57
31	L	309	LEU	CA-C-O	-7.25	113.23	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	155	MET	N-CA-C	7.24	123.44	113.16
12	5	124	ALA	CA-C-N	7.24	130.32	120.54
12	5	124	ALA	C-N-CA	7.24	130.32	120.54
24	Q	52	ASN	CA-C-N	7.24	130.30	120.38
24	Q	52	ASN	C-N-CA	7.24	130.30	120.38
1	a	209	HIS	ND1-CE1-NE2	7.24	115.64	108.40
24	Q	88	PHE	CA-CB-CG	-7.24	106.56	113.80
29	I	163	ASP	N-CA-CB	7.24	124.09	111.13
33	J	348	GLU	CB-CG-CD	-7.24	100.29	112.60
21	N	68	VAL	N-CA-C	7.24	118.00	110.62
14	n	76	ILE	CA-C-O	-7.24	112.67	119.62
17	T	89	TYR	CA-C-N	7.24	130.57	120.29
17	T	89	TYR	C-N-CA	7.24	130.57	120.29
27	O	252	PHE	O-C-N	7.24	129.79	122.12
31	L	273	HIS	CE1-NE2-CD2	-7.24	101.77	109.00
32	M	38	ASP	N-CA-CB	7.24	120.76	110.12
32	M	355	ASP	CA-CB-CG	-7.24	105.36	112.60
27	O	337	LEU	CA-C-O	7.23	129.57	121.11
28	H	198	MET	N-CA-CB	7.23	120.98	110.20
1	a	148	GLU	N-CA-C	-7.23	104.48	112.72
26	U	75	ASN	CA-C-O	7.23	128.41	120.82
27	O	118	GLY	O-C-N	7.23	130.22	122.41
27	O	145	LYS	CA-C-N	7.23	129.96	120.28
27	O	145	LYS	C-N-CA	7.23	129.96	120.28
14	n	181	ALA	CA-C-N	7.23	132.94	120.58
14	n	181	ALA	C-N-CA	7.23	132.94	120.58
27	O	58	ARG	N-CA-C	7.23	119.83	111.02
2	b	244	ASN	OD1-CG-ND2	-7.22	115.38	122.60
25	R	373	PRO	CA-C-N	7.22	130.55	120.29
25	R	373	PRO	C-N-CA	7.22	130.55	120.29
30	K	396	ARG	NE-CZ-NH2	7.22	125.70	119.20
27	O	253	GLN	N-CA-C	7.22	120.02	111.71
17	T	213	ASN	OD1-CG-ND2	7.21	129.81	122.60
26	U	210	TYR	CA-C-N	7.21	130.53	120.29
26	U	210	TYR	C-N-CA	7.21	130.53	120.29
15	W	74	ALA	CA-C-N	7.21	127.93	120.00
15	W	74	ALA	C-N-CA	7.21	127.93	120.00
17	T	11	LEU	N-CA-C	7.21	119.14	111.28
21	N	293	LEU	O-C-N	-7.21	113.93	120.71
24	Q	410	ASP	CA-CB-CG	7.21	119.81	112.60
5	e	84	ASP	CA-CB-CG	-7.21	105.39	112.60
7	G	96	ALA	CA-C-N	7.21	129.94	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	96	ALA	C-N-CA	7.21	129.94	120.28
10	3	124	PHE	N-CA-C	-7.21	98.12	109.07
10	j	149	MET	CG-SD-CE	-7.20	85.05	100.90
25	R	270	VAL	N-CA-C	-7.20	105.50	111.91
27	O	241	THR	N-CA-C	-7.20	104.64	113.50
21	N	91	ILE	N-CA-C	-7.20	106.11	113.10
22	S	55	ARG	NE-CZ-NH1	-7.20	114.30	121.50
21	N	191	THR	N-CA-C	7.20	118.92	111.14
1	A	19	PHE	N-CA-CB	7.20	120.65	110.36
9	2	203	ASP	N-CA-C	-7.20	97.67	109.40
13	m	93	SER	CA-C-N	7.20	130.64	120.42
13	m	93	SER	C-N-CA	7.20	130.64	120.42
4	d	70	HIS	ND1-CE1-NE2	7.20	115.60	108.40
4	d	96	HIS	CA-CB-CG	7.20	121.00	113.80
11	k	162	LYS	N-CA-C	-7.20	103.52	111.36
21	N	852	ASN	CA-CB-CG	7.20	119.80	112.60
7	g	112	PHE	O-C-N	-7.19	114.66	122.07
8	h	150	ASN	CA-CB-CG	-7.19	105.41	112.60
22	S	275	TYR	N-CA-CB	7.19	120.70	110.12
16	V	291	ASN	CB-CG-OD1	7.19	135.19	120.80
1	A	59	VAL	N-CA-C	-7.19	99.91	107.60
2	b	105	PRO	O-C-N	7.19	124.53	121.15
32	M	31	GLN	OE1-CD-NE2	7.19	129.79	122.60
8	1	162	ASP	N-CA-CB	7.19	120.69	110.12
21	N	832	HIS	CA-CB-CG	7.19	120.99	113.80
28	H	190	ARG	CA-C-O	7.19	130.79	120.51
5	e	232	ASP	CA-CB-CG	-7.19	105.41	112.60
14	7	77	PRO	N-CA-CB	7.18	110.02	103.34
8	1	20	GLY	N-CA-C	7.18	120.27	110.58
20	Z	255	LEU	CD1-CG-CD2	7.18	126.60	110.80
21	N	96	GLN	N-CA-C	-7.18	104.09	112.92
23	P	425	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
27	O	331	ALA	CA-C-N	7.18	130.61	120.42
27	O	331	ALA	C-N-CA	7.18	130.61	120.42
6	F	192	ALA	N-CA-C	7.18	119.10	111.28
17	T	76	ASP	CA-C-O	-7.18	113.28	120.82
3	C	153	PRO	N-CA-C	-7.17	104.58	114.27
15	W	22	PRO	CA-C-O	-7.17	112.90	122.08
21	N	102	VAL	CA-C-O	-7.17	113.57	121.17
12	l	101	VAL	CA-C-N	7.17	130.48	120.29
12	l	101	VAL	C-N-CA	7.17	130.48	120.29
5	e	243	LEU	N-CA-C	7.17	119.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	105	ARG	N-CA-C	7.17	119.09	111.28
11	4	29	LYS	CA-C-N	7.17	133.78	122.60
11	4	29	LYS	C-N-CA	7.17	133.78	122.60
30	K	169	VAL	N-CA-C	-7.17	97.00	108.90
4	D	45	GLY	N-CA-C	-7.17	100.14	111.18
4	D	182	LYS	N-CA-C	-7.17	102.66	111.40
17	T	27	LEU	CA-C-O	-7.17	111.39	118.34
33	J	47	GLN	N-CA-CB	7.17	120.37	109.91
20	Z	614	VAL	N-CA-C	-7.16	103.99	111.58
22	S	281	ALA	N-CA-CB	7.16	120.65	110.12
29	I	343	ARG	N-CA-C	-7.16	103.75	114.64
32	M	130	PRO	CA-C-O	-7.16	113.75	121.27
7	g	177	GLU	N-CA-CB	7.16	120.64	110.12
21	N	16	ASN	O-C-N	-7.16	113.53	122.19
27	O	202	SER	O-C-N	-7.16	114.47	123.06
5	e	23	GLN	OE1-CD-NE2	7.16	129.76	122.60
6	F	181	LYS	N-CA-C	7.16	119.94	111.71
21	N	202	PHE	CA-C-N	7.16	129.87	120.28
21	N	202	PHE	C-N-CA	7.16	129.87	120.28
21	N	651	PHE	CA-CB-CG	-7.16	106.64	113.80
29	I	430	GLU	N-CA-C	-7.16	104.35	113.23
27	O	283	HIS	CA-C-N	7.16	129.87	120.28
27	O	283	HIS	C-N-CA	7.16	129.87	120.28
3	C	141	ASP	N-CA-C	-7.16	97.76	108.99
13	m	203	HIS	CE1-NE2-CD2	-7.15	101.85	109.00
10	3	87	PHE	N-CA-C	-7.15	103.22	112.23
17	T	123	HIS	ND1-CE1-NE2	7.15	115.55	108.40
22	S	268	LEU	CA-C-O	-7.15	112.97	120.55
23	P	15	GLN	CA-C-N	7.15	130.26	120.46
23	P	15	GLN	C-N-CA	7.15	130.26	120.46
6	f	30	LYS	N-CA-CB	7.15	120.63	110.12
25	R	399	GLN	CA-C-N	7.15	129.85	120.28
25	R	399	GLN	C-N-CA	7.15	129.85	120.28
21	N	112	GLU	CA-C-N	7.14	129.85	120.28
21	N	112	GLU	C-N-CA	7.14	129.85	120.28
26	U	302	GLN	CA-C-N	7.14	129.73	120.44
26	U	302	GLN	C-N-CA	7.14	129.73	120.44
31	L	192	GLU	CA-C-N	7.14	130.43	120.29
31	L	192	GLU	C-N-CA	7.14	130.43	120.29
6	f	167	GLY	CA-C-O	7.14	127.92	119.50
7	G	101	LYS	CA-C-O	-7.14	113.32	120.82
26	U	212	ASP	O-C-N	7.14	129.42	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	376	PHE	CA-C-N	7.14	129.72	120.44
31	L	376	PHE	C-N-CA	7.14	129.72	120.44
27	O	326	HIS	ND1-CE1-NE2	7.14	115.54	108.40
6	f	214	ALA	N-CA-C	-7.14	96.93	109.06
3	C	194	LEU	CA-C-O	-7.14	112.99	120.55
15	W	67	ALA	CA-C-N	7.13	131.93	122.30
15	W	67	ALA	C-N-CA	7.13	131.93	122.30
33	J	103	ASN	CA-CB-CG	-7.13	105.47	112.60
29	I	199	GLU	N-CA-C	7.13	118.84	111.14
2	b	236	ARG	N-CA-C	-7.13	96.94	109.06
33	J	164	ILE	CB-CA-C	-7.13	104.67	111.44
14	7	159	PHE	CA-CB-CG	-7.12	106.68	113.80
22	S	332	PHE	N-CA-C	7.12	119.05	111.28
4	D	96	HIS	CG-CD2-NE2	7.12	114.32	107.20
4	D	220	ASP	N-CA-CB	7.12	122.03	110.42
23	P	112	LEU	CA-C-N	7.12	129.82	120.28
23	P	112	LEU	C-N-CA	7.12	129.82	120.28
27	O	281	ALA	N-CA-C	7.12	121.23	112.54
5	e	168	ASN	CA-CB-CG	-7.12	105.48	112.60
5	E	249	ALA	N-CA-C	-7.12	103.60	111.36
10	3	82	ILE	N-CA-C	-7.12	102.29	110.05
14	7	201	THR	N-CA-C	-7.12	98.13	109.59
21	N	669	GLU	CA-C-N	7.12	134.39	122.79
21	N	669	GLU	C-N-CA	7.12	134.39	122.79
25	R	239	THR	N-CA-C	-7.12	98.63	109.95
29	I	275	ALA	N-CA-C	7.12	119.74	109.84
21	N	469	VAL	CB-CA-C	-7.12	102.53	112.14
31	L	358	LEU	N-CA-C	-7.12	103.56	111.82
2	B	65	SER	N-CA-C	-7.12	96.74	108.76
29	I	95	GLN	N-CA-CB	7.11	120.69	110.16
5	E	132	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	A	27	GLN	CA-C-N	7.11	130.51	120.42
1	A	27	GLN	C-N-CA	7.11	130.51	120.42
6	F	24	TYR	CB-CG-CD2	-7.11	110.14	120.80
16	V	149	GLY	N-CA-C	-7.11	106.01	115.32
3	c	67	TYR	O-C-N	-7.11	114.60	123.27
8	1	199	PRO	CA-C-N	7.10	129.80	120.28
8	1	199	PRO	C-N-CA	7.10	129.80	120.28
17	T	85	LEU	N-CA-CB	7.10	120.31	110.01
19	Y	40	ILE	N-CA-C	-7.10	103.60	110.42
9	i	148	THR	CA-C-O	-7.10	113.66	121.33
16	V	215	ASN	N-CA-CB	7.10	120.64	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	248	ASP	CA-C-N	7.10	131.10	120.31
22	S	248	ASP	C-N-CA	7.10	131.10	120.31
27	O	235	HIS	CB-CG-ND1	7.10	133.35	122.70
6	f	72	LEU	N-CA-CB	7.09	123.51	111.66
25	R	283	THR	N-CA-C	-7.09	97.94	108.79
26	U	162	GLU	N-CA-C	-7.09	97.85	108.99
11	k	57	ALA	O-C-N	7.09	129.64	122.12
10	3	40	PHE	CA-CB-CG	-7.09	106.71	113.80
12	5	82	ARG	NE-CZ-NH2	-7.09	112.82	119.20
15	W	71	LYS	CA-C-N	7.09	130.53	120.53
15	W	71	LYS	C-N-CA	7.09	130.53	120.53
30	K	340	PHE	CA-CB-CG	-7.09	106.71	113.80
24	Q	392	GLN	OE1-CD-NE2	-7.09	115.51	122.60
17	T	64	VAL	CA-C-N	7.09	127.85	119.98
17	T	64	VAL	C-N-CA	7.09	127.85	119.98
7	G	130	ARG	O-C-N	-7.08	113.91	121.42
16	V	131	GLN	OE1-CD-NE2	7.08	129.68	122.60
22	S	164	ILE	CA-C-N	7.08	127.07	119.28
22	S	164	ILE	C-N-CA	7.08	127.07	119.28
23	P	230	HIS	CG-CD2-NE2	7.08	114.28	107.20
27	O	38	TRP	N-CA-C	-7.08	104.38	113.16
23	P	258	LYS	CA-C-N	7.08	127.07	119.28
23	P	258	LYS	C-N-CA	7.08	127.07	119.28
12	l	141	HIS	CA-C-N	7.08	131.07	120.31
12	l	141	HIS	C-N-CA	7.08	131.07	120.31
33	J	363	THR	O-C-N	7.08	130.22	122.15
10	3	107	PRO	CA-C-O	-7.08	113.23	121.86
10	j	90	LEU	CA-C-N	7.07	129.47	120.56
10	j	90	LEU	C-N-CA	7.07	129.47	120.56
24	Q	391	ASP	CA-CB-CG	7.07	119.67	112.60
4	d	199	LEU	CA-C-O	7.07	128.08	119.38
21	N	198	THR	N-CA-C	-7.07	101.86	112.54
21	N	618	ARG	N-CA-C	7.07	119.84	111.71
31	L	339	ARG	NE-CZ-NH1	7.07	128.57	121.50
2	B	17	LYS	N-CA-CB	7.07	122.44	110.49
22	S	371	LEU	CA-C-O	-7.07	112.93	120.42
8	1	162	ASP	CA-CB-CG	-7.07	105.53	112.60
21	N	445	GLY	CA-C-N	7.07	129.75	120.28
21	N	445	GLY	C-N-CA	7.07	129.75	120.28
11	k	191	GLN	CB-CG-CD	-7.06	100.59	112.60
2	B	68	THR	CA-CB-OG1	7.06	120.20	109.60
3	c	204	SER	CA-C-O	-7.06	113.43	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	185	ASN	OD1-CG-ND2	7.06	129.66	122.60
29	I	82	LEU	CA-C-N	7.06	128.92	120.09
29	I	82	LEU	C-N-CA	7.06	128.92	120.09
29	I	244	PHE	CA-CB-CG	7.06	120.86	113.80
2	B	50	LYS	N-CA-C	-7.06	98.34	109.07
21	N	719	ASN	OD1-CG-ND2	7.06	129.66	122.60
33	J	240	HIS	CB-CG-CD2	-7.06	122.02	131.20
7	G	225	ASN	OD1-CG-ND2	-7.06	115.54	122.60
17	T	182	LYS	CA-C-N	7.06	130.31	120.29
17	T	182	LYS	C-N-CA	7.06	130.31	120.29
24	Q	159	ASN	CA-CB-CG	7.05	119.65	112.60
26	U	59	ASP	CA-C-O	-7.05	112.81	120.92
11	4	94	SER	CA-C-N	7.05	129.61	120.44
11	4	94	SER	C-N-CA	7.05	129.61	120.44
10	3	134	LYS	N-CA-C	-7.05	102.71	112.30
28	H	269	ALA	O-C-N	-7.05	114.80	123.33
2	B	165	GLY	O-C-N	-7.05	116.84	122.90
33	J	207	ASP	CA-CB-CG	-7.05	105.55	112.60
22	S	385	SER	N-CA-C	7.05	118.75	111.14
8	h	33	ALA	CA-C-O	7.04	127.96	118.38
28	H	91	LEU	N-CA-C	-7.04	104.00	112.59
33	J	351	ASN	N-CA-C	-7.04	104.84	113.50
16	V	23	THR	CA-CB-OG1	7.04	120.16	109.60
21	N	444	HIS	CG-CD2-NE2	7.04	114.24	107.20
21	N	755	PRO	CA-C-O	-7.04	112.86	121.31
26	U	303	GLU	CB-CG-CD	-7.04	100.63	112.60
23	P	35	ALA	CA-C-N	7.04	130.29	120.29
23	P	35	ALA	C-N-CA	7.04	130.29	120.29
10	3	110	ALA	CA-C-O	-7.04	113.11	120.99
23	P	166	GLU	N-CA-C	-7.04	104.84	113.50
33	J	327	ILE	CA-C-N	7.04	129.59	120.44
33	J	327	ILE	C-N-CA	7.04	129.59	120.44
14	7	58	ASP	CA-CB-CG	-7.04	105.56	112.60
2	b	45	ILE	CA-C-O	-7.03	112.79	120.67
7	G	130	ARG	CA-C-N	7.03	127.45	119.92
7	G	130	ARG	C-N-CA	7.03	127.45	119.92
17	T	126	LEU	N-CA-CB	7.03	120.46	110.12
6	F	78	ALA	CA-C-N	7.03	127.02	119.28
6	F	78	ALA	C-N-CA	7.03	127.02	119.28
32	M	107	ASN	CA-C-N	7.03	129.58	120.44
32	M	107	ASN	C-N-CA	7.03	129.58	120.44
16	V	95	LEU	N-CA-C	-7.03	104.17	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	181	ILE	CA-C-N	7.03	130.00	120.44
9	i	181	ILE	C-N-CA	7.03	130.00	120.44
12	5	108	LYS	CB-CA-C	-7.03	99.64	111.02
18	X	70	PRO	CA-C-O	-7.03	113.66	121.32
6	F	5	ASN	N-CA-CB	7.03	121.73	111.54
26	U	142	GLN	CA-C-N	7.03	131.01	120.75
26	U	142	GLN	C-N-CA	7.03	131.01	120.75
27	O	230	PHE	CA-C-N	7.03	128.92	120.14
27	O	230	PHE	C-N-CA	7.03	128.92	120.14
21	N	826	GLU	N-CA-CB	7.02	120.19	110.01
13	6	205	GLN	N-CA-C	-7.02	103.28	112.41
2	b	13	SER	N-CA-CB	7.02	118.08	109.59
17	T	36	LYS	N-CA-C	-7.02	103.56	111.14
23	P	368	LEU	O-C-N	7.02	129.30	122.07
25	R	409	GLY	O-C-N	-7.02	115.45	122.19
4	d	30	GLY	CA-C-N	7.02	131.35	120.75
4	d	30	GLY	C-N-CA	7.02	131.35	120.75
23	P	52	LEU	N-CA-C	-7.01	103.64	111.28
1	A	205	PHE	CA-C-O	-7.01	113.12	120.55
4	D	168	SER	CA-C-N	7.01	129.67	120.28
4	D	168	SER	C-N-CA	7.01	129.67	120.28
18	X	86	ILE	CA-C-N	7.01	131.76	122.30
18	X	86	ILE	C-N-CA	7.01	131.76	122.30
25	R	29	LYS	N-CA-C	7.01	119.00	111.36
6	F	153	VAL	N-CA-CB	7.01	121.75	111.52
1	A	16	ILE	CA-C-O	7.00	128.21	120.71
7	G	84	ASP	N-CA-CB	-7.00	99.79	110.16
4	D	45	GLY	O-C-N	7.00	129.79	123.42
5	E	225	GLN	N-CA-C	7.00	119.80	111.33
26	U	219	LEU	N-CA-CB	7.00	119.49	110.04
27	O	323	ASN	OD1-CG-ND2	-7.00	115.60	122.60
33	J	272	MET	CA-C-N	7.00	129.54	120.44
33	J	272	MET	C-N-CA	7.00	129.54	120.44
21	N	23	TYR	CA-C-O	7.00	127.84	120.42
1	a	237	SER	CA-C-N	7.00	130.36	120.28
1	a	237	SER	C-N-CA	7.00	130.36	120.28
9	i	145	HIS	ND1-CE1-NE2	7.00	115.40	108.40
5	E	120	ALA	N-CA-C	7.00	119.76	111.71
8	1	134	ALA	CA-C-N	7.00	132.78	122.71
8	1	134	ALA	C-N-CA	7.00	132.78	122.71
3	c	194	LEU	CA-C-N	7.00	129.53	120.44
3	c	194	LEU	C-N-CA	7.00	129.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	105	PRO	CA-C-N	6.99	128.58	119.84
2	B	105	PRO	C-N-CA	6.99	128.58	119.84
17	T	123	HIS	CB-CG-CD2	-6.99	122.11	131.20
29	I	82	LEU	CA-C-O	-6.99	113.14	120.55
4	d	151	GLU	CA-C-N	6.99	126.69	119.56
4	d	151	GLU	C-N-CA	6.99	126.69	119.56
7	g	109	ILE	CA-C-O	-6.99	112.91	118.85
17	T	251	HIS	CE1-NE2-CD2	-6.99	102.01	109.00
31	L	190	ILE	O-C-N	-6.99	115.09	121.87
10	j	89	GLN	CB-CG-CD	6.98	124.47	112.60
27	O	267	ASP	N-CA-CB	6.98	120.38	110.12
32	M	337	LEU	N-CA-C	-6.98	101.99	112.04
6	f	52	ASN	CA-CB-CG	6.98	119.58	112.60
21	N	481	ALA	N-CA-C	6.98	118.54	111.07
22	S	451	ILE	N-CA-C	-6.98	105.92	112.83
10	3	149	MET	O-C-N	6.98	129.52	122.12
18	X	58	GLY	O-C-N	-6.98	113.07	122.35
21	N	378	ASN	CA-C-N	6.98	129.63	120.28
21	N	378	ASN	C-N-CA	6.98	129.63	120.28
24	Q	31	LEU	O-C-N	-6.98	114.83	122.09
1	A	150	LEU	N-CA-C	-6.97	104.42	114.12
13	6	97	ALA	O-C-N	6.97	129.51	122.12
29	I	236	VAL	CA-C-O	6.97	127.23	119.42
14	n	57	ALA	CA-C-N	6.97	131.28	120.75
14	n	57	ALA	C-N-CA	6.97	131.28	120.75
7	G	91	ARG	CA-C-N	6.97	127.84	120.03
7	G	91	ARG	C-N-CA	6.97	127.84	120.03
30	K	348	GLU	CA-C-N	6.97	129.62	120.28
30	K	348	GLU	C-N-CA	6.97	129.62	120.28
25	R	367	ASP	CA-CB-CG	-6.97	105.63	112.60
30	K	271	ILE	CA-C-O	6.97	127.64	120.39
9	2	239	THR	CA-C-N	6.97	130.76	120.87
9	2	239	THR	C-N-CA	6.97	130.76	120.87
16	V	215	ASN	CB-CA-C	-6.97	99.81	110.26
21	N	885	ILE	O-C-N	-6.97	114.75	122.83
32	M	67	GLU	CB-CA-C	-6.97	99.01	110.85
33	J	200	ARG	CA-C-N	6.97	129.61	120.28
33	J	200	ARG	C-N-CA	6.97	129.61	120.28
11	k	184	VAL	O-C-N	-6.96	115.74	123.26
15	W	39	ALA	CA-C-N	6.96	129.61	120.28
15	W	39	ALA	C-N-CA	6.96	129.61	120.28
4	d	59	ILE	CA-C-O	6.96	125.58	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	104	ARG	CA-C-N	6.96	130.00	120.46
9	2	104	ARG	C-N-CA	6.96	130.00	120.46
21	N	760	GLY	N-CA-C	-6.96	100.71	111.64
24	Q	226	HIS	CA-CB-CG	-6.96	106.84	113.80
33	J	233	LEU	CA-C-N	6.96	129.49	120.44
33	J	233	LEU	C-N-CA	6.96	129.49	120.44
24	Q	207	SER	N-CA-CB	6.96	120.74	109.95
30	K	161	MET	N-CA-C	-6.96	103.90	112.88
21	N	891	VAL	CA-C-N	6.96	127.36	119.92
21	N	891	VAL	C-N-CA	6.96	127.36	119.92
9	2	191	GLY	CA-C-N	6.96	129.32	120.56
9	2	191	GLY	C-N-CA	6.96	129.32	120.56
13	6	87	HIS	CE1-NE2-CD2	-6.96	102.05	109.00
22	S	337	ASN	CA-CB-CG	-6.96	105.64	112.60
5	E	222	ILE	N-CA-CB	6.95	120.66	111.90
17	T	217	THR	CA-C-N	6.95	130.88	120.31
17	T	217	THR	C-N-CA	6.95	130.88	120.31
33	J	57	PHE	N-CA-CB	6.95	120.45	110.16
9	2	117	PHE	CA-CB-CG	6.95	120.75	113.80
19	Y	15	ASP	CA-CB-CG	-6.95	105.65	112.60
9	i	88	ILE	N-CA-C	-6.95	103.43	111.00
3	C	193	ALA	O-C-N	-6.95	114.91	122.07
4	D	167	ASN	CA-CB-CG	-6.95	105.65	112.60
21	N	469	VAL	N-CA-C	6.95	117.71	110.62
27	O	92	PHE	CA-C-N	6.95	129.59	120.28
27	O	92	PHE	C-N-CA	6.95	129.59	120.28
2	B	122	THR	N-CA-C	-6.95	104.68	113.43
11	k	110	LYS	CA-C-N	6.95	132.71	122.08
11	k	110	LYS	C-N-CA	6.95	132.71	122.08
13	6	108	LYS	N-CA-C	-6.95	96.95	108.34
5	e	10	ARG	NE-CZ-NH1	6.94	128.44	121.50
10	3	177	ARG	NE-CZ-NH1	-6.94	114.56	121.50
14	7	228	PHE	O-C-N	-6.94	115.99	123.42
22	S	461	PHE	CA-C-N	6.94	130.15	120.29
22	S	461	PHE	C-N-CA	6.94	130.15	120.29
28	H	225	VAL	CA-CB-CG2	-6.94	98.60	110.40
22	S	323	LEU	CA-C-N	6.94	130.15	120.29
22	S	323	LEU	C-N-CA	6.94	130.15	120.29
23	P	354	SER	N-CA-CB	6.94	120.28	109.94
25	R	357	PHE	CA-CB-CG	-6.94	106.86	113.80
29	I	273	GLU	N-CA-C	-6.94	103.15	111.69
30	K	197	LEU	O-C-N	6.94	130.06	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	300	VAL	N-CA-CB	6.94	119.97	110.54
9	2	170	HIS	CA-CB-CG	-6.93	106.86	113.80
21	N	740	TRP	N-CA-C	-6.93	104.82	113.28
27	O	130	ASP	CA-C-N	6.93	129.57	120.28
27	O	130	ASP	C-N-CA	6.93	129.57	120.28
6	f	121	GLN	N-CA-C	6.93	118.49	111.07
6	f	166	GLN	N-CA-CB	6.93	120.98	110.30
21	N	499	HIS	CE1-NE2-CD2	-6.93	102.07	109.00
11	k	69	ILE	CA-C-N	6.93	129.87	120.44
11	k	69	ILE	C-N-CA	6.93	129.87	120.44
10	j	64	ASN	N-CA-C	-6.93	103.66	111.07
13	m	108	LYS	N-CA-C	-6.93	95.66	107.23
15	W	89	THR	CA-C-N	6.93	129.57	120.28
15	W	89	THR	C-N-CA	6.93	129.57	120.28
21	N	405	LEU	CA-C-N	6.93	129.57	120.28
21	N	405	LEU	C-N-CA	6.93	129.57	120.28
4	D	200	LEU	CA-C-N	6.93	129.56	120.28
4	D	200	LEU	C-N-CA	6.93	129.56	120.28
22	S	379	LEU	CA-C-N	6.93	129.56	120.28
22	S	379	LEU	C-N-CA	6.93	129.56	120.28
23	P	221	TYR	CA-C-N	6.93	130.13	120.29
23	P	221	TYR	C-N-CA	6.93	130.13	120.29
12	l	141	HIS	ND1-CE1-NE2	6.92	115.32	108.40
12	5	134	LEU	CA-C-N	6.92	128.79	120.14
12	5	134	LEU	C-N-CA	6.92	128.79	120.14
7	g	87	HIS	CB-CG-CD2	-6.92	122.20	131.20
6	f	230	VAL	O-C-N	6.92	128.91	122.06
11	k	159	ASP	CA-C-O	6.92	127.88	120.55
4	D	11	PHE	CA-CB-CG	-6.92	106.88	113.80
6	F	126	ARG	O-C-N	-6.92	117.01	121.85
6	F	224	ILE	N-CA-CB	6.91	120.63	111.64
21	N	264	SER	N-CA-C	6.91	118.61	111.14
21	N	858	LYS	N-CA-C	-6.91	98.52	109.23
33	J	35	ARG	CA-C-O	-6.91	112.57	120.24
10	3	188	TYR	CA-CB-CG	-6.91	101.46	113.90
18	X	55	LYS	O-C-N	-6.91	116.08	121.47
21	N	759	ILE	CA-C-N	6.91	128.52	120.71
21	N	759	ILE	C-N-CA	6.91	128.52	120.71
23	P	124	VAL	O-C-N	6.91	128.95	121.83
13	m	99	ARG	CA-C-N	6.91	129.84	120.44
13	m	99	ARG	C-N-CA	6.91	129.84	120.44
2	B	219	PRO	N-CA-C	-6.91	104.94	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	388	GLY	CA-C-N	6.91	130.81	120.31
27	O	388	GLY	C-N-CA	6.91	130.81	120.31
29	I	380	LEU	CA-C-N	6.91	129.93	120.46
29	I	380	LEU	C-N-CA	6.91	129.93	120.46
31	L	230	LEU	CA-C-N	6.91	129.54	120.28
31	L	230	LEU	C-N-CA	6.91	129.54	120.28
24	Q	315	ASN	CA-CB-CG	-6.91	105.69	112.60
5	e	130	GLU	N-CA-C	-6.91	98.85	109.14
8	h	164	ILE	O-C-N	6.91	128.68	121.91
21	N	539	MET	CA-C-N	6.90	130.80	120.31
21	N	539	MET	C-N-CA	6.90	130.80	120.31
25	R	408	ASP	CA-C-N	6.90	127.64	119.98
25	R	408	ASP	C-N-CA	6.90	127.64	119.98
1	A	90	ALA	CA-C-N	6.90	130.09	120.29
1	A	90	ALA	C-N-CA	6.90	130.09	120.29
6	F	114	ASP	CA-C-N	6.90	129.41	120.44
6	F	114	ASP	C-N-CA	6.90	129.41	120.44
22	S	377	TYR	N-CA-C	-6.90	103.84	111.36
33	J	298	ASP	CA-CB-CG	-6.90	105.70	112.60
8	h	162	ASP	N-CA-C	6.90	118.80	111.28
10	3	186	VAL	N-CA-C	-6.90	98.24	108.45
21	N	607	GLN	CA-C-N	6.90	130.09	120.29
21	N	607	GLN	C-N-CA	6.90	130.09	120.29
23	P	338	TRP	CA-C-O	6.90	127.73	120.42
30	K	223	VAL	CA-C-O	-6.90	113.33	120.71
31	L	73	GLN	N-CA-C	-6.90	103.86	112.90
31	L	273	HIS	CG-CD2-NE2	6.90	114.10	107.20
28	H	135	ASP	N-CA-C	-6.89	103.51	112.68
28	H	220	LYS	N-CA-C	-6.89	103.84	111.36
2	B	79	GLY	O-C-N	-6.89	114.88	121.77
13	6	228	LYS	CA-C-O	-6.89	113.45	120.96
21	N	313	LEU	N-CA-C	-6.89	103.69	111.14
24	Q	315	ASN	OD1-CG-ND2	6.89	129.49	122.60
33	J	15	HIS	CA-C-N	6.89	130.08	120.29
33	J	15	HIS	C-N-CA	6.89	130.08	120.29
1	a	205	PHE	N-CA-C	6.89	118.44	111.07
14	n	129	LEU	N-CA-C	6.89	118.79	111.28
25	R	173	THR	N-CA-CB	6.89	120.25	110.12
15	W	33	VAL	CA-C-N	6.89	129.40	120.44
15	W	33	VAL	C-N-CA	6.89	129.40	120.44
32	M	425	ARG	NE-CZ-NH1	-6.89	114.61	121.50
11	k	98	TYR	CB-CA-C	-6.88	98.73	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	43	ASP	N-CA-CB	6.88	122.12	110.49
21	N	223	LEU	CA-C-N	6.88	129.80	120.44
21	N	223	LEU	C-N-CA	6.88	129.80	120.44
28	H	211	VAL	CA-C-O	-6.88	113.17	120.53
1	a	87	ILE	O-C-N	-6.88	116.02	120.42
3	c	84	ALA	CA-C-N	6.88	129.50	120.28
3	c	84	ALA	C-N-CA	6.88	129.50	120.28
21	N	608	LEU	CB-CA-C	-6.88	99.15	110.85
2	B	11	THR	CA-CB-OG1	6.88	119.92	109.60
6	F	56	LEU	N-CA-C	-6.88	105.04	113.50
21	N	810	ALA	N-CA-C	6.88	120.93	112.54
32	M	405	ASN	CA-C-N	6.88	131.29	122.00
32	M	405	ASN	C-N-CA	6.88	131.29	122.00
33	J	290	ILE	N-CA-CB	6.88	120.34	111.67
6	f	19	LEU	N-CA-CB	6.88	121.37	110.57
25	R	21	VAL	CA-C-O	-6.88	110.74	119.95
13	6	159	ASP	N-CA-C	-6.87	104.78	113.02
19	Y	47	GLU	N-CA-C	-6.87	106.10	114.75
9	i	133	ASP	CA-CB-CG	6.87	119.47	112.60
14	7	172	SER	CA-C-N	6.86	126.83	119.28
14	7	172	SER	C-N-CA	6.86	126.83	119.28
17	T	162	ASP	CA-C-O	-6.86	113.14	120.42
20	Z	861	THR	N-CA-C	-6.86	106.80	114.62
19	Y	24	ILE	N-CA-C	-6.86	103.62	110.62
26	U	293	GLU	N-CA-C	6.86	118.76	111.28
26	U	212	ASP	CA-CB-CG	-6.86	105.74	112.60
26	U	225	ILE	CA-C-N	6.86	130.16	120.28
26	U	225	ILE	C-N-CA	6.86	130.16	120.28
29	I	174	ASP	CA-CB-CG	-6.86	105.74	112.60
21	N	826	GLU	CB-CA-C	-6.86	100.11	110.88
21	N	404	SER	N-CA-C	-6.86	103.26	111.69
16	V	107	TRP	CD2-CE2-CZ2	-6.85	115.55	122.40
30	K	338	ILE	N-CA-CB	6.85	119.74	111.31
15	W	12	ASN	CA-CB-CG	-6.85	105.75	112.60
19	Y	40	ILE	N-CA-CB	6.85	118.56	110.55
15	W	72	ILE	CA-C-N	6.85	129.46	120.28
15	W	72	ILE	C-N-CA	6.85	129.46	120.28
26	U	295	LYS	CA-C-N	6.85	130.14	120.42
26	U	295	LYS	C-N-CA	6.85	130.14	120.42
13	m	38	ILE	CA-C-O	-6.85	114.85	121.63
28	H	232	PRO	N-CA-C	-6.84	105.08	114.80
21	N	33	ASP	N-CA-C	-6.84	104.84	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	175	GLU	CA-C-N	6.84	129.45	120.28
23	P	175	GLU	C-N-CA	6.84	129.45	120.28
4	d	53	LYS	N-CA-C	-6.84	104.55	113.17
25	R	185	LEU	CA-C-N	6.84	129.45	120.28
25	R	185	LEU	C-N-CA	6.84	129.45	120.28
30	K	289	ASP	O-C-N	6.84	131.12	122.23
32	M	228	LYS	N-CA-CB	6.84	119.93	110.01
33	J	153	LEU	CA-C-N	6.84	130.00	120.29
33	J	153	LEU	C-N-CA	6.84	130.00	120.29
2	b	143	ASN	CA-C-O	6.84	126.55	118.69
7	G	195	GLN	N-CA-C	6.83	118.73	111.28
15	W	127	ARG	CA-C-N	6.83	130.70	120.31
15	W	127	ARG	C-N-CA	6.83	130.70	120.31
10	j	19	ASP	CA-CB-CG	-6.83	105.77	112.60
14	n	236	ASN	CA-CB-CG	6.83	119.43	112.60
22	S	261	HIS	CE1-NE2-CD2	-6.83	102.17	109.00
25	R	75	GLY	N-CA-C	-6.83	105.64	115.27
5	E	223	THR	N-CA-C	-6.83	97.22	108.76
10	3	40	PHE	N-CA-CB	6.83	122.03	110.49
25	R	356	ALA	CA-C-O	-6.83	113.65	120.82
10	j	41	GLU	CB-CG-CD	-6.83	101.00	112.60
30	K	198	TYR	CA-C-O	-6.83	113.65	120.82
11	k	23	ARG	NE-CZ-NH1	-6.82	114.68	121.50
22	S	82	TYR	N-CA-C	-6.82	98.48	109.40
13	m	21	LEU	CA-C-N	-6.82	115.97	122.66
13	m	21	LEU	C-N-CA	-6.82	115.97	122.66
12	l	241	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
14	n	215	ARG	CA-C-N	6.82	129.15	120.56
14	n	215	ARG	C-N-CA	6.82	129.15	120.56
8	1	94	LEU	CA-C-O	-6.82	113.19	120.42
11	4	34	LYS	N-CA-C	-6.82	103.10	112.03
22	S	404	LEU	CA-C-N	6.82	129.42	120.28
22	S	404	LEU	C-N-CA	6.82	129.42	120.28
23	P	221	TYR	N-CA-CB	6.82	120.15	110.12
23	P	227	ILE	N-CA-CB	-6.82	101.84	110.57
29	I	240	THR	CA-C-O	-6.82	113.19	120.42
7	G	223	GLU	N-CA-C	-6.82	102.86	113.02
21	N	654	GLN	CB-CA-C	-6.82	100.18	110.88
32	M	171	GLU	CA-C-N	6.82	129.82	120.35
32	M	171	GLU	C-N-CA	6.82	129.82	120.35
29	I	96	LEU	CA-C-N	6.81	129.97	120.29
29	I	96	LEU	C-N-CA	6.81	129.97	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	391	ASP	CA-CB-CG	-6.81	105.79	112.60
3	c	19	LEU	CA-C-N	6.81	130.66	120.31
3	c	19	LEU	C-N-CA	6.81	130.66	120.31
6	f	212	SER	N-CA-C	-6.81	97.87	109.24
10	3	48	HIS	ND1-CE1-NE2	6.81	115.21	108.40
32	M	47	GLU	N-CA-C	6.81	118.78	111.36
17	T	97	SER	N-CA-C	-6.80	106.18	114.75
21	N	543	ASP	N-CA-C	-6.80	104.18	113.30
16	V	289	GLU	CA-C-N	6.80	129.95	120.29
16	V	289	GLU	C-N-CA	6.80	129.95	120.29
22	S	89	LYS	CA-C-N	6.80	129.39	120.28
22	S	89	LYS	C-N-CA	6.80	129.39	120.28
31	L	170	MET	N-CA-CB	6.80	120.23	110.16
4	D	179	TYR	CA-C-N	6.80	133.21	122.74
4	D	179	TYR	C-N-CA	6.80	133.21	122.74
5	E	108	ASN	CA-CB-CG	-6.80	105.80	112.60
16	V	230	TYR	N-CA-C	-6.80	104.98	113.28
25	R	43	ARG	NE-CZ-NH2	-6.80	113.08	119.20
31	L	313	ASP	O-C-N	-6.80	115.07	123.36
6	f	101	ARG	N-CA-C	-6.80	98.98	109.24
6	f	135	ILE	CA-CB-CG1	6.80	121.95	110.40
4	D	62	SER	CA-C-O	-6.80	114.15	121.56
10	3	40	PHE	N-CA-C	-6.80	96.32	110.80
6	F	149	PRO	N-CA-C	6.79	123.66	113.81
8	1	127	SER	CB-CA-C	-6.79	104.61	114.87
21	N	212	ASP	CA-CB-CG	-6.79	105.81	112.60
24	Q	255	TYR	CA-C-N	6.79	129.93	120.29
24	Q	255	TYR	C-N-CA	6.79	129.93	120.29
25	R	259	PHE	CA-C-O	-6.79	113.70	120.70
4	d	17	ILE	O-C-N	-6.79	115.87	123.20
4	d	183	GLU	CA-C-N	6.79	124.62	119.66
4	d	183	GLU	C-N-CA	6.79	124.62	119.66
10	3	179	ALA	CA-C-O	-6.79	113.22	120.42
14	7	105	THR	CA-C-N	6.79	129.67	120.44
14	7	105	THR	C-N-CA	6.79	129.67	120.44
7	g	140	GLY	CA-C-N	6.79	132.37	122.94
7	g	140	GLY	C-N-CA	6.79	132.37	122.94
14	n	221	ASP	N-CA-C	-6.79	97.29	108.76
24	Q	146	TYR	CA-C-O	-6.79	113.23	120.42
33	J	165	GLU	CA-C-O	6.79	127.69	120.70
1	a	65	ASP	CA-C-O	-6.78	113.66	119.36
9	i	138	HIS	CE1-NE2-CD2	-6.78	102.22	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	145	GLY	CA-C-N	6.78	130.50	120.87
3	C	145	GLY	C-N-CA	6.78	130.50	120.87
33	J	44	LEU	CA-C-O	6.78	127.21	119.27
14	n	108	ALA	CA-C-N	6.78	130.46	120.90
14	n	108	ALA	C-N-CA	6.78	130.46	120.90
14	n	76	ILE	CA-C-N	6.78	127.31	119.99
14	n	76	ILE	C-N-CA	6.78	127.31	119.99
3	C	240	VAL	N-CA-CB	6.78	120.75	110.58
29	I	382	THR	CA-C-N	6.78	129.66	120.44
29	I	382	THR	C-N-CA	6.78	129.66	120.44
5	E	232	ASP	CA-CB-CG	-6.78	105.83	112.60
22	S	250	ALA	CA-C-N	6.78	129.91	120.29
22	S	250	ALA	C-N-CA	6.78	129.91	120.29
27	O	165	LEU	CA-C-N	6.78	129.36	120.28
27	O	165	LEU	C-N-CA	6.78	129.36	120.28
28	H	187	LEU	CA-C-N	6.78	124.61	119.66
28	H	187	LEU	C-N-CA	6.78	124.61	119.66
29	I	350	PHE	CA-CB-CG	-6.78	107.03	113.80
31	L	99	GLN	CG-CD-NE2	-6.78	106.23	116.40
31	L	371	THR	N-CA-C	-6.78	105.05	113.38
32	M	384	ASP	CA-CB-CG	-6.77	105.83	112.60
32	M	39	ASN	CA-C-N	6.77	129.36	120.28
32	M	39	ASN	C-N-CA	6.77	129.36	120.28
4	D	35	GLY	CA-C-O	-6.77	115.66	120.94
33	J	186	ILE	N-CA-C	-6.77	97.87	108.23
14	7	152	VAL	N-CA-CB	6.77	123.17	111.39
26	U	260	ASN	CA-CB-CG	6.77	119.37	112.60
29	I	191	ILE	CA-C-N	6.77	129.35	120.28
29	I	191	ILE	C-N-CA	6.77	129.35	120.28
11	k	36	ARG	NE-CZ-NH1	-6.77	114.73	121.50
9	2	68	PRO	CA-C-O	-6.76	109.51	119.18
17	T	207	ALA	CA-C-N	6.76	129.34	120.28
17	T	207	ALA	C-N-CA	6.76	129.34	120.28
24	Q	226	HIS	CA-C-N	6.76	129.34	120.28
24	Q	226	HIS	C-N-CA	6.76	129.34	120.28
26	U	106	ILE	O-C-N	6.76	128.43	121.87
1	A	137	LEU	O-C-N	-6.76	115.37	122.94
18	X	39	GLU	O-C-N	6.76	129.85	122.15
21	N	187	ASN	OD1-CG-ND2	6.76	129.36	122.60
10	3	48	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
14	7	158	GLN	OE1-CD-NE2	6.76	129.36	122.60
22	S	230	LYS	N-CA-C	6.76	118.30	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	74	GLU	CA-C-N	6.75	129.22	120.44
29	I	74	GLU	C-N-CA	6.75	129.22	120.44
13	m	226	GLU	N-CA-C	-6.75	100.49	110.48
18	X	35	ILE	N-CA-CB	6.75	118.70	111.00
21	N	240	GLN	CB-CG-CD	-6.75	101.12	112.60
21	N	650	ASP	N-CA-C	6.75	119.65	111.82
15	W	103	ASN	N-CA-CB	6.75	124.08	111.53
32	M	264	ARG	N-CA-C	6.75	119.47	111.71
6	f	190	ILE	CA-C-N	6.75	129.87	120.29
6	f	190	ILE	C-N-CA	6.75	129.87	120.29
17	T	133	ILE	N-CA-CB	6.75	118.31	110.82
1	A	169	THR	N-CA-C	-6.74	99.06	109.24
27	O	33	TYR	CA-C-N	6.74	129.32	120.28
27	O	33	TYR	C-N-CA	6.74	129.32	120.28
31	L	324	ILE	N-CA-CB	6.74	120.41	111.64
15	W	33	VAL	N-CA-C	6.74	117.44	110.36
28	H	95	HIS	CG-CD2-NE2	6.74	113.94	107.20
13	m	84	HIS	CG-CD2-NE2	6.74	113.94	107.20
10	3	181	SER	N-CA-C	-6.74	98.41	108.99
14	7	127	GLU	N-CA-C	-6.74	104.00	111.82
21	N	239	LEU	CA-C-N	6.74	130.56	120.31
21	N	239	LEU	C-N-CA	6.74	130.56	120.31
25	R	227	ALA	CA-C-N	6.74	129.31	120.28
25	R	227	ALA	C-N-CA	6.74	129.31	120.28
31	L	357	ARG	CB-CA-C	-6.74	99.39	110.85
7	g	112	PHE	CA-C-N	6.74	129.31	120.28
7	g	112	PHE	C-N-CA	6.74	129.31	120.28
8	h	44	THR	CA-C-O	6.74	127.80	120.32
11	k	133	HIS	CE1-NE2-CD2	-6.74	102.26	109.00
1	A	209	HIS	CG-CD2-NE2	6.74	113.94	107.20
21	N	410	LEU	N-CA-CB	6.74	120.03	110.12
5	E	181	ALA	CA-C-N	6.74	129.31	120.28
5	E	181	ALA	C-N-CA	6.74	129.31	120.28
33	J	363	THR	CA-C-O	-6.74	113.28	120.42
8	h	88	ALA	N-CA-C	6.74	118.42	111.14
8	h	93	GLU	CA-C-O	-6.74	113.41	120.55
10	j	48	HIS	ND1-CE1-NE2	6.73	115.13	108.40
16	V	67	ASP	O-C-N	-6.73	115.57	123.25
4	d	110	THR	CA-C-N	6.73	129.30	120.28
4	d	110	THR	C-N-CA	6.73	129.30	120.28
13	6	92	LEU	N-CA-C	-6.73	97.55	108.52
31	L	164	ASP	CA-C-O	-6.73	113.09	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	129	LEU	O-C-N	6.73	129.82	122.15
21	N	154	LEU	CA-C-N	6.73	127.40	120.00
21	N	154	LEU	C-N-CA	6.73	127.40	120.00
6	f	193	GLY	CA-C-N	6.73	129.97	120.42
6	f	193	GLY	C-N-CA	6.73	129.97	120.42
26	U	164	GLU	CA-C-N	6.72	129.84	120.29
26	U	164	GLU	C-N-CA	6.72	129.84	120.29
32	M	317	SER	N-CA-CB	6.72	121.85	110.49
3	c	25	ALA	CA-C-N	6.72	129.29	120.28
3	c	25	ALA	C-N-CA	6.72	129.29	120.28
26	U	114	THR	CA-C-N	6.72	132.72	122.37
26	U	114	THR	C-N-CA	6.72	132.72	122.37
32	M	105	ASN	CA-CB-CG	-6.72	105.88	112.60
3	c	87	LEU	CA-C-N	6.72	129.96	120.42
3	c	87	LEU	C-N-CA	6.72	129.96	120.42
6	f	93	ASN	CA-CB-CG	-6.72	105.88	112.60
32	M	335	PRO	N-CA-CB	6.72	110.29	102.76
21	N	881	TYR	N-CA-C	-6.72	104.21	112.88
22	S	122	ASN	N-CA-C	6.72	118.26	111.07
15	W	64	THR	CA-C-N	6.71	130.96	121.02
15	W	64	THR	C-N-CA	6.71	130.96	121.02
20	Z	628	ASN	CA-C-N	6.71	129.66	120.46
20	Z	628	ASN	C-N-CA	6.71	129.66	120.46
7	G	64	ASN	O-C-N	-6.71	115.42	123.27
23	P	339	GLU	CA-C-N	6.71	130.51	120.31
23	P	339	GLU	C-N-CA	6.71	130.51	120.31
6	F	13	PHE	CB-CA-C	-6.71	98.19	109.53
33	J	244	ILE	CA-C-N	6.71	130.87	122.48
33	J	244	ILE	C-N-CA	6.71	130.87	122.48
3	C	20	TYR	CA-C-N	6.71	130.51	120.31
3	C	20	TYR	C-N-CA	6.71	130.51	120.31
20	Z	918	ASP	CA-C-N	6.71	129.27	120.28
20	Z	918	ASP	C-N-CA	6.71	129.27	120.28
14	n	257	ASP	CA-C-N	6.71	130.24	120.91
14	n	257	ASP	C-N-CA	6.71	130.24	120.91
14	n	258	ILE	N-CA-C	-6.71	100.93	109.58
13	6	61	SER	N-CA-C	-6.71	96.81	108.69
20	Z	733	VAL	CA-C-N	6.71	129.81	120.29
20	Z	733	VAL	C-N-CA	6.71	129.81	120.29
19	Y	5	VAL	N-CA-CB	6.71	119.12	110.13
25	R	124	ASP	CA-CB-CG	-6.71	105.89	112.60
31	L	381	LYS	N-CA-C	6.71	118.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	97	TYR	CA-C-O	-6.71	114.99	121.02
28	H	247	LEU	CA-C-O	6.71	127.69	120.38
16	V	30	SER	N-CA-CB	6.70	119.85	110.26
18	X	56	PRO	N-CA-CB	-6.70	97.35	103.25
24	Q	48	ASP	CA-C-N	6.70	130.23	120.71
24	Q	48	ASP	C-N-CA	6.70	130.23	120.71
30	K	44	ASN	N-CA-CB	6.70	120.11	110.06
32	M	143	ASN	N-CA-CB	6.70	121.82	110.49
12	5	254	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
17	T	122	PHE	CA-CB-CG	-6.70	107.10	113.80
21	N	378	ASN	CA-CB-CG	-6.70	105.90	112.60
21	N	475	ALA	N-CA-C	6.70	118.24	111.07
1	A	237	SER	N-CA-CB	6.70	119.56	110.38
21	N	911	LYS	N-CA-C	-6.70	104.42	112.59
22	S	148	ASP	O-C-N	-6.70	115.02	122.12
13	m	112	PRO	CA-C-O	-6.70	113.45	121.48
27	O	318	HIS	CB-CG-CD2	-6.70	122.50	131.20
24	Q	303	ALA	CB-CA-C	-6.69	97.82	110.67
28	H	126	ASN	CA-C-O	6.69	126.41	119.05
10	j	48	HIS	CE1-NE2-CD2	-6.69	102.31	109.00
2	B	180	ASN	N-CA-C	-6.69	99.14	109.24
8	1	171	ALA	N-CA-CB	6.69	120.65	110.28
29	I	83	LYS	CA-C-O	-6.69	111.85	118.34
16	V	231	GLU	O-C-N	6.69	129.21	122.12
21	N	820	GLU	CA-C-N	6.69	129.14	120.44
21	N	820	GLU	C-N-CA	6.69	129.14	120.44
14	n	51	ASN	CA-C-O	6.69	126.59	119.03
17	T	236	ASN	CA-C-N	6.69	129.13	120.44
17	T	236	ASN	C-N-CA	6.69	129.13	120.44
27	O	249	ASP	CA-C-N	6.69	129.78	120.29
27	O	249	ASP	C-N-CA	6.69	129.78	120.29
1	A	248	ILE	CB-CA-C	-6.69	102.99	112.22
7	g	30	ALA	N-CA-C	6.68	118.57	111.28
1	A	91	ARG	N-CA-CB	6.68	120.05	110.16
12	5	241	HIS	ND1-CE1-NE2	6.68	115.08	108.40
27	O	46	THR	CA-C-N	6.68	129.24	120.28
27	O	46	THR	C-N-CA	6.68	129.24	120.28
16	V	199	LEU	N-CA-CB	6.68	122.46	110.83
21	N	900	ASN	OD1-CG-ND2	6.68	129.28	122.60
31	L	194	ARG	CA-C-O	-6.68	112.55	120.10
17	T	158	GLN	CA-C-N	6.68	129.23	120.28
17	T	158	GLN	C-N-CA	6.68	129.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	275	ASP	N-CA-C	-6.68	103.34	113.89
32	M	65	ASN	N-CA-CB	6.68	119.94	110.12
11	k	13	VAL	N-CA-C	-6.68	98.76	108.11
5	E	77	ALA	N-CA-C	-6.67	99.79	110.14
20	Z	626	PRO	CA-C-N	6.67	129.22	120.28
20	Z	626	PRO	C-N-CA	6.67	129.22	120.28
24	Q	321	TYR	CA-C-N	6.67	129.22	120.28
24	Q	321	TYR	C-N-CA	6.67	129.22	120.28
33	J	123	HIS	ND1-CE1-NE2	6.67	115.08	108.40
7	G	189	ALA	N-CA-C	-6.67	103.82	112.23
29	I	410	GLN	O-C-N	6.67	130.58	122.84
4	D	61	PRO	N-CA-C	6.67	122.13	111.26
4	D	112	TYR	CB-CG-CD1	6.67	130.81	120.80
20	Z	248	TYR	N-CA-CB	6.67	119.93	110.12
21	N	57	ASP	CA-CB-CG	-6.67	105.93	112.60
11	k	27	VAL	N-CA-CB	6.67	118.22	110.82
18	X	92	SER	N-CA-C	-6.67	97.40	108.34
25	R	44	LYS	CA-C-O	-6.67	113.35	120.42
6	f	152	ASN	CA-CB-CG	6.67	119.27	112.60
7	g	152	GLU	CA-C-N	6.67	126.80	119.87
7	g	152	GLU	C-N-CA	6.67	126.80	119.87
25	R	146	ASP	CA-CB-CG	-6.67	105.93	112.60
27	O	91	ASP	CA-CB-CG	-6.67	105.93	112.60
27	O	140	LYS	CA-C-N	6.67	132.16	122.36
27	O	140	LYS	C-N-CA	6.67	132.16	122.36
28	H	385	ARG	NE-CZ-NH2	-6.67	113.20	119.20
4	D	44	LEU	CA-C-O	6.67	127.31	120.24
12	5	213	GLY	CA-C-N	6.66	129.59	120.46
12	5	213	GLY	C-N-CA	6.66	129.59	120.46
23	P	49	ALA	N-CA-C	6.66	118.54	111.28
5	E	222	ILE	N-CA-C	-6.66	96.69	107.28
7	g	47	VAL	N-CA-C	-6.66	98.54	108.46
7	G	16	SER	N-CA-C	-6.66	102.47	110.13
7	g	230	PHE	CA-CB-CG	-6.66	107.14	113.80
8	h	192	VAL	CA-C-O	6.66	127.42	120.36
22	S	243	ASN	N-CA-C	6.66	119.54	111.82
26	U	70	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
11	k	67	TYR	CA-C-N	6.65	129.19	120.28
11	k	67	TYR	C-N-CA	6.65	129.19	120.28
2	B	230	ASP	CA-CB-CG	6.65	119.25	112.60
12	5	92	ASP	CA-CB-CG	6.65	119.25	112.60
27	O	326	HIS	CE1-NE2-CD2	-6.65	102.35	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	349	THR	N-CA-C	-6.65	96.22	107.99
30	K	242	PHE	CA-C-N	6.65	129.48	120.63
30	K	242	PHE	C-N-CA	6.65	129.48	120.63
21	N	226	ASN	CA-C-N	6.65	129.49	120.38
21	N	226	ASN	C-N-CA	6.65	129.49	120.38
24	Q	127	ARG	NE-CZ-NH1	6.65	128.15	121.50
5	e	136	ARG	CA-C-N	6.65	128.15	119.84
5	e	136	ARG	C-N-CA	6.65	128.15	119.84
12	l	88	ILE	N-CA-C	-6.65	98.86	108.36
3	C	13	PHE	N-CA-C	-6.65	98.07	108.90
33	J	349	LYS	CA-C-N	6.65	131.36	121.72
33	J	349	LYS	C-N-CA	6.65	131.36	121.72
13	m	92	LEU	N-CA-C	-6.64	99.08	109.25
1	A	125	SER	CA-C-O	6.64	127.59	120.55
20	Z	743	ILE	CA-C-N	6.64	129.18	120.28
20	Z	743	ILE	C-N-CA	6.64	129.18	120.28
23	P	373	GLU	O-C-N	-6.64	115.08	122.12
28	H	49	LEU	N-CA-C	-6.64	104.12	111.36
33	J	179	ILE	N-CA-CB	6.64	118.20	110.82
33	J	190	PRO	O-C-N	-6.64	118.25	121.31
7	G	66	LYS	N-CA-CB	6.64	120.32	110.49
8	1	123	PRO	O-C-N	6.64	131.61	122.64
20	Z	254	PRO	CA-C-O	-6.64	108.51	120.60
20	Z	747	ALA	O-C-N	6.64	128.91	122.07
22	S	484	ASP	CA-CB-CG	-6.64	105.96	112.60
32	M	267	PHE	CA-CB-CG	-6.64	107.16	113.80
33	J	313	LYS	CA-C-O	-6.64	113.20	120.24
16	V	63	VAL	CA-C-O	-6.64	113.35	120.59
7	G	16	SER	CA-C-N	6.64	126.23	119.19
7	G	16	SER	C-N-CA	6.64	126.23	119.19
16	V	237	ASN	CA-C-N	6.64	129.72	120.29
16	V	237	ASN	C-N-CA	6.64	129.72	120.29
25	R	78	ASP	CA-C-O	-6.64	113.89	121.19
3	c	146	TYR	N-CA-CB	6.64	119.85	109.83
5	E	216	ASN	CA-CB-CG	-6.64	105.96	112.60
32	M	169	ALA	CA-C-N	6.64	129.71	120.29
32	M	169	ALA	C-N-CA	6.64	129.71	120.29
3	c	13	PHE	CB-CA-C	-6.63	100.06	110.74
25	R	352	SER	CA-C-N	6.63	129.71	120.29
25	R	352	SER	C-N-CA	6.63	129.71	120.29
6	f	47	VAL	N-CA-C	-6.63	98.58	108.46
10	3	80	ARG	CA-C-N	6.63	131.35	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	80	ARG	C-N-CA	6.63	131.35	120.94
1	a	166	TYR	O-C-N	-6.63	115.48	123.10
10	j	36	VAL	N-CA-C	-6.63	105.86	111.56
9	2	96	SER	CA-C-N	6.63	129.70	120.29
9	2	96	SER	C-N-CA	6.63	129.70	120.29
13	6	74	LYS	CA-C-N	6.63	130.38	120.31
13	6	74	LYS	C-N-CA	6.63	130.38	120.31
16	V	60	ASP	N-CA-C	-6.63	102.72	113.19
2	b	97	TYR	O-C-N	6.62	128.74	122.18
15	W	33	VAL	CA-CB-CG1	6.62	121.66	110.40
25	R	105	LYS	CB-CA-C	-6.62	100.48	110.88
27	O	169	ASN	CA-CB-CG	-6.62	105.98	112.60
29	I	60	LEU	CA-C-N	6.62	129.45	120.44
29	I	60	LEU	C-N-CA	6.62	129.45	120.44
32	M	310	ASN	CA-C-O	-6.62	112.36	119.97
32	M	364	HIS	CG-CD2-NE2	6.62	113.82	107.20
4	D	103	PRO	CA-C-N	6.62	129.98	120.98
4	D	103	PRO	C-N-CA	6.62	129.98	120.98
12	5	109	VAL	N-CA-C	-6.62	98.84	108.11
22	S	371	LEU	O-C-N	6.62	129.69	122.15
1	A	182	LEU	O-C-N	6.62	129.69	122.15
6	F	113	CYS	CA-C-N	6.62	129.04	120.44
6	F	113	CYS	C-N-CA	6.62	129.04	120.44
19	Y	9	GLN	CB-CG-CD	-6.61	101.36	112.60
26	U	145	ASP	CA-CB-CG	6.61	119.21	112.60
5	e	167	TYR	N-CA-C	-6.61	99.11	108.96
23	P	195	GLN	CA-C-O	-6.61	113.54	120.55
3	c	116	SER	CA-C-N	6.61	129.14	120.28
3	c	116	SER	C-N-CA	6.61	129.14	120.28
14	7	249	ASN	CA-C-N	6.61	130.10	120.71
14	7	249	ASN	C-N-CA	6.61	130.10	120.71
16	V	158	LEU	CB-CA-C	6.61	120.69	109.72
24	Q	332	ARG	N-CA-C	6.61	118.56	111.36
29	I	322	VAL	N-CA-C	-6.61	97.99	107.77
26	U	8	VAL	N-CA-C	-6.61	98.10	107.75
29	I	287	ILE	CB-CA-C	6.61	118.08	110.88
1	a	124	LEU	O-C-N	-6.61	114.95	122.09
28	H	95	HIS	CE1-NE2-CD2	-6.61	102.39	109.00
29	I	327	ALA	N-CA-C	-6.61	98.95	109.59
29	I	58	LYS	CA-C-N	6.60	129.42	120.44
29	I	58	LYS	C-N-CA	6.60	129.42	120.44
6	F	110	HIS	CE1-NE2-CD2	-6.60	102.40	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	220	ARG	NE-CZ-NH1	-6.60	114.90	121.50
22	S	107	SER	N-CA-C	-6.60	102.36	112.99
2	b	201	GLU	N-CA-C	-6.60	97.84	109.06
21	N	190	LEU	O-C-N	-6.60	114.63	122.15
31	L	123	SER	O-C-N	6.60	131.57	122.46
6	f	21	GLN	CA-C-N	6.60	129.79	120.42
6	f	21	GLN	C-N-CA	6.60	129.79	120.42
1	A	73	PHE	CA-CB-CG	-6.60	107.20	113.80
32	M	367	LYS	O-C-N	-6.60	113.81	122.59
30	K	353	PHE	N-CA-C	6.60	118.47	111.28
31	L	162	GLU	CB-CG-CD	-6.60	101.39	112.60
31	L	253	ASP	O-C-N	6.60	130.64	122.92
9	i	145	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
12	l	267	ASP	CA-C-N	6.59	129.49	120.46
12	l	267	ASP	C-N-CA	6.59	129.49	120.46
5	E	52	LYS	N-CA-C	-6.59	97.61	108.76
21	N	730	VAL	CB-CA-C	-6.59	103.53	111.97
28	H	50	LYS	O-C-N	-6.59	115.13	122.12
21	N	649	VAL	O-C-N	-6.59	115.94	122.93
31	L	223	PRO	N-CA-C	-6.59	102.66	110.70
6	f	99	PHE	CA-CB-CG	-6.59	107.21	113.80
8	h	17	PHE	CA-CB-CG	6.59	120.39	113.80
11	4	159	ASP	CA-CB-CG	-6.59	106.01	112.60
16	V	294	SER	CA-C-N	6.59	129.49	120.46
16	V	294	SER	C-N-CA	6.59	129.49	120.46
24	Q	278	VAL	O-C-N	6.59	128.62	121.83
26	U	28	LYS	N-CA-C	-6.59	99.48	108.38
10	3	120	PHE	CA-C-N	6.59	133.16	122.69
10	3	120	PHE	C-N-CA	6.59	133.16	122.69
21	N	532	ALA	N-CA-C	-6.59	104.87	113.17
22	S	482	PRO	N-CA-C	-6.59	105.02	114.18
25	R	24	TYR	N-CA-C	-6.59	104.72	112.89
5	E	16	SER	CA-C-O	-6.59	111.78	121.46
20	Z	915	ALA	N-CA-C	-6.59	104.87	113.17
21	N	194	ILE	CA-C-O	-6.59	113.74	121.05
23	P	10	ASP	CA-CB-CG	-6.59	106.01	112.60
25	R	169	ASP	CA-C-N	6.59	129.77	120.42
25	R	169	ASP	C-N-CA	6.59	129.77	120.42
30	K	99	PHE	CA-CB-CG	-6.59	107.21	113.80
32	M	372	ASP	CA-CB-CG	6.59	119.19	112.60
4	D	191	CYS	CA-C-N	6.58	128.85	120.56
4	D	191	CYS	C-N-CA	6.58	128.85	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	178	ASN	N-CA-C	6.58	118.53	111.36
33	J	15	HIS	CE1-NE2-CD2	-6.58	102.42	109.00
11	k	21	VAL	O-C-N	6.58	130.18	123.20
23	P	165	VAL	N-CA-C	-6.58	103.36	113.16
22	S	405	ARG	NE-CZ-NH1	-6.58	114.92	121.50
33	J	88	VAL	N-CA-CB	6.58	118.06	110.49
26	U	3	LEU	N-CA-C	-6.58	104.88	113.17
3	C	200	THR	N-CA-C	6.58	119.27	111.71
31	L	223	PRO	CA-C-N	6.58	126.60	119.89
31	L	223	PRO	C-N-CA	6.58	126.60	119.89
15	W	117	PRO	CA-C-N	6.57	129.37	120.63
15	W	117	PRO	C-N-CA	6.57	129.37	120.63
16	V	109	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
27	O	86	LEU	CA-C-O	6.57	126.64	119.15
8	1	164	ILE	N-CA-C	6.57	117.32	110.62
16	V	269	ARG	N-CA-C	6.57	118.44	111.28
24	Q	83	GLU	N-CA-C	-6.57	104.05	111.14
32	M	261	LYS	CA-C-O	6.57	127.46	119.38
2	b	224	TYR	N-CA-C	-6.57	98.74	108.79
4	d	97	ARG	NE-CZ-NH2	6.57	125.11	119.20
14	n	256	LYS	CA-C-N	6.57	131.84	120.68
14	n	256	LYS	C-N-CA	6.57	131.84	120.68
13	6	200	THR	N-CA-C	-6.57	103.61	111.69
25	R	394	ASP	CA-CB-CG	-6.57	106.03	112.60
9	i	88	ILE	CA-C-O	-6.56	113.69	120.71
11	k	97	PRO	CB-CA-C	-6.56	101.54	110.60
10	3	30	GLY	N-CA-C	-6.56	101.07	111.18
7	G	90	ASN	CA-C-N	6.56	128.97	120.44
7	G	90	ASN	C-N-CA	6.56	128.97	120.44
28	H	356	ASN	N-CA-C	-6.56	103.62	111.69
5	e	63	SER	N-CA-C	-6.56	106.48	114.75
3	c	6	TYR	N-CA-C	-6.56	105.85	114.31
7	G	55	THR	N-CA-C	-6.56	104.06	111.14
17	T	54	ASP	CA-CB-CG	-6.56	106.04	112.60
24	Q	127	ARG	N-CA-C	-6.56	103.62	111.69
31	L	168	TYR	CA-C-N	6.56	131.79	120.58
31	L	168	TYR	C-N-CA	6.56	131.79	120.58
7	g	183	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
32	M	63	LYS	CA-C-O	-6.56	113.47	120.42
5	e	244	LYS	O-C-N	6.55	129.62	122.15
3	C	76	ALA	N-CA-C	-6.55	99.62	110.17
17	T	125	GLU	CB-CG-CD	-6.55	101.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	92	VAL	CA-CB-CG1	-6.55	99.26	110.40
30	K	256	ASP	N-CA-C	6.55	118.08	111.07
1	A	175	GLN	N-CA-C	6.55	119.26	111.33
8	1	185	VAL	CA-C-N	6.55	130.82	122.37
8	1	185	VAL	C-N-CA	6.55	130.82	122.37
10	3	139	SER	N-CA-C	-6.55	99.20	108.96
14	n	190	LYS	CA-C-N	6.55	128.94	120.56
14	n	190	LYS	C-N-CA	6.55	128.94	120.56
16	V	91	MET	CA-C-N	6.55	129.06	120.28
16	V	91	MET	C-N-CA	6.55	129.06	120.28
21	N	359	ALA	N-CA-C	6.55	118.76	110.24
28	H	274	VAL	N-CA-C	-6.55	98.70	108.46
13	m	103	HIS	CA-CB-CG	-6.55	107.25	113.80
14	n	105	THR	CA-C-N	6.55	129.59	120.29
14	n	105	THR	C-N-CA	6.55	129.59	120.29
10	3	136	PHE	N-CA-CB	6.55	121.56	110.49
12	5	280	GLY	N-CA-C	-6.55	104.81	114.90
13	6	155	MET	N-CA-C	6.55	122.46	113.16
2	b	214	ILE	N-CA-CB	6.55	120.14	112.35
11	k	53	THR	N-CA-CB	6.55	119.74	110.12
5	E	43	LYS	N-CA-C	-6.55	105.17	113.02
16	V	180	LEU	CA-C-N	6.55	131.22	120.94
16	V	180	LEU	C-N-CA	6.55	131.22	120.94
2	b	116	LYS	N-CA-C	-6.54	104.23	111.82
2	B	244	ASN	CB-CA-C	-6.54	99.72	110.85
5	E	54	ALA	N-CA-C	-6.54	97.61	108.34
9	2	101	ARG	CA-C-N	6.54	130.61	120.60
9	2	101	ARG	C-N-CA	6.54	130.61	120.60
6	f	54	ASP	N-CA-CB	6.54	121.55	110.49
13	6	84	HIS	N-CA-CB	6.54	119.74	110.12
27	O	53	LYS	CB-CA-C	-6.54	99.93	110.79
32	M	394	VAL	CB-CA-C	-6.54	103.70	111.94
7	g	13	SER	CA-C-O	6.54	125.82	119.08
25	R	125	GLU	N-CA-C	-6.54	96.87	110.80
29	I	56	LYS	N-CA-CB	6.54	119.84	110.16
2	b	30	GLN	O-C-N	6.54	130.18	122.34
5	e	163	THR	CA-C-N	6.54	131.41	122.19
5	e	163	THR	C-N-CA	6.54	131.41	122.19
22	S	420	GLU	N-CA-CB	6.54	119.68	109.94
26	U	213	LYS	N-CA-C	6.54	118.41	111.28
7	G	22	PHE	O-C-N	6.54	128.83	122.03
26	U	29	GLU	CA-C-N	6.54	134.00	123.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	29	GLU	C-N-CA	6.54	134.00	123.93
27	O	235	HIS	ND1-CE1-NE2	6.54	114.94	108.40
10	j	49	VAL	CA-C-O	-6.53	113.33	120.71
16	V	140	VAL	N-CA-CB	6.53	118.83	110.99
21	N	164	ASP	CA-C-O	6.53	127.43	120.70
21	N	746	ALA	N-CA-C	-6.53	104.49	114.16
23	P	351	ARG	N-CA-CB	6.53	119.72	110.12
3	c	160	TRP	CA-C-O	6.53	128.44	121.45
2	B	214	ILE	CA-C-O	6.53	127.37	120.51
16	V	109	HIS	ND1-CE1-NE2	6.53	114.93	108.40
22	S	73	THR	CA-C-N	6.53	129.56	120.29
22	S	73	THR	C-N-CA	6.53	129.56	120.29
15	W	69	PHE	N-CA-CB	6.53	119.82	110.16
4	D	113	VAL	N-CA-C	-6.53	104.13	110.72
22	S	49	ASP	N-CA-CB	6.53	118.12	110.42
24	Q	167	LYS	N-CA-CB	6.53	120.40	110.28
28	H	345	PRO	N-CA-CB	6.53	109.03	103.35
9	2	78	ALA	CB-CA-C	-6.52	99.96	110.79
17	T	35	ILE	CA-C-N	6.52	129.31	120.44
17	T	35	ILE	C-N-CA	6.52	129.31	120.44
23	P	51	ASP	CA-CB-CG	6.52	119.12	112.60
31	L	163	THR	CA-C-N	6.52	130.58	120.60
31	L	163	THR	C-N-CA	6.52	130.58	120.60
8	h	38	ARG	N-CA-C	-6.52	105.24	113.72
3	C	165	VAL	N-CA-C	-6.52	100.86	108.82
11	4	146	HIS	CA-CB-CG	-6.52	107.28	113.80
22	S	239	ARG	CA-C-N	6.52	129.31	120.44
22	S	239	ARG	C-N-CA	6.52	129.31	120.44
30	K	385	ALA	CB-CA-C	-6.52	100.59	110.90
26	U	269	THR	N-CA-C	6.52	120.97	112.89
33	J	31	GLU	N-CA-C	6.52	118.05	111.07
22	S	375	ASP	N-CA-CB	6.52	121.97	112.13
23	P	96	MET	N-CA-CB	6.52	119.46	110.01
28	H	105	ILE	N-CA-CB	6.52	118.43	111.46
32	M	239	THR	N-CA-C	6.52	119.38	111.82
32	M	240	ASN	N-CA-CB	6.52	121.51	110.49
13	m	48	GLU	CA-C-N	6.52	126.54	119.89
13	m	48	GLU	C-N-CA	6.52	126.54	119.89
4	D	52	LEU	O-C-N	-6.52	116.42	123.26
9	2	122	HIS	N-CA-C	-6.52	105.20	113.02
2	B	127	VAL	CA-CB-CG2	-6.51	99.33	110.40
15	W	86	HIS	CE1-NE2-CD2	-6.51	102.49	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	131	GLN	CB-CG-CD	-6.51	101.53	112.60
23	P	21	PHE	CA-CB-CG	-6.51	107.28	113.80
33	J	165	GLU	CB-CA-C	-6.51	100.61	110.90
20	Z	727	GLU	N-CA-CB	-6.51	100.00	109.83
21	N	270	LEU	CA-C-N	6.51	129.01	120.28
21	N	270	LEU	C-N-CA	6.51	129.01	120.28
25	R	124	ASP	N-CA-CB	6.51	120.79	110.57
7	G	22	PHE	N-CA-CB	6.51	119.42	109.91
8	1	63	ALA	O-C-N	6.51	129.57	122.15
17	T	107	SER	O-C-N	6.51	128.77	122.07
24	Q	75	ARG	CA-C-N	6.51	129.30	120.38
24	Q	75	ARG	C-N-CA	6.51	129.30	120.38
29	I	224	ALA	CA-C-O	-6.51	113.71	120.87
15	W	174	VAL	CA-C-N	6.51	129.50	120.65
15	W	174	VAL	C-N-CA	6.51	129.50	120.65
29	I	260	GLY	CA-C-N	6.51	126.09	119.19
29	I	260	GLY	C-N-CA	6.51	126.09	119.19
5	E	176	SER	N-CA-C	6.51	119.20	111.33
28	H	269	ALA	CA-C-N	6.50	129.99	120.82
28	H	269	ALA	C-N-CA	6.50	129.99	120.82
29	I	376	ASN	N-CA-C	-6.50	102.52	112.99
5	E	51	GLU	N-CA-C	-6.50	99.12	109.59
21	N	455	MET	CA-C-O	6.50	129.81	120.51
24	Q	130	ARG	O-C-N	6.50	130.36	122.75
12	5	272	PHE	CA-C-O	-6.50	113.66	120.55
21	N	233	ASN	CA-C-O	-6.50	113.67	121.40
10	3	71	THR	N-CA-C	6.50	118.44	111.36
17	T	162	ASP	O-C-N	6.50	129.56	122.15
21	N	690	HIS	CB-CA-C	-6.50	99.52	110.44
9	i	234	PHE	CA-C-N	6.50	127.96	119.84
9	i	234	PHE	C-N-CA	6.50	127.96	119.84
24	Q	66	VAL	CA-CB-CG1	6.50	121.44	110.40
29	I	126	PRO	N-CA-CB	6.50	109.00	103.35
32	M	249	PRO	CA-C-N	6.50	128.98	120.28
32	M	249	PRO	C-N-CA	6.50	128.98	120.28
2	B	149	GLN	N-CA-C	-6.50	98.31	108.90
26	U	61	LYS	O-C-N	6.50	130.03	122.17
5	e	176	SER	N-CA-C	6.49	119.19	111.33
7	g	183	HIS	CA-C-N	6.49	126.18	119.82
7	g	183	HIS	C-N-CA	6.49	126.18	119.82
33	J	240	HIS	ND1-CE1-NE2	6.49	114.89	108.40
20	Z	727	GLU	CA-C-N	6.49	133.94	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	727	GLU	C-N-CA	6.49	133.94	121.54
24	Q	295	GLY	CA-C-N	6.49	129.64	120.42
24	Q	295	GLY	C-N-CA	6.49	129.64	120.42
24	Q	321	TYR	N-CA-C	-6.49	103.01	111.71
9	i	229	GLN	CA-C-O	-6.49	112.13	119.79
13	m	13	TYR	CA-C-O	-6.49	114.48	121.94
22	S	97	THR	N-CA-CB	6.49	121.46	110.49
30	K	257	VAL	CB-CA-C	6.49	120.52	112.02
32	M	188	LYS	N-CA-C	6.49	118.35	111.28
11	k	21	VAL	CA-C-O	-6.49	113.64	120.39
16	V	134	SER	CA-C-O	6.49	127.42	119.11
23	P	133	GLU	CA-C-N	6.49	129.35	120.46
23	P	133	GLU	C-N-CA	6.49	129.35	120.46
33	J	391	ASN	CA-C-O	-6.49	113.54	120.42
7	g	123	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	A	220	LYS	N-CA-C	6.49	118.35	111.28
3	C	76	ALA	O-C-N	-6.49	115.64	123.10
20	Z	744	ALA	CA-C-N	6.49	128.97	120.28
20	Z	744	ALA	C-N-CA	6.49	128.97	120.28
25	R	31	PHE	CA-C-O	6.49	127.43	120.10
27	O	212	GLN	CG-CD-NE2	-6.49	106.67	116.40
31	L	401	PHE	CA-C-N	6.49	128.97	120.28
31	L	401	PHE	C-N-CA	6.49	128.97	120.28
33	J	165	GLU	N-CA-C	6.48	118.14	111.14
12	l	109	VAL	O-C-N	6.48	130.07	123.20
9	2	180	ALA	CA-C-O	-6.48	113.55	120.42
11	4	41	HIS	CA-CB-CG	-6.48	107.32	113.80
14	7	246	GLN	CA-C-O	6.48	127.45	120.38
29	I	54	ARG	CA-C-N	6.48	129.49	120.29
29	I	54	ARG	C-N-CA	6.48	129.49	120.29
30	K	242	PHE	N-CA-C	-6.48	105.33	112.72
5	e	168	ASN	N-CA-C	-6.48	105.29	113.72
6	f	220	THR	CA-C-N	6.48	126.94	120.52
6	f	220	THR	C-N-CA	6.48	126.94	120.52
5	E	197	GLU	CA-C-O	-6.48	113.68	120.55
23	P	72	TRP	CA-C-N	6.48	128.96	120.28
23	P	72	TRP	C-N-CA	6.48	128.96	120.28
3	C	234	GLU	CA-C-N	6.48	129.34	120.46
3	C	234	GLU	C-N-CA	6.48	129.34	120.46
19	Y	61	GLU	N-CA-CB	6.48	119.70	110.44
21	N	575	ALA	O-C-N	6.48	128.74	122.07
33	J	266	SER	CA-C-N	6.48	128.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	266	SER	C-N-CA	6.48	128.96	120.28
27	O	392	TRP	CA-C-O	6.48	127.19	118.38
14	n	141	ASN	CA-C-N	6.47	127.93	119.84
14	n	141	ASN	C-N-CA	6.47	127.93	119.84
3	c	160	TRP	O-C-N	-6.47	115.66	123.10
10	3	54	THR	N-CA-C	-6.47	100.88	110.46
17	T	94	HIS	CE1-NE2-CD2	-6.47	102.53	109.00
24	Q	305	ALA	CA-C-O	-6.47	113.06	120.24
31	L	216	LYS	N-CA-C	-6.47	99.23	109.07
5	e	39	GLY	O-C-N	-6.47	118.31	123.49
23	P	227	ILE	CA-C-O	-6.47	113.87	121.05
28	H	298	ALA	CA-C-N	6.47	129.48	120.29
28	H	298	ALA	C-N-CA	6.47	129.48	120.29
3	c	218	LYS	N-CA-C	-6.47	104.59	114.16
21	N	7	ALA	CA-C-O	-6.47	112.07	118.34
25	R	401	HIS	CA-C-N	6.47	128.85	120.44
25	R	401	HIS	C-N-CA	6.47	128.85	120.44
33	J	207	ASP	N-CA-CB	6.47	121.42	110.49
7	G	65	VAL	CA-CB-CG2	6.46	121.39	110.40
10	3	62	THR	N-CA-CB	6.46	119.62	110.12
21	N	366	THR	CA-C-O	-6.46	114.03	120.82
13	6	97	ALA	N-CA-CB	6.46	119.62	110.12
14	7	207	GLU	CA-C-O	-6.46	113.57	120.42
21	N	747	HIS	ND1-CE1-NE2	6.46	114.86	108.40
22	S	18	LEU	CA-C-N	6.46	128.94	120.28
22	S	18	LEU	C-N-CA	6.46	128.94	120.28
26	U	116	ASN	CA-CB-CG	-6.46	106.14	112.60
30	K	426	PHE	CA-CB-CG	-6.46	107.34	113.80
9	i	206	VAL	N-CA-CB	6.46	118.75	110.99
6	F	137	TYR	CA-C-O	-6.46	113.35	120.33
21	N	293	LEU	CA-C-N	6.46	126.69	119.32
21	N	293	LEU	C-N-CA	6.46	126.69	119.32
25	R	363	PHE	N-CA-C	6.46	118.32	111.28
12	l	141	HIS	CE1-NE2-CD2	-6.46	102.54	109.00
5	E	77	ALA	N-CA-CB	6.46	120.80	110.85
24	Q	92	LYS	N-CA-C	-6.46	104.97	112.92
1	a	244	ARG	N-CA-C	6.46	118.32	111.28
14	n	135	GLN	CA-C-N	6.46	129.46	120.29
14	n	135	GLN	C-N-CA	6.46	129.46	120.29
1	A	136	PRO	CA-C-O	-6.46	113.79	121.67
17	T	93	ASN	CA-C-N	6.46	131.30	122.19
17	T	93	ASN	C-N-CA	6.46	131.30	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	348	VAL	N-CA-C	-6.46	98.82	108.12
30	K	347	ARG	CG-CD-NE	-6.46	97.79	112.00
21	N	891	VAL	CA-C-O	-6.46	111.30	119.95
9	2	237	GLY	N-CA-C	-6.46	106.41	115.32
28	H	256	LYS	O-C-N	6.46	128.96	122.12
16	V	245	VAL	CA-CB-CG2	-6.45	99.43	110.40
22	S	121	VAL	O-C-N	-6.45	115.19	121.90
24	Q	4	PRO	CA-C-N	6.45	127.28	119.99
24	Q	4	PRO	C-N-CA	6.45	127.28	119.99
24	Q	265	MET	N-CA-C	-6.45	104.33	111.36
27	O	168	THR	N-CA-C	-6.45	104.33	111.82
33	J	16	GLU	CA-C-N	6.45	128.93	120.28
33	J	16	GLU	C-N-CA	6.45	128.93	120.28
10	3	158	LEU	O-C-N	6.45	130.29	123.06
24	Q	126	LYS	CA-C-O	6.45	125.55	118.65
24	Q	280	ASN	O-C-N	-6.45	114.80	122.15
23	P	415	TRP	O-C-N	-6.45	114.34	122.27
6	F	82	ARG	CA-C-N	6.45	128.81	120.56
6	F	82	ARG	C-N-CA	6.45	128.81	120.56
19	Y	53	ALA	N-CA-C	6.45	118.31	111.28
26	U	28	LYS	O-C-N	6.45	129.89	122.99
17	T	113	LEU	CA-C-N	6.44	128.91	120.28
17	T	113	LEU	C-N-CA	6.44	128.91	120.28
2	b	147	LEU	N-CA-C	-6.44	97.73	108.75
4	D	38	GLY	N-CA-C	-6.44	97.91	113.18
10	j	97	GLU	N-CA-C	6.44	117.96	111.07
17	T	242	LYS	O-C-N	-6.44	115.29	122.12
22	S	280	ASN	O-C-N	-6.44	115.44	122.07
33	J	171	PRO	CB-CA-C	6.44	117.81	109.89
10	j	84	PRO	N-CA-C	6.44	122.34	113.65
3	c	6	TYR	CA-C-N	6.43	135.18	122.31
3	c	6	TYR	C-N-CA	6.43	135.18	122.31
10	j	88	THR	N-CA-C	-6.43	104.27	111.28
12	l	260	TRP	CE2-CD2-CE3	6.43	125.23	118.80
4	D	193	LYS	O-C-N	6.43	129.75	122.22
7	G	242	PHE	CA-C-N	6.43	128.80	120.44
7	G	242	PHE	C-N-CA	6.43	128.80	120.44
18	X	78	ILE	N-CA-CB	6.43	121.85	111.23
15	W	165	GLN	CA-C-N	6.43	134.02	122.38
15	W	165	GLN	C-N-CA	6.43	134.02	122.38
26	U	42	ASN	CA-CB-CG	-6.43	106.17	112.60
11	4	84	VAL	CA-C-N	6.43	128.90	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	84	VAL	C-N-CA	6.43	128.90	120.28
20	Z	153	TYR	CA-C-N	6.43	129.27	120.46
20	Z	153	TYR	C-N-CA	6.43	129.27	120.46
23	P	403	GLU	N-CA-CB	6.43	121.35	110.49
28	H	263	VAL	CA-C-O	6.43	127.82	119.85
12	l	121	ALA	CA-C-N	6.43	127.35	121.31
12	l	121	ALA	C-N-CA	6.43	127.35	121.31
9	2	43	ILE	N-CA-C	-6.43	98.79	108.17
10	3	48	HIS	CG-CD2-NE2	6.43	113.63	107.20
25	R	217	HIS	ND1-CE1-NE2	6.43	114.83	108.40
29	I	386	ASP	N-CA-C	6.42	120.75	111.56
6	F	120	THR	CA-C-O	-6.42	113.68	120.55
15	W	18	ASN	O-C-N	6.42	130.44	122.86
6	f	3	ARG	CD-NE-CZ	-6.42	115.41	124.40
3	C	197	LEU	CA-C-N	6.42	128.79	120.44
3	C	197	LEU	C-N-CA	6.42	128.79	120.44
13	m	146	ALA	CA-C-O	-6.42	113.39	120.38
9	2	182	LYS	CA-C-N	6.42	128.88	120.28
9	2	182	LYS	C-N-CA	6.42	128.88	120.28
9	2	202	VAL	CB-CA-C	-6.42	101.13	110.63
24	Q	226	HIS	ND1-CE1-NE2	6.42	114.82	108.40
32	M	98	GLU	CB-CA-C	-6.42	100.80	110.88
11	4	99	GLN	N-CA-C	-6.42	97.90	108.49
24	Q	351	ILE	CA-C-N	6.42	128.86	120.26
24	Q	351	ILE	C-N-CA	6.42	128.86	120.26
1	A	208	THR	CA-C-N	6.41	129.40	120.29
1	A	208	THR	C-N-CA	6.41	129.40	120.29
2	B	58	SER	N-CA-CB	6.41	120.08	110.65
5	E	168	ASN	N-CA-C	-6.41	105.61	113.50
21	N	191	THR	CA-C-N	6.41	129.51	120.28
21	N	191	THR	C-N-CA	6.41	129.51	120.28
31	L	115	GLU	N-CA-C	-6.41	106.42	114.56
7	g	105	THR	N-CA-C	-6.41	97.84	108.23
13	m	77	LYS	N-CA-CB	-6.41	100.70	110.12
11	4	95	ARG	O-C-N	6.41	128.67	122.07
20	Z	207	ILE	N-CA-C	-6.41	105.33	113.22
6	f	173	GLU	CA-C-N	6.41	128.87	120.28
6	f	173	GLU	C-N-CA	6.41	128.87	120.28
14	7	145	ASN	CB-CA-C	-6.41	98.70	110.62
20	Z	806	GLU	N-CA-C	-6.41	101.79	111.34
22	S	180	ASN	N-CA-CB	6.41	121.17	110.41
5	e	51	GLU	CA-C-O	-6.41	113.78	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	131	GLU	CA-C-N	6.41	130.46	121.24
5	e	131	GLU	C-N-CA	6.41	130.46	121.24
6	F	93	ASN	CA-CB-CG	6.41	119.00	112.60
10	3	102	PRO	N-CA-CB	-6.41	96.53	103.25
20	Z	748	LEU	CA-CB-CG	6.41	138.72	116.30
21	N	316	LYS	CA-C-N	6.41	129.39	120.29
21	N	316	LYS	C-N-CA	6.41	129.39	120.29
24	Q	175	VAL	O-C-N	6.41	128.08	121.87
30	K	133	PRO	CA-C-O	-6.41	114.04	121.34
10	3	151	GLU	CA-C-N	6.40	128.76	120.44
10	3	151	GLU	C-N-CA	6.40	128.76	120.44
7	G	161	LYS	CA-C-N	6.40	133.96	121.41
7	G	161	LYS	C-N-CA	6.40	133.96	121.41
25	R	209	ARG	CA-C-N	6.40	128.86	120.28
25	R	209	ARG	C-N-CA	6.40	128.86	120.28
25	R	171	MET	CA-C-N	6.40	128.86	120.28
25	R	171	MET	C-N-CA	6.40	128.86	120.28
6	F	217	GLY	CA-C-N	6.40	128.85	120.28
6	F	217	GLY	C-N-CA	6.40	128.85	120.28
21	N	886	LYS	N-CA-C	-6.40	105.47	113.28
16	V	100	ARG	NE-CZ-NH2	-6.40	113.44	119.20
21	N	129	ILE	N-CA-CB	6.40	117.50	110.53
22	S	338	MET	N-CA-C	-6.40	105.43	112.72
2	b	28	VAL	CB-CA-C	-6.40	103.50	112.14
30	K	66	ASP	N-CA-C	6.40	118.25	111.28
6	F	11	VAL	CA-C-O	6.39	124.94	119.38
21	N	15	GLU	CB-CG-CD	-6.39	101.73	112.60
31	L	137	ARG	N-CA-C	-6.39	102.89	112.54
32	M	93	ASP	N-CA-C	-6.39	105.06	112.92
6	F	3	ARG	CA-C-N	6.39	133.21	121.70
6	F	3	ARG	C-N-CA	6.39	133.21	121.70
21	N	634	LEU	N-CA-C	-6.39	97.96	108.76
23	P	433	ILE	CA-C-N	6.39	128.85	120.28
23	P	433	ILE	C-N-CA	6.39	128.85	120.28
26	U	200	LEU	CA-C-N	6.39	128.85	120.28
26	U	200	LEU	C-N-CA	6.39	128.85	120.28
27	O	300	VAL	CA-C-O	-6.39	114.39	121.17
29	I	81	ILE	CA-C-N	6.39	128.84	120.28
29	I	81	ILE	C-N-CA	6.39	128.84	120.28
6	F	63	ILE	N-CA-C	-6.39	99.16	108.11
18	X	123	ASN	CB-CG-ND2	-6.39	106.81	116.40
3	c	33	GLY	N-CA-C	6.39	122.28	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	93	ALA	O-C-N	-6.39	115.35	122.12
19	Y	67	VAL	CA-CB-CG2	6.39	121.26	110.40
21	N	759	ILE	N-CA-CB	6.39	119.94	111.64
4	d	120	TYR	N-CA-CB	6.38	119.71	110.20
19	Y	52	ASN	OD1-CG-ND2	6.38	128.98	122.60
21	N	579	SER	N-CA-C	-6.38	105.53	113.38
1	a	221	ASN	CA-C-N	6.38	131.65	121.18
1	a	221	ASN	C-N-CA	6.38	131.65	121.18
21	N	35	LEU	CA-C-N	6.38	128.83	120.28
21	N	35	LEU	C-N-CA	6.38	128.83	120.28
31	L	139	LYS	CA-C-O	6.38	127.01	119.48
6	F	24	TYR	CB-CG-CD1	6.38	130.37	120.80
25	R	308	LEU	CA-C-N	6.38	129.35	120.29
25	R	308	LEU	C-N-CA	6.38	129.35	120.29
27	O	77	SER	N-CA-C	6.38	118.24	111.28
31	L	423	ALA	CB-CA-C	-6.38	100.86	110.88
9	2	94	LEU	CA-C-N	6.38	128.83	120.28
9	2	94	LEU	C-N-CA	6.38	128.83	120.28
7	G	111	ALA	O-C-N	-6.38	115.50	122.07
16	V	293	VAL	CA-C-O	-6.38	114.32	120.95
30	K	159	SER	CA-C-N	6.38	129.22	120.35
30	K	159	SER	C-N-CA	6.38	129.22	120.35
7	g	241	ASP	CA-C-N	6.38	129.11	120.44
7	g	241	ASP	C-N-CA	6.38	129.11	120.44
4	D	170	THR	N-CA-CB	6.38	119.70	110.20
9	2	188	ILE	O-C-N	6.38	130.56	121.82
27	O	12	SER	N-CA-C	6.38	118.23	111.28
29	I	402	LEU	CA-C-N	6.38	128.82	120.28
29	I	402	LEU	C-N-CA	6.38	128.82	120.28
33	J	87	LYS	N-CA-CB	6.38	119.85	110.35
1	a	62	LYS	CA-C-O	6.37	126.99	119.28
5	E	210	GLU	N-CA-C	-6.37	101.09	110.52
9	2	226	GLU	N-CA-CB	6.37	120.95	110.69
25	R	268	SER	N-CA-CB	6.37	120.16	110.28
11	k	41	HIS	CE1-NE2-CD2	-6.37	102.63	109.00
1	A	38	THR	CA-C-O	-6.37	111.70	118.77
11	4	141	PHE	CA-C-N	6.37	129.34	120.29
11	4	141	PHE	C-N-CA	6.37	129.34	120.29
5	E	62	ASP	N-CA-C	-6.37	105.44	113.72
23	P	219	GLU	N-CA-C	-6.37	103.86	111.69
11	k	133	HIS	ND1-CE1-NE2	6.37	114.77	108.40
1	A	174	LYS	N-CA-C	-6.37	104.13	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	91	GLU	CA-C-N	6.37	129.10	120.44
29	I	91	GLU	C-N-CA	6.37	129.10	120.44
28	H	244	LYS	N-CA-C	-6.37	104.46	112.93
11	k	110	LYS	CB-CA-C	-6.36	98.38	109.07
16	V	183	ALA	N-CA-CB	6.36	121.24	110.49
28	H	426	ALA	N-CA-CB	6.36	120.14	110.28
6	f	219	ASP	N-CA-C	-6.36	105.17	114.39
2	B	100	ILE	CA-C-N	6.36	131.46	120.58
2	B	100	ILE	C-N-CA	6.36	131.46	120.58
5	E	24	VAL	CA-C-N	6.36	128.80	120.28
5	E	24	VAL	C-N-CA	6.36	128.80	120.28
7	G	76	CYS	O-C-N	-6.36	115.63	123.33
24	Q	40	ALA	CA-C-O	-6.36	114.21	121.65
27	O	279	ILE	CB-CA-C	-6.36	103.72	112.24
10	3	112	ILE	CA-C-N	6.36	130.35	120.75
10	3	112	ILE	C-N-CA	6.36	130.35	120.75
10	j	145	GLN	OE1-CD-NE2	6.36	128.96	122.60
11	4	158	LEU	N-CA-C	-6.36	103.87	111.69
22	S	274	PHE	CA-CB-CG	6.36	120.16	113.80
31	L	375	ASP	N-CA-C	-6.36	105.10	112.92
13	m	56	ASP	N-CA-C	-6.36	104.83	112.58
21	N	642	ASP	CA-C-N	6.36	126.04	119.56
21	N	642	ASP	C-N-CA	6.36	126.04	119.56
22	S	51	ARG	N-CA-CB	6.36	119.59	110.06
22	S	60	LEU	CA-C-N	6.36	128.79	120.28
22	S	60	LEU	C-N-CA	6.36	128.79	120.28
25	R	72	VAL	CA-C-O	6.36	128.72	120.78
30	K	199	GLU	CA-C-N	6.36	129.31	120.29
30	K	199	GLU	C-N-CA	6.36	129.31	120.29
21	N	45	ASP	CA-C-O	6.35	127.15	120.42
9	2	102	GLU	CA-C-N	6.35	126.57	119.90
9	2	102	GLU	C-N-CA	6.35	126.57	119.90
10	3	73	LEU	CA-C-N	6.35	128.70	120.44
10	3	73	LEU	C-N-CA	6.35	128.70	120.44
22	S	432	ILE	N-CA-C	-6.35	104.66	110.82
13	6	214	ILE	N-CA-C	-6.35	99.22	108.11
30	K	202	GLY	N-CA-C	-6.35	105.86	115.00
32	M	136	ASP	CA-C-N	6.35	126.47	119.87
32	M	136	ASP	C-N-CA	6.35	126.47	119.87
33	J	251	ASP	N-CA-CB	6.35	121.10	111.70
12	l	231	LEU	O-C-N	6.35	128.85	122.12
2	B	111	VAL	CA-C-N	6.35	128.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	111	VAL	C-N-CA	6.35	128.79	120.28
14	7	81	ASN	OD1-CG-ND2	6.35	128.95	122.60
24	Q	427	PHE	O-C-N	6.35	130.94	122.43
9	i	75	ALA	N-CA-C	-6.35	99.91	108.86
13	6	70	ASP	N-CA-C	-6.35	104.23	112.23
29	I	296	SER	N-CA-C	-6.35	104.33	113.21
8	h	86	THR	CA-C-N	6.34	128.78	120.28
8	h	86	THR	C-N-CA	6.34	128.78	120.28
14	n	193	ASP	CA-CB-CG	-6.34	106.26	112.60
17	T	208	LEU	O-C-N	-6.34	115.39	122.12
21	N	510	HIS	ND1-CE1-NE2	6.34	114.75	108.40
33	J	400	VAL	N-CA-CB	6.34	121.70	111.23
4	D	187	THR	N-CA-CB	6.34	122.48	111.00
16	V	120	SER	N-CA-C	6.34	119.00	111.33
4	d	186	ALA	N-CA-C	-6.34	104.85	112.59
26	U	26	GLN	CA-C-N	6.34	129.83	120.95
26	U	26	GLN	C-N-CA	6.34	129.83	120.95
29	I	320	GLY	N-CA-C	-6.34	105.36	112.33
29	I	383	THR	CA-C-N	6.34	129.76	120.82
29	I	383	THR	C-N-CA	6.34	129.76	120.82
1	a	212	ASP	CB-CA-C	-6.34	100.88	110.90
3	c	187	ASP	N-CA-C	-6.34	104.47	111.82
4	D	57	THR	N-CA-C	-6.34	104.10	113.61
31	L	306	MET	N-CA-CB	6.34	119.54	110.16
24	Q	89	ALA	N-CA-CB	6.34	121.20	110.49
10	j	134	LYS	N-CA-C	-6.34	103.73	112.03
22	S	74	LEU	O-C-N	6.34	129.37	122.15
25	R	220	ALA	N-CA-C	6.33	119.17	111.82
31	L	387	ASN	N-CA-C	-6.33	99.83	108.38
14	7	134	TYR	CA-C-O	6.33	127.26	120.10
17	T	53	ASN	CA-CB-CG	6.33	118.93	112.60
17	T	89	TYR	CB-CG-CD1	6.33	130.30	120.80
17	T	77	SER	CA-C-N	6.33	128.67	120.44
17	T	77	SER	C-N-CA	6.33	128.67	120.44
20	Z	729	GLU	N-CA-CB	6.33	121.19	110.49
27	O	172	TYR	N-CA-CB	6.33	120.09	110.28
21	N	235	ALA	CA-C-N	6.33	126.96	120.00
21	N	235	ALA	C-N-CA	6.33	126.96	120.00
13	m	166	ASN	CA-CB-CG	-6.33	106.27	112.60
27	O	115	ARG	NE-CZ-NH2	6.33	124.89	119.20
29	I	124	THR	CA-C-O	6.33	126.71	119.18
11	k	89	ALA	CA-C-N	6.33	129.27	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	89	ALA	C-N-CA	6.33	129.27	120.29
27	O	157	LEU	CA-C-O	6.33	127.46	120.82
30	K	223	VAL	CA-C-N	6.33	129.27	120.29
30	K	223	VAL	C-N-CA	6.33	129.27	120.29
8	h	94	LEU	CA-C-N	6.32	128.75	120.28
8	h	94	LEU	C-N-CA	6.32	128.75	120.28
14	n	99	LEU	O-C-N	-6.32	114.82	122.22
9	2	166	VAL	N-CA-C	-6.32	104.17	110.62
21	N	768	ILE	O-C-N	6.32	126.39	121.46
24	Q	432	VAL	CB-CA-C	-6.32	103.49	112.22
31	L	345	ARG	N-CA-C	-6.32	99.90	109.95
9	2	38	ASN	CA-CB-CG	-6.32	106.28	112.60
12	l	227	ASP	CA-CB-CG	6.32	118.92	112.60
26	U	286	ILE	N-CA-CB	6.32	119.13	110.54
4	D	185	PRO	N-CA-CB	6.32	108.93	103.31
15	W	167	GLU	N-CA-C	-6.32	98.90	109.07
21	N	322	ASP	CA-CB-CG	6.32	118.92	112.60
11	k	176	PHE	CA-CB-CG	-6.32	107.48	113.80
13	m	215	VAL	CB-CA-C	-6.32	103.32	111.53
1	A	121	MET	CA-C-N	6.32	129.26	120.29
1	A	121	MET	C-N-CA	6.32	129.26	120.29
27	O	391	ILE	N-CA-CB	6.32	119.30	111.41
18	X	58	GLY	CA-C-O	6.31	127.33	119.25
24	Q	110	SER	CA-C-N	6.31	129.57	120.79
24	Q	110	SER	C-N-CA	6.31	129.57	120.79
3	C	81	THR	O-C-N	-6.31	113.81	122.46
25	R	328	PHE	N-CA-CB	-6.31	100.84	110.12
28	H	463	TYR	CA-C-N	6.31	132.91	122.62
28	H	463	TYR	C-N-CA	6.31	132.91	122.62
30	K	306	PHE	CA-CB-CG	6.31	120.11	113.80
32	M	333	LEU	N-CA-CB	6.31	119.26	110.17
27	O	283	HIS	CE1-NE2-CD2	-6.31	102.69	109.00
2	b	130	PHE	N-CA-CB	6.31	119.26	110.17
11	k	182	LYS	CA-C-O	6.31	127.52	120.70
21	N	547	LEU	N-CA-C	-6.31	104.48	111.36
21	N	839	ARG	NE-CZ-NH2	6.31	124.88	119.20
21	N	649	VAL	CA-CB-CG2	-6.31	99.68	110.40
22	S	100	HIS	ND1-CE1-NE2	6.31	114.71	108.40
3	c	129	ARG	NE-CZ-NH2	6.31	124.88	119.20
2	B	179	TRP	O-C-N	6.31	130.09	122.96
18	X	75	TRP	N-CA-CB	6.31	120.70	110.42
21	N	55	PHE	CA-CB-CG	-6.30	107.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	748	PHE	CA-CB-CG	-6.30	107.50	113.80
7	g	100	LYS	CA-C-O	-6.30	113.87	120.55
5	E	65	GLU	CA-C-O	-6.30	114.28	121.40
21	N	300	ASN	OD1-CG-ND2	6.30	128.90	122.60
13	m	103	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
14	n	199	PRO	N-CA-CB	6.30	109.19	103.20
23	P	237	VAL	CA-C-N	6.30	129.01	120.44
23	P	237	VAL	C-N-CA	6.30	129.01	120.44
23	P	400	VAL	N-CA-C	-6.30	99.29	108.11
24	Q	177	VAL	CA-CB-CG2	-6.30	99.69	110.40
25	R	363	PHE	N-CA-CB	6.30	119.38	110.12
1	a	115	ASP	O-C-N	-6.30	115.58	122.07
5	e	232	ASP	N-CA-C	-6.30	101.14	110.46
21	N	112	GLU	N-CA-C	6.30	118.23	111.36
33	J	60	ASP	CA-CB-CG	-6.30	106.30	112.60
21	N	885	ILE	CA-C-O	6.30	129.02	121.02
24	Q	233	LYS	CA-C-N	6.30	128.72	120.28
24	Q	233	LYS	C-N-CA	6.30	128.72	120.28
31	L	100	SER	CA-C-N	6.30	129.10	120.35
31	L	100	SER	C-N-CA	6.30	129.10	120.35
1	a	111	ASP	CA-CB-CG	-6.30	106.30	112.60
6	F	115	LYS	N-CA-C	-6.30	104.33	111.07
17	T	225	ASN	OD1-CG-ND2	6.30	128.90	122.60
21	N	315	ASN	CA-CB-CG	-6.30	106.30	112.60
22	S	325	GLY	N-CA-C	-6.30	106.45	115.64
17	T	251	HIS	ND1-CE1-NE2	6.29	114.69	108.40
3	c	113	ARG	CB-CA-C	-6.29	100.34	110.79
24	Q	337	ALA	CA-C-N	6.29	128.71	120.28
24	Q	337	ALA	C-N-CA	6.29	128.71	120.28
6	f	39	ARG	N-CA-C	6.29	116.75	107.88
18	X	98	PHE	N-CA-C	-6.29	99.15	109.40
21	N	500	ASP	CA-CB-CG	-6.29	106.31	112.60
24	Q	418	GLN	CA-C-O	-6.29	113.75	120.42
28	H	448	ASP	CA-CB-CG	6.29	118.89	112.60
2	B	129	PRO	CA-C-N	6.29	130.07	120.82
2	B	129	PRO	C-N-CA	6.29	130.07	120.82
8	1	169	SER	CA-C-N	6.29	129.87	120.31
8	1	169	SER	C-N-CA	6.29	129.87	120.31
29	I	68	HIS	CA-CB-CG	6.29	120.09	113.80
9	i	86	GLN	N-CA-C	6.29	118.21	111.36
1	A	212	ASP	CA-CB-CG	-6.29	106.31	112.60
24	Q	155	LEU	CA-C-N	6.29	128.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	155	LEU	C-N-CA	6.29	128.70	120.28
7	g	87	HIS	N-CA-C	6.29	118.13	111.28
7	g	107	ILE	N-CA-CB	6.29	120.01	111.21
2	b	37	ILE	N-CA-C	-6.28	99.00	108.17
12	l	184	GLY	CA-C-N	6.28	126.23	119.76
12	l	184	GLY	C-N-CA	6.28	126.23	119.76
4	D	13	PRO	CA-C-N	6.28	133.13	122.26
4	D	13	PRO	C-N-CA	6.28	133.13	122.26
19	Y	43	TRP	N-CA-CB	6.28	121.11	110.49
21	N	82	ALA	CB-CA-C	-6.28	100.17	110.85
25	R	291	SER	CA-C-N	6.28	128.70	120.28
25	R	291	SER	C-N-CA	6.28	128.70	120.28
2	b	27	ALA	CA-C-N	6.28	129.07	120.46
2	b	27	ALA	C-N-CA	6.28	129.07	120.46
8	h	172	ILE	N-CA-C	-6.28	104.38	110.72
4	D	231	GLN	CA-C-N	6.28	129.21	120.29
4	D	231	GLN	C-N-CA	6.28	129.21	120.29
21	N	121	GLU	N-CA-C	6.28	117.79	111.07
25	R	49	PHE	N-CA-C	6.28	118.12	111.28
10	j	94	SER	CA-C-N	6.28	129.32	120.28
10	j	94	SER	C-N-CA	6.28	129.32	120.28
10	3	202	MET	CA-C-N	6.28	130.79	120.94
10	3	202	MET	C-N-CA	6.28	130.79	120.94
32	M	375	ASN	N-CA-C	-6.28	97.84	108.26
20	Z	85	VAL	CA-C-O	-6.28	111.54	119.95
1	A	193	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
5	e	135	SER	N-CA-CB	6.27	120.04	110.44
2	B	130	PHE	CA-CB-CG	-6.27	107.53	113.80
3	C	94	HIS	CG-CD2-NE2	6.27	113.47	107.20
13	6	48	GLU	CA-C-N	6.27	126.64	119.93
13	6	48	GLU	C-N-CA	6.27	126.64	119.93
7	g	204	HIS	CA-CB-CG	6.27	120.07	113.80
2	b	23	TYR	CB-CG-CD1	6.27	130.20	120.80
2	b	94	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
12	l	136	SER	O-C-N	6.27	129.30	122.15
28	H	444	LEU	N-CA-CB	6.27	119.10	110.01
16	V	202	ASP	CA-CB-CG	-6.27	106.33	112.60
28	H	418	GLU	N-CA-CB	6.27	119.95	110.30
4	D	238	GLN	OE1-CD-NE2	6.26	128.86	122.60
12	5	275	VAL	O-C-N	6.26	128.88	121.80
21	N	337	GLY	CA-C-N	6.26	129.19	120.29
21	N	337	GLY	C-N-CA	6.26	129.19	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	765	ASP	CA-CB-CG	6.26	118.86	112.60
28	H	118	ASP	N-CA-C	-6.26	105.28	113.17
32	M	392	LYS	N-CA-C	-6.26	104.55	111.82
2	B	209	ILE	CA-CB-CG1	-6.26	99.75	110.40
25	R	246	TYR	CA-C-O	6.26	127.08	119.38
30	K	131	LEU	CB-CA-C	-6.26	101.05	110.88
32	M	361	LEU	N-CA-C	6.26	118.11	111.28
10	j	15	MET	N-CA-C	-6.26	99.46	108.60
25	R	185	LEU	N-CA-CB	6.26	119.42	110.16
25	R	308	LEU	N-CA-C	6.26	118.90	111.33
2	B	155	SER	N-CA-C	-6.26	99.71	109.72
1	a	214	LEU	N-CA-CB	6.26	119.93	110.30
13	m	201	GLU	CB-CG-CD	-6.26	101.96	112.60
22	S	203	SER	CA-C-N	6.26	128.66	120.28
22	S	203	SER	C-N-CA	6.26	128.66	120.28
26	U	281	LEU	CA-C-N	6.26	128.44	120.56
26	U	281	LEU	C-N-CA	6.26	128.44	120.56
4	d	91	VAL	N-CA-CB	6.25	119.96	110.58
4	d	109	LEU	N-CA-CB	6.25	119.14	110.07
22	S	243	ASN	CA-CB-CG	-6.25	106.35	112.60
5	E	151	ASP	CB-CA-C	-6.25	100.97	109.28
6	F	107	ARG	CA-CB-CG	6.25	126.60	114.10
10	3	85	GLU	CA-CB-CG	-6.25	101.60	114.10
21	N	380	LEU	CA-C-O	-6.25	113.92	120.55
25	R	319	CYS	N-CA-C	-6.25	101.23	110.48
32	M	222	GLY	CA-C-N	6.25	126.82	120.38
32	M	222	GLY	C-N-CA	6.25	126.82	120.38
16	V	53	MET	CG-SD-CE	-6.25	87.15	100.90
17	T	177	PHE	N-CA-C	-6.25	105.97	113.97
29	I	231	LEU	N-CA-C	-6.25	104.57	111.82
13	m	49	PRO	CA-C-O	-6.25	114.44	121.43
20	Z	206	ASP	N-CA-C	6.25	124.10	110.80
25	R	327	ASP	CA-C-N	6.25	128.65	120.28
25	R	327	ASP	C-N-CA	6.25	128.65	120.28
10	j	54	THR	O-C-N	-6.24	115.05	123.10
11	k	104	ILE	N-CA-C	-6.24	98.63	107.75
16	V	274	GLN	CB-CA-C	-6.24	101.07	110.06
17	T	235	PHE	CA-CB-CG	-6.24	107.56	113.80
21	N	884	PHE	N-CA-CB	6.24	120.74	110.69
25	R	109	LYS	CG-CD-CE	6.24	125.66	111.30
17	T	135	ASN	CA-CB-CG	-6.24	106.36	112.60
24	Q	393	GLY	N-CA-C	-6.24	105.92	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	52	LYS	CA-C-N	6.24	130.74	120.94
7	G	52	LYS	C-N-CA	6.24	130.74	120.94
17	T	188	GLU	CB-CG-CD	-6.24	101.99	112.60
20	Z	745	LEU	N-CA-C	-6.24	104.48	111.28
20	Z	746	ILE	CB-CA-C	6.24	122.37	112.26
27	O	121	ASP	CA-CB-CG	-6.24	106.36	112.60
28	H	403	ARG	CA-C-N	6.24	129.80	120.31
28	H	403	ARG	C-N-CA	6.24	129.80	120.31
31	L	364	HIS	ND1-CE1-NE2	6.24	114.64	108.40
7	g	112	PHE	CB-CG-CD1	6.24	131.30	120.70
14	n	261	TYR	N-CA-C	-6.24	105.71	113.38
7	G	14	VAL	CA-C-O	-6.24	113.66	120.71
2	b	190	HIS	CA-CB-CG	-6.24	107.56	113.80
14	n	73	GLU	CB-CA-C	-6.24	101.18	110.16
16	V	175	SER	CA-C-N	6.24	133.45	121.54
16	V	175	SER	C-N-CA	6.24	133.45	121.54
31	L	164	ASP	CA-CB-CG	-6.24	106.36	112.60
6	F	110	HIS	ND1-CE1-NE2	6.23	114.63	108.40
14	n	85	GLY	CA-C-N	6.23	131.79	122.75
14	n	85	GLY	C-N-CA	6.23	131.79	122.75
10	3	203	ARG	N-CA-CB	6.23	119.15	110.17
25	R	36	SER	N-CA-C	-6.23	103.34	113.19
27	O	392	TRP	O-C-N	-6.23	116.05	121.85
17	T	183	SER	CA-C-N	6.23	129.78	120.31
17	T	183	SER	C-N-CA	6.23	129.78	120.31
7	g	123	HIS	CG-CD2-NE2	6.23	113.43	107.20
5	E	72	ARG	CA-C-O	6.23	126.83	119.48
5	E	166	ARG	NE-CZ-NH1	6.23	127.73	121.50
12	5	105	THR	N-CA-C	-6.23	104.16	112.94
21	N	842	ASN	OD1-CG-ND2	-6.23	116.37	122.60
27	O	24	PRO	CA-C-N	6.23	129.13	120.29
27	O	24	PRO	C-N-CA	6.23	129.13	120.29
30	K	315	ILE	N-CA-C	-6.23	99.43	108.71
31	L	261	ARG	N-CA-C	6.23	117.73	111.07
5	E	234	GLU	CB-CG-CD	-6.23	102.02	112.60
13	m	93	SER	N-CA-C	-6.22	102.15	110.55
1	A	220	LYS	CA-C-N	6.22	132.03	121.14
1	A	220	LYS	C-N-CA	6.22	132.03	121.14
28	H	155	PHE	CA-CB-CG	-6.22	107.58	113.80
32	M	165	SER	N-CA-C	-6.22	105.17	112.89
4	D	34	VAL	CA-C-N	6.22	125.88	121.65
4	D	34	VAL	C-N-CA	6.22	125.88	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	182	HIS	CG-CD2-NE2	6.22	113.42	107.20
23	P	205	LYS	N-CA-C	-6.22	105.52	113.23
24	Q	298	ALA	O-C-N	6.22	129.49	122.22
4	d	128	PRO	CA-C-O	-6.21	114.28	121.86
21	N	198	THR	CA-C-O	6.21	125.97	119.51
21	N	380	LEU	O-C-N	6.21	128.71	122.12
29	I	375	VAL	CA-C-N	6.21	130.61	120.23
29	I	375	VAL	C-N-CA	6.21	130.61	120.23
33	J	40	ASN	CA-CB-CG	-6.21	106.39	112.60
12	l	234	ARG	N-CA-CB	6.21	119.25	110.12
16	V	226	LYS	N-CA-CB	6.21	119.21	109.83
17	T	179	ASP	CB-CA-C	-6.21	100.29	110.85
28	H	453	GLY	CA-C-N	6.21	128.60	120.28
28	H	453	GLY	C-N-CA	6.21	128.60	120.28
5	e	205	LYS	O-C-N	-6.21	115.07	122.15
14	n	158	GLN	OE1-CD-NE2	6.21	128.81	122.60
16	V	131	GLN	CA-C-N	6.21	129.11	120.29
16	V	131	GLN	C-N-CA	6.21	129.11	120.29
19	Y	82	ASP	CA-CB-CG	-6.21	106.39	112.60
25	R	378	ASN	CA-CB-CG	6.21	118.81	112.60
26	U	196	SER	CA-C-N	6.21	128.60	120.28
26	U	196	SER	C-N-CA	6.21	128.60	120.28
12	l	236	ILE	CA-C-O	-6.21	114.27	120.85
3	C	11	THR	CA-C-N	6.21	129.54	120.91
3	C	11	THR	C-N-CA	6.21	129.54	120.91
21	N	182	ASN	OD1-CG-ND2	-6.21	116.39	122.60
9	i	210	GLY	N-CA-C	-6.21	106.67	115.30
5	E	92	ALA	O-C-N	-6.21	115.07	122.15
5	E	188	HIS	ND1-CE1-NE2	6.21	114.61	108.40
21	N	807	THR	CA-C-O	-6.21	114.30	120.82
22	S	271	ARG	NE-CZ-NH2	6.21	124.78	119.20
28	H	74	THR	O-C-N	-6.21	116.26	123.27
30	K	107	THR	CA-C-N	6.21	128.06	121.48
30	K	107	THR	C-N-CA	6.21	128.06	121.48
30	K	285	GLN	N-CA-C	-6.21	103.86	112.30
4	d	188	VAL	N-CA-C	-6.21	103.33	111.09
8	1	116	LYS	N-CA-CB	6.21	120.98	110.49
16	V	301	ASN	N-CA-C	6.20	118.04	111.28
17	T	123	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
21	N	718	GLU	CA-C-N	6.20	129.68	120.87
21	N	718	GLU	C-N-CA	6.20	129.68	120.87
22	S	377	TYR	N-CA-CB	6.20	119.34	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	190	ARG	N-CA-C	6.20	124.01	110.80
33	J	114	CYS	N-CA-CB	6.20	120.74	110.63
16	V	160	ASP	CA-C-O	-6.20	114.98	121.55
25	R	111	LYS	O-C-N	6.20	128.69	122.12
33	J	295	ASN	CA-CB-CG	-6.20	106.40	112.60
5	e	113	THR	N-CA-CB	6.20	119.33	110.16
10	j	177	ARG	N-CA-C	-6.20	105.56	112.57
26	U	64	ASP	CA-C-N	6.20	131.61	122.99
26	U	64	ASP	C-N-CA	6.20	131.61	122.99
4	d	219	SER	N-CA-C	-6.20	105.02	112.58
28	H	434	ARG	NE-CZ-NH1	6.20	127.70	121.50
11	k	122	LEU	N-CA-C	-6.20	104.61	111.36
6	F	127	PRO	N-CA-CB	-6.20	97.80	103.31
23	P	87	GLY	CA-C-N	6.20	132.20	122.78
23	P	87	GLY	C-N-CA	6.20	132.20	122.78
25	R	31	PHE	CA-CB-CG	-6.20	107.60	113.80
25	R	225	LYS	CA-C-N	6.20	129.09	120.29
25	R	225	LYS	C-N-CA	6.20	129.09	120.29
11	k	57	ALA	CB-CA-C	-6.19	100.51	110.79
2	b	110	LEU	CA-C-N	6.19	128.94	120.46
2	b	110	LEU	C-N-CA	6.19	128.94	120.46
26	U	52	PHE	CA-CB-CG	-6.19	107.61	113.80
27	O	85	SER	N-CA-C	6.19	118.03	111.28
32	M	40	GLU	N-CA-C	6.19	118.03	111.28
4	D	29	ARG	NE-CZ-NH2	-6.19	113.63	119.20
7	G	116	LEU	CB-CA-C	-6.19	100.52	110.79
21	N	9	LEU	CA-C-N	6.19	128.49	120.44
21	N	9	LEU	C-N-CA	6.19	128.49	120.44
22	S	412	ASN	CA-CB-CG	-6.19	106.41	112.60
10	j	45	HIS	CA-C-O	-6.19	114.08	120.89
14	7	106	GLU	CA-C-O	-6.19	114.33	120.70
10	3	170	ALA	CB-CA-C	-6.19	100.52	110.79
32	M	64	ASP	N-CA-C	6.19	118.03	111.28
5	e	161	SER	N-CA-C	-6.19	105.01	113.30
15	W	111	VAL	N-CA-C	-6.19	99.45	108.11
9	i	222	PRO	N-CA-C	-6.18	105.95	114.98
13	6	106	TYR	N-CA-C	-6.18	105.73	113.28
21	N	6	ALA	CA-C-N	6.18	127.82	120.09
21	N	6	ALA	C-N-CA	6.18	127.82	120.09
22	S	49	ASP	CA-C-N	6.18	125.91	119.05
22	S	49	ASP	C-N-CA	6.18	125.91	119.05
23	P	419	VAL	CA-C-O	-6.18	114.52	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	241	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
6	f	29	ILE	CA-C-N	6.18	128.56	120.28
6	f	29	ILE	C-N-CA	6.18	128.56	120.28
3	C	111	LEU	N-CA-C	6.18	118.10	111.36
3	C	203	SER	CA-C-N	6.18	128.84	120.44
3	C	203	SER	C-N-CA	6.18	128.84	120.44
20	Z	952	SER	N-CA-C	-6.18	99.29	108.99
24	Q	2	SER	CA-C-O	6.18	127.06	120.70
30	K	105	GLN	CA-CB-CG	6.18	126.46	114.10
5	e	194	LYS	CA-C-N	6.18	128.56	120.28
5	e	194	LYS	C-N-CA	6.18	128.56	120.28
11	k	117	TYR	CA-CB-CG	-6.18	102.78	113.90
14	7	245	LEU	N-CA-C	-6.18	100.44	110.20
1	a	241	ILE	CA-C-N	6.18	128.56	120.28
1	a	241	ILE	C-N-CA	6.18	128.56	120.28
6	f	95	SER	CA-C-O	6.18	127.10	120.55
23	P	177	ILE	CA-C-O	-6.18	114.62	121.17
32	M	236	ALA	N-CA-C	6.18	118.09	111.36
30	K	322	ASP	N-CA-C	-6.17	103.44	111.71
2	b	63	LYS	N-CA-C	-6.17	105.03	113.30
23	P	232	ARG	NE-CZ-NH2	-6.17	113.64	119.20
25	R	20	ARG	NE-CZ-NH2	-6.17	113.64	119.20
3	c	183	ASP	N-CA-C	-6.17	101.64	111.02
11	k	133	HIS	CG-CD2-NE2	6.17	113.37	107.20
21	N	510	HIS	CE1-NE2-CD2	-6.17	102.83	109.00
29	I	269	LYS	CA-C-N	6.17	128.34	120.56
29	I	269	LYS	C-N-CA	6.17	128.34	120.56
21	N	179	THR	CA-C-N	6.17	129.05	120.29
21	N	179	THR	C-N-CA	6.17	129.05	120.29
20	Z	210	TYR	N-CA-C	-6.17	104.64	111.36
20	Z	780	MET	CA-C-N	6.17	126.83	119.98
20	Z	780	MET	C-N-CA	6.17	126.83	119.98
21	N	421	ASP	CA-CB-CG	-6.17	106.43	112.60
33	J	398	ILE	CA-C-N	6.17	133.32	121.54
33	J	398	ILE	C-N-CA	6.17	133.32	121.54
26	U	169	ILE	CA-C-O	-6.17	114.31	120.85
2	B	157	PHE	CA-CB-CG	-6.17	107.64	113.80
9	i	95	HIS	CA-C-N	6.16	128.54	120.28
9	i	95	HIS	C-N-CA	6.16	128.54	120.28
15	W	154	LEU	CA-C-N	6.16	128.54	120.28
15	W	154	LEU	C-N-CA	6.16	128.54	120.28
20	Z	413	ASP	CA-C-N	6.16	126.82	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	413	ASP	C-N-CA	6.16	126.82	119.98
26	U	54	LEU	CA-C-O	-6.16	113.50	120.46
28	H	256	LYS	N-CA-CB	6.16	119.18	110.12
12	5	273	TRP	CA-C-N	6.16	128.82	120.44
12	5	273	TRP	C-N-CA	6.16	128.82	120.44
10	j	23	ILE	N-CA-C	-6.16	99.18	108.17
21	N	638	ILE	CA-C-N	6.16	128.53	120.28
21	N	638	ILE	C-N-CA	6.16	128.53	120.28
23	P	75	LEU	CA-C-N	6.16	128.45	120.44
23	P	75	LEU	C-N-CA	6.16	128.45	120.44
28	H	273	ARG	NE-CZ-NH2	6.16	124.74	119.20
33	J	298	ASP	CB-CA-C	-6.16	100.56	110.79
23	P	104	LEU	CA-C-N	6.16	128.53	120.28
23	P	104	LEU	C-N-CA	6.16	128.53	120.28
5	e	54	ALA	N-CA-C	-6.16	99.68	109.59
21	N	553	PHE	CA-CB-CG	-6.16	107.64	113.80
21	N	834	GLU	N-CA-C	-6.16	104.94	112.88
22	S	353	LYS	O-C-N	6.16	128.65	122.12
33	J	185	VAL	N-CA-C	-6.16	98.61	107.78
11	4	89	ALA	CA-C-N	6.15	128.81	120.44
11	4	89	ALA	C-N-CA	6.15	128.81	120.44
33	J	288	ILE	N-CA-CB	6.15	119.40	111.83
13	m	76	PHE	O-C-N	-6.15	115.14	122.15
14	7	178	GLY	CA-C-N	6.15	128.53	120.28
14	7	178	GLY	C-N-CA	6.15	128.53	120.28
25	R	158	LEU	CA-C-O	-6.15	114.03	120.55
30	K	235	ILE	N-CA-C	-6.15	96.55	109.34
5	e	229	LYS	CA-C-N	6.15	130.94	121.71
5	e	229	LYS	C-N-CA	6.15	130.94	121.71
13	m	107	GLY	N-CA-C	-6.15	106.72	114.16
25	R	305	PHE	CA-C-N	6.15	125.88	119.05
25	R	305	PHE	C-N-CA	6.15	125.88	119.05
1	a	161	GLY	O-C-N	-6.15	115.67	122.50
29	I	196	GLU	CA-C-O	-6.15	113.15	120.10
10	j	28	ARG	CB-CA-C	-6.15	101.31	110.16
13	m	13	TYR	CB-CG-CD2	6.15	130.02	120.80
2	B	26	THR	N-CA-CB	6.15	119.16	110.12
9	2	212	ASP	CA-CB-CG	6.15	118.75	112.60
5	E	196	ALA	N-CA-CB	6.15	119.15	110.12
23	P	183	GLN	CB-CA-C	-6.15	100.59	110.79
33	J	236	MET	CA-C-N	6.15	131.13	120.68
33	J	236	MET	C-N-CA	6.15	131.13	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	170	THR	N-CA-C	-6.14	104.13	111.69
31	L	223	PRO	O-C-N	-6.14	114.21	121.46
14	7	65	SER	CA-C-O	-6.14	113.91	120.42
22	S	92	LEU	N-CA-C	6.14	117.98	111.28
14	n	89	ASP	CA-CB-CG	6.14	118.74	112.60
12	5	203	CYS	N-CA-C	-6.14	97.82	108.69
16	V	291	ASN	OD1-CG-ND2	-6.14	116.46	122.60
31	L	281	ASP	CA-CB-CG	-6.14	106.46	112.60
1	a	69	VAL	N-CA-C	-6.14	99.58	108.36
7	G	109	ILE	N-CA-CB	6.14	114.37	110.50
27	O	91	ASP	N-CA-C	-6.14	98.72	108.73
4	D	235	GLN	CA-C-N	6.14	129.14	120.42
4	D	235	GLN	C-N-CA	6.14	129.14	120.42
33	J	112	ARG	NE-CZ-NH2	-6.14	113.68	119.20
4	d	81	ASP	CA-C-N	6.14	129.64	120.31
4	d	81	ASP	C-N-CA	6.14	129.64	120.31
5	e	27	SER	CA-CB-OG	6.14	123.37	111.10
7	G	158	TRP	N-CA-C	-6.14	99.40	108.79
26	U	223	HIS	CA-CB-CG	-6.14	107.66	113.80
25	R	152	LYS	N-CA-CB	6.13	118.91	110.01
29	I	417	LYS	CA-C-N	6.13	128.50	120.28
29	I	417	LYS	C-N-CA	6.13	128.50	120.28
23	P	311	TRP	CG-CD2-CE3	-6.13	127.77	133.90
24	Q	155	LEU	CB-CA-C	-6.13	100.42	110.85
2	b	19	GLY	CA-C-O	-6.13	113.56	120.30
6	F	211	LEU	N-CA-CB	6.13	118.99	109.85
13	6	87	HIS	ND1-CE1-NE2	6.13	114.53	108.40
13	6	169	GLU	CA-C-O	-6.13	113.76	120.69
2	B	13	SER	N-CA-CB	6.13	116.71	109.72
29	I	71	LEU	N-CA-C	-6.13	104.52	111.14
33	J	139	VAL	O-C-N	6.13	127.82	121.87
13	6	191	LEU	CA-C-N	6.13	129.12	120.42
13	6	191	LEU	C-N-CA	6.13	129.12	120.42
5	e	157	HIS	CG-CD2-NE2	6.13	113.33	107.20
15	W	157	PHE	CA-C-N	6.13	129.12	120.42
15	W	157	PHE	C-N-CA	6.13	129.12	120.42
17	T	148	LEU	CA-C-N	6.13	128.49	120.28
17	T	148	LEU	C-N-CA	6.13	128.49	120.28
6	f	205	SER	N-CA-C	-6.12	100.01	109.14
7	g	42	CYS	N-CA-C	-6.12	100.10	109.41
21	N	311	ILE	CA-C-N	6.12	128.06	120.34
21	N	311	ILE	C-N-CA	6.12	128.06	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	110	TYR	CA-C-N	6.12	129.53	120.90
1	a	110	TYR	C-N-CA	6.12	129.53	120.90
12	5	194	GLY	CA-C-O	6.12	126.68	119.46
32	M	373	ASP	CA-C-N	6.12	128.86	120.35
32	M	373	ASP	C-N-CA	6.12	128.86	120.35
7	g	26	TYR	N-CA-C	-6.12	105.30	112.89
1	a	71	TYR	N-CA-C	-6.12	107.65	114.62
5	E	88	MET	CA-C-N	6.12	129.11	120.42
5	E	88	MET	C-N-CA	6.12	129.11	120.42
5	E	157	HIS	CE1-NE2-CD2	-6.12	102.88	109.00
32	M	109	ASP	N-CA-CB	6.12	120.83	110.49
12	5	147	GLU	CB-CG-CD	-6.12	102.20	112.60
17	T	60	ARG	CA-C-N	6.12	129.10	120.42
17	T	60	ARG	C-N-CA	6.12	129.10	120.42
22	S	171	TYR	CB-CG-CD2	-6.12	111.63	120.80
27	O	42	SER	CA-C-N	6.12	128.48	120.28
27	O	42	SER	C-N-CA	6.12	128.48	120.28
8	1	184	MET	CA-C-O	6.11	128.15	121.06
20	Z	913	ILE	N-CA-C	-6.11	104.89	110.82
33	J	331	HIS	ND1-CE1-NE2	6.11	114.51	108.40
3	c	69	LEU	N-CA-C	-6.11	105.78	113.72
3	c	200	THR	N-CA-C	6.11	118.74	111.71
7	g	221	LEU	N-CA-C	6.11	117.94	111.28
21	N	832	HIS	CG-CD2-NE2	6.11	113.31	107.20
29	I	367	SER	O-C-N	-6.11	115.19	122.15
16	V	29	ILE	CA-C-N	6.11	131.19	120.87
16	V	29	ILE	C-N-CA	6.11	131.19	120.87
24	Q	157	LEU	CA-C-O	-6.11	114.41	120.82
7	g	32	GLU	O-C-N	6.11	128.59	122.12
1	A	217	GLU	N-CA-CB	6.11	119.09	110.36
24	Q	312	LEU	CA-C-N	6.11	128.46	120.28
24	Q	312	LEU	C-N-CA	6.11	128.46	120.28
27	O	81	TYR	CB-CG-CD1	6.11	129.96	120.80
27	O	319	LEU	CB-CA-C	-6.11	99.62	108.84
33	J	69	GLY	N-CA-C	-6.11	105.81	112.04
21	N	658	ILE	CA-C-N	6.11	128.46	120.28
21	N	658	ILE	C-N-CA	6.11	128.46	120.28
24	Q	126	LYS	CA-C-N	6.11	131.02	120.58
24	Q	126	LYS	C-N-CA	6.11	131.02	120.58
18	X	66	LEU	CA-C-O	6.10	126.81	120.40
25	R	22	PRO	CA-C-N	6.10	128.46	120.28
25	R	22	PRO	C-N-CA	6.10	128.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	262	GLN	N-CA-C	-6.10	104.71	111.36
28	H	74	THR	CA-C-O	6.10	127.08	120.43
16	V	251	TYR	CA-C-N	6.10	128.74	120.44
16	V	251	TYR	C-N-CA	6.10	128.74	120.44
32	M	319	ASP	CA-C-O	6.10	126.89	120.42
6	f	107	ARG	CA-C-N	6.10	128.46	120.28
6	f	107	ARG	C-N-CA	6.10	128.46	120.28
25	R	406	GLN	OE1-CD-NE2	-6.10	116.50	122.60
5	e	233	ASN	CA-C-N	6.10	128.95	120.29
5	e	233	ASN	C-N-CA	6.10	128.95	120.29
12	l	154	ALA	O-C-N	6.10	128.59	122.12
12	l	279	GLU	O-C-N	-6.10	115.20	122.15
21	N	583	VAL	N-CA-C	-6.10	104.56	110.72
23	P	9	ALA	CA-C-O	-6.10	114.42	120.82
24	Q	330	LEU	CA-C-O	6.10	127.01	120.55
28	H	198	MET	CA-C-O	6.10	127.01	120.24
26	U	24	ARG	N-CA-C	-6.10	105.13	113.30
27	O	254	LEU	CA-C-O	6.10	127.01	120.55
15	W	78	ASP	CA-C-N	6.09	129.78	120.82
15	W	78	ASP	C-N-CA	6.09	129.78	120.82
21	N	621	THR	O-C-N	6.09	129.10	122.15
22	S	392	ILE	CA-C-N	6.09	129.06	120.28
22	S	392	ILE	C-N-CA	6.09	129.06	120.28
26	U	197	LEU	O-C-N	6.09	128.58	122.12
21	N	492	THR	CA-CB-OG1	6.09	118.74	109.60
8	h	198	TYR	CA-CB-CG	-6.09	102.94	113.90
2	B	57	MET	N-CA-C	-6.09	100.58	110.20
19	Y	25	ASN	OD1-CG-ND2	6.09	128.69	122.60
21	N	76	GLU	CB-CG-CD	-6.09	102.25	112.60
23	P	43	GLU	CA-C-O	6.09	126.80	119.43
5	e	119	LEU	CA-C-N	6.09	129.05	120.28
5	e	119	LEU	C-N-CA	6.09	129.05	120.28
5	E	143	LEU	N-CA-C	-6.09	98.80	108.73
7	G	138	PHE	N-CA-C	-6.09	99.71	108.60
11	4	192	VAL	CA-CB-CG1	-6.09	100.05	110.40
28	H	133	SER	N-CA-CB	6.09	119.45	110.56
30	K	68	ILE	CA-C-N	6.09	128.94	120.29
30	K	68	ILE	C-N-CA	6.09	128.94	120.29
22	S	354	LEU	N-CA-CB	6.09	120.32	110.40
33	J	58	ILE	O-C-N	-6.09	115.97	121.87
25	R	236	ALA	N-CA-C	6.09	117.92	111.28
22	S	210	LEU	CB-CA-C	-6.08	101.33	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	218	LEU	N-CA-CB	-6.08	101.15	110.16
10	j	129	CYS	N-CA-CB	6.08	120.99	111.56
5	e	61	SER	N-CA-C	-6.08	104.50	112.41
6	f	94	TYR	N-CA-C	6.08	117.91	111.28
10	j	153	LEU	CA-C-N	6.08	129.46	120.95
10	j	153	LEU	C-N-CA	6.08	129.46	120.95
11	k	116	LEU	N-CA-C	-6.08	98.48	108.76
22	S	395	ILE	CB-CA-C	6.08	120.61	112.22
29	I	339	ILE	CA-C-O	6.08	125.93	119.91
9	2	81	THR	CA-C-N	6.08	128.34	120.44
9	2	81	THR	C-N-CA	6.08	128.34	120.44
10	3	145	GLN	O-C-N	6.08	128.33	122.07
15	W	149	GLN	N-CA-CB	6.08	120.76	110.49
9	i	229	GLN	O-C-N	6.08	130.47	122.33
4	D	204	GLN	N-CA-CB	6.08	120.76	110.49
32	M	121	THR	O-C-N	6.08	129.79	122.68
1	a	104	PHE	CA-C-O	6.07	126.99	120.55
5	E	151	ASP	N-CA-C	-6.07	107.69	114.62
14	7	75	LEU	N-CA-C	-6.07	99.80	109.76
21	N	784	TYR	CA-C-N	6.07	126.91	120.11
21	N	784	TYR	C-N-CA	6.07	126.91	120.11
21	N	812	ALA	CA-C-N	6.07	128.70	120.44
21	N	812	ALA	C-N-CA	6.07	128.70	120.44
28	H	81	LEU	CB-CA-C	-6.07	99.01	110.67
30	K	234	PHE	CA-C-O	6.07	127.64	120.66
21	N	544	GLU	N-CA-CB	6.07	120.32	110.42
16	V	174	THR	CA-CB-OG1	6.07	118.71	109.60
28	H	257	THR	CA-C-N	6.07	129.54	120.31
28	H	257	THR	C-N-CA	6.07	129.54	120.31
31	L	58	ASN	CA-C-N	6.07	128.91	120.29
31	L	58	ASN	C-N-CA	6.07	128.91	120.29
10	j	89	GLN	CA-C-N	6.07	128.33	120.44
10	j	89	GLN	C-N-CA	6.07	128.33	120.44
18	X	100	TRP	CD2-CE2-CZ2	-6.07	116.33	122.40
22	S	488	GLN	N-CA-CB	6.07	119.14	110.16
27	O	74	ASN	CA-C-N	6.07	128.41	120.28
27	O	74	ASN	C-N-CA	6.07	128.41	120.28
29	I	171	MET	N-CA-C	-6.07	104.59	111.14
5	e	102	TYR	CA-C-O	6.07	126.83	119.31
1	A	180	THR	N-CA-C	6.07	117.89	111.28
2	B	47	THR	CA-CB-OG1	6.07	118.70	109.60
9	2	121	GLY	O-C-N	6.07	129.99	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	181	ALA	N-CA-C	6.07	117.97	111.36
23	P	187	SER	CA-C-O	-6.07	111.79	119.31
23	P	431	HIS	CG-CD2-NE2	6.07	113.27	107.20
28	H	53	GLU	CA-C-O	-6.07	113.99	120.42
15	W	166	GLU	CB-CG-CD	-6.06	102.29	112.60
29	I	316	PHE	CA-C-O	-6.06	114.45	120.82
31	L	327	THR	CA-C-O	-6.06	114.34	121.44
6	f	94	TYR	CA-C-N	6.06	128.40	120.28
6	f	94	TYR	C-N-CA	6.06	128.40	120.28
8	h	118	GLU	CA-C-O	-6.06	114.78	121.33
8	1	43	LEU	CA-C-O	6.06	126.99	120.32
24	Q	34	ASP	N-CA-CB	6.06	119.13	110.16
1	A	250	GLU	O-C-N	6.06	130.13	123.04
18	X	123	ASN	CA-CB-CG	6.06	118.66	112.60
21	N	667	GLN	OE1-CD-NE2	6.06	128.66	122.60
2	b	230	ASP	N-CA-C	-6.06	100.54	109.81
24	Q	66	VAL	CA-C-O	-6.06	113.93	120.47
25	R	310	GLU	N-CA-C	6.06	117.96	111.36
32	M	52	SER	O-C-N	6.06	128.63	122.09
5	E	176	SER	O-C-N	6.06	128.54	122.12
24	Q	421	LYS	N-CA-C	6.06	117.96	111.36
14	n	94	GLN	OE1-CD-NE2	6.05	128.65	122.60
11	4	117	TYR	N-CA-CB	6.05	120.10	110.65
11	4	122	LEU	CA-C-O	-6.05	114.00	120.42
25	R	194	VAL	O-C-N	6.05	128.07	121.83
26	U	223	HIS	CG-CD2-NE2	6.05	113.25	107.20
4	D	173	GLU	CA-C-N	6.05	128.71	120.54
4	D	173	GLU	C-N-CA	6.05	128.71	120.54
22	S	384	ARG	CA-C-N	6.05	128.67	120.44
22	S	384	ARG	C-N-CA	6.05	128.67	120.44
1	a	39	ASN	OD1-CG-ND2	6.05	128.65	122.60
9	i	83	ALA	CB-CA-C	-6.05	100.74	110.79
21	N	233	ASN	OD1-CG-ND2	6.05	128.65	122.60
29	I	95	GLN	N-CA-C	-6.05	104.77	111.36
30	K	377	SER	O-C-N	6.05	130.38	122.15
10	j	58	THR	CA-C-O	-6.05	114.14	120.55
14	n	165	LEU	CA-C-N	6.05	128.30	120.44
14	n	165	LEU	C-N-CA	6.05	128.30	120.44
8	1	103	THR	N-CA-C	-6.05	98.55	108.41
27	O	361	ASP	N-CA-C	6.05	118.65	111.33
32	M	90	GLU	N-CA-C	-6.05	105.76	113.02
32	M	151	ASP	CA-CB-CG	-6.05	106.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	313	ASP	CA-C-O	-6.05	114.15	121.05
5	e	119	LEU	N-CA-C	-6.05	104.81	111.82
23	P	266	TYR	CB-CG-CD1	6.05	129.87	120.80
28	H	448	ASP	CA-C-N	6.05	128.38	120.28
28	H	448	ASP	C-N-CA	6.05	128.38	120.28
15	W	97	THR	CA-C-N	6.05	133.37	121.58
15	W	97	THR	C-N-CA	6.05	133.37	121.58
26	U	77	ASN	CA-C-N	6.05	128.38	120.28
26	U	77	ASN	C-N-CA	6.05	128.38	120.28
29	I	324	VAL	CB-CA-C	6.05	119.63	110.62
9	2	186	ASP	CA-C-N	6.04	128.87	120.29
9	2	186	ASP	C-N-CA	6.04	128.87	120.29
23	P	404	LYS	CA-C-N	6.04	127.40	119.84
23	P	404	LYS	C-N-CA	6.04	127.40	119.84
32	M	367	LYS	CA-CB-CG	6.04	126.19	114.10
2	b	51	SER	O-C-N	6.04	130.28	123.27
7	G	183	HIS	ND1-CE1-NE2	6.04	114.44	108.40
17	T	211	PHE	CA-CB-CG	6.04	119.84	113.80
22	S	298	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	a	139	VAL	CA-CB-CG1	-6.04	100.13	110.40
8	1	157	LYS	N-CA-C	6.04	117.86	111.28
23	P	295	SER	CA-C-N	6.04	128.37	120.28
23	P	295	SER	C-N-CA	6.04	128.37	120.28
14	7	208	GLU	CA-C-N	6.04	128.87	120.29
14	7	208	GLU	C-N-CA	6.04	128.87	120.29
31	L	61	LYS	CA-C-N	6.04	128.37	120.28
31	L	61	LYS	C-N-CA	6.04	128.37	120.28
14	n	136	ARG	NE-CZ-NH1	-6.04	115.46	121.50
6	F	15	PRO	N-CA-CB	-6.04	97.12	103.52
15	W	177	GLY	O-C-N	-6.04	115.73	121.77
22	S	34	LEU	CA-C-N	6.04	128.37	120.28
22	S	34	LEU	C-N-CA	6.04	128.37	120.28
25	R	373	PRO	N-CA-CB	6.04	109.07	103.46
29	I	313	LEU	CA-C-O	-6.04	112.27	119.15
4	d	199	LEU	O-C-N	-6.04	114.34	122.43
12	l	111	GLU	CA-C-N	6.04	128.29	120.56
12	l	111	GLU	C-N-CA	6.04	128.29	120.56
12	5	174	THR	CA-C-O	6.04	127.96	120.54
19	Y	40	ILE	CA-C-N	6.04	128.97	120.28
19	Y	40	ILE	C-N-CA	6.04	128.97	120.28
31	L	368	VAL	CA-CB-CG1	-6.04	100.14	110.40
29	I	246	ARG	NE-CZ-NH2	-6.03	113.77	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	124	PHE	CA-C-N	6.03	129.55	123.04
10	3	124	PHE	C-N-CA	6.03	129.55	123.04
21	N	630	ALA	N-CA-CB	6.03	118.75	110.01
6	f	131	GLY	CA-C-O	-6.03	115.68	121.11
3	C	66	LEU	N-CA-C	-6.03	98.25	108.26
17	T	57	ILE	N-CA-CB	6.03	117.60	110.55
21	N	696	LYS	CA-C-N	6.03	128.28	120.44
21	N	696	LYS	C-N-CA	6.03	128.28	120.44
4	D	155	ILE	N-CA-C	-6.03	99.80	108.48
13	6	44	ASN	CB-CA-C	-6.03	99.67	110.70
17	T	256	LYS	CA-C-N	6.03	133.05	121.54
17	T	256	LYS	C-N-CA	6.03	133.05	121.54
21	N	456	GLY	CA-C-N	6.03	128.27	120.44
21	N	456	GLY	C-N-CA	6.03	128.27	120.44
22	S	407	ILE	CA-C-N	6.03	128.35	120.28
22	S	407	ILE	C-N-CA	6.03	128.35	120.28
3	c	219	GLY	N-CA-C	-6.02	107.43	115.32
13	6	197	THR	CA-C-O	-6.02	114.17	120.55
24	Q	185	TYR	O-C-N	6.02	129.68	122.27
29	I	335	ASP	CA-C-N	6.02	125.91	119.28
29	I	335	ASP	C-N-CA	6.02	125.91	119.28
9	i	155	SER	N-CA-C	-6.02	99.53	108.99
32	M	77	TYR	O-C-N	-6.02	116.53	123.33
6	f	113	CYS	N-CA-C	-6.02	104.80	111.36
2	B	227	ILE	N-CA-CB	6.02	117.56	111.36
9	2	37	PHE	CA-CB-CG	-6.02	107.78	113.80
11	4	54	VAL	CB-CA-C	-6.02	104.15	112.04
16	V	251	TYR	CA-C-O	-6.02	113.05	119.97
21	N	625	LEU	CA-C-N	6.02	126.79	119.99
21	N	625	LEU	C-N-CA	6.02	126.79	119.99
23	P	155	GLU	CA-C-N	6.02	128.95	120.28
23	P	155	GLU	C-N-CA	6.02	128.95	120.28
1	a	174	LYS	CA-C-N	6.02	128.62	120.38
1	a	174	LYS	C-N-CA	6.02	128.62	120.38
8	h	202	TYR	N-CA-CB	6.02	119.17	110.20
17	T	161	TRP	CB-CG-CD2	-6.02	118.38	126.80
4	D	46	CYS	CA-C-N	6.02	129.37	120.95
4	D	46	CYS	C-N-CA	6.02	129.37	120.95
7	G	174	ALA	O-C-N	-6.02	115.29	122.15
21	N	793	GLY	CA-C-N	6.02	128.83	120.29
21	N	793	GLY	C-N-CA	6.02	128.83	120.29
27	O	313	ILE	CA-C-N	6.02	128.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	313	ILE	C-N-CA	6.02	128.34	120.28
6	f	229	ALA	CB-CA-C	-6.01	100.01	110.17
12	5	215	LEU	CA-C-O	-6.01	114.11	120.55
21	N	297	ASP	CA-CB-CG	-6.01	106.59	112.60
28	H	90	ARG	NE-CZ-NH2	-6.01	113.79	119.20
5	E	161	SER	N-CA-C	-6.01	105.98	113.38
33	J	70	SER	N-CA-C	-6.01	99.38	108.52
14	n	66	LEU	CA-C-N	6.01	131.67	122.77
14	n	66	LEU	C-N-CA	6.01	131.67	122.77
17	T	245	TYR	N-CA-C	6.01	117.83	111.28
26	U	258	SER	CA-C-O	-6.01	114.18	120.55
5	e	32	LYS	CB-CG-CD	6.01	125.12	111.30
13	m	42	SER	CA-C-N	6.01	131.18	123.13
13	m	42	SER	C-N-CA	6.01	131.18	123.13
17	T	75	PHE	CA-CB-CG	-6.01	107.79	113.80
23	P	288	ASN	CA-C-N	6.01	128.33	120.28
23	P	288	ASN	C-N-CA	6.01	128.33	120.28
31	L	349	ILE	CA-C-O	-6.01	115.60	119.15
1	a	107	LYS	N-CA-CB	6.01	118.72	110.01
28	H	46	ALA	CA-C-N	6.01	128.25	120.44
28	H	46	ALA	C-N-CA	6.01	128.25	120.44
4	d	97	ARG	NH1-CZ-NH2	-6.01	111.49	119.30
9	i	118	LYS	O-C-N	6.01	128.49	122.12
21	N	649	VAL	CA-C-N	6.01	129.44	120.31
21	N	649	VAL	C-N-CA	6.01	129.44	120.31
24	Q	135	HIS	CA-CB-CG	6.01	119.81	113.80
25	R	144	ILE	CA-CB-CG1	6.01	120.61	110.40
15	W	87	MET	CA-C-N	6.00	128.33	120.28
15	W	87	MET	C-N-CA	6.00	128.33	120.28
27	O	242	ILE	O-C-N	-6.00	115.59	122.62
2	b	40	THR	N-CA-CB	6.00	120.53	110.92
4	d	33	ALA	O-C-N	-6.00	116.55	123.33
4	d	135	ILE	CA-CB-CG1	-6.00	100.19	110.40
5	E	82	THR	CA-CB-OG1	6.00	118.61	109.60
6	f	20	PHE	CA-C-N	6.00	128.32	120.28
6	f	20	PHE	C-N-CA	6.00	128.32	120.28
12	l	182	LYS	O-C-N	-6.00	115.57	121.93
21	N	701	VAL	CA-C-N	6.00	129.43	120.31
21	N	701	VAL	C-N-CA	6.00	129.43	120.31
29	I	408	ARG	N-CA-C	-6.00	101.64	110.52
22	S	49	ASP	O-C-N	-6.00	115.64	120.38
29	I	365	HIS	CE1-NE2-CD2	-6.00	103.00	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	319	SER	O-C-N	6.00	128.99	122.15
25	R	175	ALA	CA-C-N	6.00	129.43	120.31
25	R	175	ALA	C-N-CA	6.00	129.43	120.31
28	H	444	LEU	CA-C-O	-6.00	114.52	120.82
7	g	169	ARG	NE-CZ-NH2	-6.00	113.80	119.20
8	h	129	HIS	CA-CB-CG	-6.00	107.80	113.80
2	B	89	SER	CA-C-N	6.00	128.24	120.44
2	B	89	SER	C-N-CA	6.00	128.24	120.44
10	3	201	LYS	N-CA-C	-6.00	99.13	108.90
21	N	270	LEU	CA-C-O	6.00	126.78	120.42
28	H	267	THR	CA-CB-OG1	6.00	118.59	109.60
29	I	380	LEU	CA-C-O	6.00	126.88	120.70
3	C	9	ARG	NE-CZ-NH2	-6.00	113.81	119.20
21	N	419	THR	CA-C-N	6.00	128.31	120.28
21	N	419	THR	C-N-CA	6.00	128.31	120.28
22	S	359	LYS	N-CA-CB	6.00	119.03	110.16
22	S	437	ASN	O-C-N	-5.99	116.39	123.22
31	L	141	LYS	N-CA-C	-5.99	100.03	108.96
32	M	340	SER	N-CA-C	5.99	118.50	110.35
5	e	166	ARG	NE-CZ-NH1	5.99	127.49	121.50
22	S	438	HIS	CG-CD2-NE2	5.99	113.19	107.20
23	P	350	LEU	N-CA-C	-5.99	104.75	111.28
26	U	278	ILE	CA-C-N	5.99	128.31	120.28
26	U	278	ILE	C-N-CA	5.99	128.31	120.28
30	K	79	LEU	N-CA-C	-5.99	104.83	111.36
10	j	32	GLN	N-CA-CB	5.99	120.61	110.49
17	T	125	GLU	CA-C-N	5.99	128.31	120.28
17	T	125	GLU	C-N-CA	5.99	128.31	120.28
17	T	163	LEU	CA-C-N	5.99	128.80	120.29
17	T	163	LEU	C-N-CA	5.99	128.80	120.29
25	R	26	VAL	CA-C-N	5.99	128.31	120.28
25	R	26	VAL	C-N-CA	5.99	128.31	120.28
32	M	342	ARG	NE-CZ-NH1	-5.99	115.51	121.50
3	C	112	VAL	CA-C-N	5.99	128.30	120.28
3	C	112	VAL	C-N-CA	5.99	128.30	120.28
16	V	125	THR	CA-C-N	5.99	128.31	120.28
16	V	125	THR	C-N-CA	5.99	128.31	120.28
22	S	67	GLU	CB-CA-C	-5.99	98.16	110.38
22	S	204	ASP	N-CA-C	-5.99	104.75	111.28
23	P	263	HIS	N-CA-CB	5.99	119.02	110.16
28	H	166	THR	CA-C-N	5.99	128.31	120.28
28	H	166	THR	C-N-CA	5.99	128.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	47	VAL	N-CA-CB	5.99	119.67	111.41
16	V	281	SER	CA-C-N	5.99	128.30	120.28
16	V	281	SER	C-N-CA	5.99	128.30	120.28
31	L	414	ASP	CA-CB-CG	5.99	118.59	112.60
18	X	131	ASN	OD1-CG-ND2	5.99	128.59	122.60
22	S	286	TYR	N-CA-C	-5.99	105.94	113.72
28	H	220	LYS	N-CA-CB	5.99	119.02	110.16
33	J	384	LEU	N-CA-C	-5.99	104.84	111.36
2	B	67	LEU	N-CA-C	-5.98	104.33	111.69
2	B	113	GLU	CA-C-N	5.98	128.66	120.46
2	B	113	GLU	C-N-CA	5.98	128.66	120.46
11	4	148	TYR	CB-CG-CD1	5.98	129.77	120.80
16	V	99	GLY	N-CA-C	-5.98	106.99	115.43
25	R	58	GLU	O-C-N	-5.98	115.72	123.32
26	U	277	TYR	CA-C-N	5.98	128.66	120.46
26	U	277	TYR	C-N-CA	5.98	128.66	120.46
11	k	39	SER	CA-C-N	5.98	126.76	120.12
11	k	39	SER	C-N-CA	5.98	126.76	120.12
12	l	258	ASP	N-CA-C	-5.98	105.64	113.17
16	V	20	ARG	NE-CZ-NH2	-5.98	113.82	119.20
27	O	51	ASP	O-C-N	5.98	129.43	122.19
31	L	274	GLU	CA-C-O	5.98	125.82	120.02
18	X	16	GLU	CA-C-N	5.98	128.29	120.28
18	X	16	GLU	C-N-CA	5.98	128.29	120.28
12	l	237	LEU	N-CA-C	5.98	117.88	111.36
12	5	251	ASN	CA-CB-CG	-5.98	106.62	112.60
19	Y	48	THR	N-CA-C	-5.98	103.31	111.56
24	Q	388	GLY	CA-C-N	5.98	131.32	122.71
24	Q	388	GLY	C-N-CA	5.98	131.32	122.71
27	O	350	ILE	N-CA-C	-5.98	99.78	108.87
7	g	236	LEU	CA-C-N	5.98	128.57	120.44
7	g	236	LEU	C-N-CA	5.98	128.57	120.44
14	n	178	GLY	CA-C-N	5.98	128.78	120.29
14	n	178	GLY	C-N-CA	5.98	128.78	120.29
9	2	227	GLU	N-CA-CB	5.98	120.02	110.46
10	j	33	SER	N-CA-CB	5.97	118.94	111.00
25	R	102	LEU	CA-C-O	-5.97	114.50	121.07
1	a	159	PRO	N-CA-C	-5.97	108.47	114.68
7	g	163	ALA	N-CA-C	-5.97	99.97	109.23
8	h	102	LEU	N-CA-C	-5.97	99.61	108.99
1	A	54	ILE	CB-CA-C	-5.97	102.00	110.12
20	Z	455	ILE	CA-C-N	5.97	126.74	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	455	ILE	C-N-CA	5.97	126.74	119.99
21	N	243	LYS	N-CA-CB	-5.97	101.02	110.28
21	N	499	HIS	CG-CD2-NE2	5.97	113.17	107.20
33	J	310	ILE	N-CA-C	-5.97	99.45	108.17
7	g	175	GLU	CB-CG-CD	-5.97	102.45	112.60
9	i	115	HIS	CE1-NE2-CD2	-5.97	103.03	109.00
25	R	279	LEU	N-CA-C	-5.97	106.16	113.50
9	i	111	MET	CA-C-N	5.97	128.20	120.44
9	i	111	MET	C-N-CA	5.97	128.20	120.44
7	G	204	HIS	CE1-NE2-CD2	-5.97	103.03	109.00
17	T	87	PRO	CA-C-N	5.97	128.28	120.28
17	T	87	PRO	C-N-CA	5.97	128.28	120.28
21	N	12	LEU	N-CA-C	5.97	117.87	111.36
22	S	387	VAL	N-CA-C	-5.97	104.53	110.62
33	J	271	THR	CA-C-N	5.97	128.28	120.28
33	J	271	THR	C-N-CA	5.97	128.28	120.28
11	k	189	ILE	N-CA-CB	5.97	121.77	111.39
21	N	99	GLU	O-C-N	5.97	129.41	122.19
21	N	535	LEU	N-CA-CB	5.97	118.99	110.16
23	P	405	PRO	N-CA-CB	5.97	109.52	103.25
5	e	185	ASN	N-CA-C	-5.97	104.16	112.45
22	S	48	LEU	N-CA-C	5.97	117.78	111.28
29	I	75	PHE	O-C-N	-5.97	115.92	122.07
30	K	392	LEU	N-CA-CB	5.97	119.28	110.33
10	j	150	CYS	N-CA-C	5.96	117.86	111.36
22	S	313	SER	CA-C-O	5.96	126.87	120.55
29	I	85	PHE	CA-CB-CG	-5.96	107.83	113.80
5	E	13	SER	CA-C-N	5.96	131.23	123.00
5	E	13	SER	C-N-CA	5.96	131.23	123.00
2	B	60	THR	N-CA-C	-5.96	106.62	114.31
24	Q	280	ASN	N-CA-CB	5.96	118.98	110.16
12	l	285	VAL	CA-C-N	5.96	129.67	122.16
12	l	285	VAL	C-N-CA	5.96	129.67	122.16
6	F	32	GLY	CA-C-O	-5.96	116.03	122.47
20	Z	809	MET	CB-CA-C	-5.96	100.72	110.85
20	Z	913	ILE	CB-CA-C	-5.96	104.23	112.04
25	R	276	LEU	O-C-N	5.96	128.53	122.09
32	M	189	GLN	CA-C-N	5.96	128.88	120.42
32	M	189	GLN	C-N-CA	5.96	128.88	120.42
11	4	103	LEU	CA-C-O	5.96	126.79	120.36
20	Z	208	VAL	CA-C-O	-5.96	114.70	118.69
32	M	26	SER	CA-C-N	5.96	128.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	26	SER	C-N-CA	5.96	128.26	120.28
32	M	39	ASN	N-CA-C	5.96	117.44	111.07
4	D	96	HIS	CE1-NE2-CD2	-5.96	103.05	109.00
7	G	224	THR	O-C-N	-5.96	115.72	121.85
25	R	98	LEU	CA-C-N	5.96	128.54	120.44
25	R	98	LEU	C-N-CA	5.96	128.54	120.44
2	b	94	HIS	N-CA-C	5.95	117.57	111.14
6	f	123	TYR	O-C-N	-5.95	116.07	123.04
21	N	690	HIS	ND1-CE1-NE2	5.95	114.35	108.40
14	n	255	ALA	CA-C-O	5.95	126.14	119.41
18	X	75	TRP	CB-CA-C	-5.95	100.55	110.19
26	U	164	GLU	N-CA-C	-5.95	102.67	110.53
29	I	374	ASP	CA-CB-CG	-5.95	106.65	112.60
21	N	651	PHE	N-CA-CB	5.95	119.50	110.28
23	P	195	GLN	CA-C-N	5.95	128.74	120.29
23	P	195	GLN	C-N-CA	5.95	128.74	120.29
23	P	314	VAL	CA-C-N	5.95	128.18	120.44
23	P	314	VAL	C-N-CA	5.95	128.18	120.44
12	l	102	ALA	N-CA-C	5.95	117.84	111.36
1	A	135	ARG	CA-C-N	5.95	125.86	119.85
1	A	135	ARG	C-N-CA	5.95	125.86	119.85
16	V	304	ALA	CB-CA-C	-5.95	99.81	110.70
11	4	158	LEU	N-CA-CB	5.95	119.06	110.20
21	N	653	ARG	NE-CZ-NH1	5.95	127.45	121.50
22	S	118	PHE	CA-C-N	5.95	129.73	120.75
22	S	118	PHE	C-N-CA	5.95	129.73	120.75
4	d	195	THR	CA-C-N	5.95	128.61	120.46
4	d	195	THR	C-N-CA	5.95	128.61	120.46
9	2	63	LEU	N-CA-C	-5.95	97.52	107.80
17	T	13	ILE	CA-C-N	5.95	128.73	120.29
17	T	13	ILE	C-N-CA	5.95	128.73	120.29
21	N	192	LEU	CA-C-N	5.95	128.17	120.44
21	N	192	LEU	C-N-CA	5.95	128.17	120.44
21	N	537	THR	O-C-N	-5.95	115.37	122.15
21	N	592	GLY	CA-C-N	5.95	128.17	120.44
21	N	592	GLY	C-N-CA	5.95	128.17	120.44
31	L	380	VAL	O-C-N	5.95	127.95	121.83
7	G	152	GLU	CA-C-N	5.94	125.64	119.82
7	G	152	GLU	C-N-CA	5.94	125.64	119.82
31	L	287	GLY	CA-C-N	5.94	126.92	120.44
31	L	287	GLY	C-N-CA	5.94	126.92	120.44
1	a	223	LEU	N-CA-CB	5.94	122.03	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	128	VAL	N-CA-CB	5.94	118.12	110.99
13	m	84	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
7	G	101	LYS	N-CA-CB	5.94	118.63	110.01
10	3	8	ASN	N-CA-C	-5.94	105.34	113.30
10	3	44	PHE	N-CA-C	-5.94	100.28	109.14
23	P	298	SER	CA-C-O	-5.94	113.14	119.97
26	U	220	PRO	CB-CA-C	5.94	119.11	111.21
29	I	65	ILE	CA-C-O	5.94	127.15	120.85
33	J	210	PHE	CA-CB-CG	5.94	119.74	113.80
10	3	163	LEU	CA-C-O	5.94	126.80	119.97
31	L	408	ASP	CA-CB-CG	-5.94	106.66	112.60
27	O	381	GLY	CA-C-N	5.94	128.72	120.29
27	O	381	GLY	C-N-CA	5.94	128.72	120.29
3	C	138	ALA	N-CA-C	-5.94	98.72	108.76
21	N	484	GLY	CA-C-N	5.94	128.24	120.28
21	N	484	GLY	C-N-CA	5.94	128.24	120.28
31	L	328	ASN	OD1-CG-ND2	5.94	128.54	122.60
23	P	240	TYR	CA-C-O	-5.94	114.13	120.42
26	U	160	THR	N-CA-C	-5.94	100.55	108.74
27	O	102	LEU	N-CA-CB	5.93	118.94	110.16
28	H	80	HIS	CA-CB-CG	-5.93	107.87	113.80
29	I	255	LYS	N-CA-C	-5.93	106.28	112.93
33	J	81	ASP	N-CA-C	-5.93	105.22	112.88
9	i	41	VAL	O-C-N	-5.93	117.49	123.19
10	j	10	GLY	CA-C-O	-5.93	114.27	121.98
10	j	200	LEU	N-CA-CB	5.93	119.14	109.95
21	N	422	TYR	N-CA-CB	5.93	118.84	110.12
29	I	151	HIS	CA-C-O	5.93	127.05	120.82
3	c	176	LEU	N-CA-CB	5.93	118.61	110.01
5	E	22	PHE	CA-CB-CG	5.93	119.73	113.80
23	P	258	LYS	O-C-N	-5.93	115.69	120.38
27	O	329	MET	CA-C-O	-5.93	114.26	120.55
3	c	90	THR	CA-C-N	5.93	128.15	120.44
3	c	90	THR	C-N-CA	5.93	128.15	120.44
29	I	316	PHE	CB-CG-CD1	-5.93	110.62	120.70
31	L	187	THR	CA-C-N	5.93	128.71	120.29
31	L	187	THR	C-N-CA	5.93	128.71	120.29
31	L	228	LYS	CA-C-O	-5.93	114.23	120.63
7	G	21	ASN	CA-C-N	5.93	128.47	120.65
7	G	21	ASN	C-N-CA	5.93	128.47	120.65
15	W	18	ASN	CA-C-O	-5.93	115.10	121.56
17	T	250	MET	N-CA-C	5.93	118.41	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	109	ILE	CA-C-N	5.93	125.63	119.05
7	g	109	ILE	C-N-CA	5.93	125.63	119.05
21	N	4	THR	CA-CB-OG1	5.93	118.49	109.60
21	N	137	PHE	N-CA-C	5.93	117.41	111.07
27	O	38	TRP	CG-CD2-CE3	-5.93	127.97	133.90
2	b	240	SER	CA-C-O	5.92	126.83	120.55
4	d	102	ASP	N-CA-C	-5.92	99.92	109.58
4	D	129	PHE	CA-C-N	5.92	133.02	121.41
4	D	129	PHE	C-N-CA	5.92	133.02	121.41
22	S	458	GLN	OE1-CD-NE2	-5.92	116.68	122.60
24	Q	76	GLU	CA-C-N	5.92	128.70	120.29
24	Q	76	GLU	C-N-CA	5.92	128.70	120.29
6	f	168	ALA	N-CA-C	-5.92	104.22	112.45
12	l	87	ILE	CA-C-O	5.92	126.64	120.36
1	a	244	ARG	N-CA-CB	5.92	118.82	110.12
17	T	29	PRO	O-C-N	5.92	129.05	122.24
18	X	70	PRO	O-C-N	5.92	130.07	122.85
22	S	302	HIS	CA-CB-CG	-5.92	107.88	113.80
27	O	106	PHE	N-CA-CB	5.92	118.83	110.12
30	K	357	ALA	N-CA-C	-5.92	105.24	112.88
14	7	189	ARG	CD-NE-CZ	-5.92	116.11	124.40
11	k	85	ARG	CA-C-N	5.92	128.21	120.28
11	k	85	ARG	C-N-CA	5.92	128.21	120.28
12	5	191	ASP	N-CA-C	-5.92	100.76	109.81
28	H	435	ARG	N-CA-C	-5.92	100.54	109.95
4	D	213	THR	O-C-N	-5.92	116.41	123.27
7	G	120	VAL	CA-CB-CG2	-5.92	100.34	110.40
23	P	135	GLU	CA-C-N	5.92	128.21	120.28
23	P	135	GLU	C-N-CA	5.92	128.21	120.28
27	O	179	PHE	CA-C-O	-5.92	113.17	119.97
30	K	380	GLY	CA-C-O	-5.92	114.01	120.40
7	G	236	LEU	O-C-N	-5.92	115.41	122.15
1	a	70	SER	CA-C-O	-5.91	114.37	120.99
4	d	64	VAL	N-CA-CB	5.91	119.29	111.25
6	F	101	ARG	N-CA-C	-5.91	98.64	108.75
11	4	133	HIS	ND1-CE1-NE2	5.91	114.31	108.40
4	d	254	HIS	CE1-NE2-CD2	-5.91	103.09	109.00
13	m	130	VAL	CB-CA-C	-5.91	101.70	110.33
19	Y	55	THR	CA-C-N	5.91	128.13	120.44
19	Y	55	THR	C-N-CA	5.91	128.13	120.44
2	b	244	ASN	N-CA-C	-5.91	104.92	111.36
5	E	136	ARG	NE-CZ-NH2	5.91	124.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	83	GLN	CA-C-N	5.91	128.20	120.28
30	K	83	GLN	C-N-CA	5.91	128.20	120.28
30	K	353	PHE	CA-CB-CG	5.91	119.71	113.80
8	1	166	HIS	CE1-NE2-CD2	-5.91	103.09	109.00
9	2	178	GLU	N-CA-CB	-5.91	101.44	110.01
15	W	52	ILE	CA-C-O	-5.91	115.47	121.67
17	T	234	TYR	CA-CB-CG	-5.91	103.26	113.90
21	N	489	MET	N-CA-C	-5.91	105.38	112.59
25	R	392	ARG	NE-CZ-NH2	-5.91	113.88	119.20
26	U	15	LEU	CB-CA-C	-5.91	100.81	110.85
11	4	87	GLU	CA-C-N	5.91	128.68	120.29
11	4	87	GLU	C-N-CA	5.91	128.68	120.29
25	R	327	ASP	CA-CB-CG	5.91	118.50	112.60
4	d	132	SER	N-CA-C	-5.90	100.08	109.59
7	g	211	ASP	N-CA-C	-5.90	101.72	110.46
16	V	84	ASP	N-CA-CB	5.90	120.47	110.49
24	Q	296	ILE	CA-C-N	5.90	128.67	120.29
24	Q	296	ILE	C-N-CA	5.90	128.67	120.29
8	h	93	GLU	O-C-N	5.90	128.37	122.12
10	j	31	SER	N-CA-CB	5.90	119.97	110.65
7	G	62	GLN	CG-CD-NE2	-5.90	107.55	116.40
7	G	116	LEU	N-CA-CB	5.90	118.79	110.12
12	5	100	TRP	N-CA-CB	5.90	122.11	111.37
17	T	37	ASN	N-CA-CB	5.90	118.79	110.12
21	N	428	VAL	CA-C-N	5.90	128.19	120.28
21	N	428	VAL	C-N-CA	5.90	128.19	120.28
22	S	22	GLU	O-C-N	-5.90	115.42	122.15
22	S	204	ASP	CA-C-O	-5.90	114.30	120.55
25	R	338	TYR	CA-C-N	5.90	128.19	120.28
25	R	338	TYR	C-N-CA	5.90	128.19	120.28
28	H	114	GLU	N-CA-C	-5.90	99.28	108.90
8	h	153	GLU	CA-C-N	5.90	131.23	122.74
8	h	153	GLU	C-N-CA	5.90	131.23	122.74
4	D	195	THR	N-CA-C	5.90	117.71	111.28
12	5	169	GLY	CA-C-N	5.90	129.14	120.82
12	5	169	GLY	C-N-CA	5.90	129.14	120.82
21	N	779	GLU	N-CA-CB	5.90	118.91	110.06
27	O	352	TRP	CB-CG-CD2	-5.90	118.54	126.80
32	M	136	ASP	O-C-N	-5.90	114.92	121.53
33	J	179	ILE	O-C-N	-5.90	115.88	122.66
33	J	394	GLN	CA-C-O	5.90	126.66	119.11
6	f	119	ASN	OD1-CG-ND2	-5.90	116.70	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	161	ALA	N-CA-C	-5.90	99.73	108.99
21	N	572	LEU	CA-C-N	5.90	128.10	120.44
21	N	572	LEU	C-N-CA	5.90	128.10	120.44
25	R	162	ILE	N-CA-C	-5.90	99.80	108.23
30	K	186	GLU	CA-C-N	5.90	128.66	120.29
30	K	186	GLU	C-N-CA	5.90	128.66	120.29
4	d	220	ASP	CA-CB-CG	5.89	118.49	112.60
6	f	124	GLY	CA-C-O	-5.89	115.10	122.65
6	F	157	TYR	CA-C-O	5.89	126.19	119.18
5	e	187	TRP	N-CA-C	-5.89	99.00	108.55
16	V	36	LYS	CA-C-N	5.89	128.10	120.44
16	V	36	LYS	C-N-CA	5.89	128.10	120.44
22	S	87	SER	CA-C-N	5.89	128.66	120.29
22	S	87	SER	C-N-CA	5.89	128.66	120.29
24	Q	305	ALA	CA-C-N	5.89	128.46	120.44
24	Q	305	ALA	C-N-CA	5.89	128.46	120.44
31	L	389	ALA	CA-C-N	5.89	128.77	120.28
31	L	389	ALA	C-N-CA	5.89	128.77	120.28
32	M	56	ASN	N-CA-C	-5.89	104.21	111.40
32	M	242	THR	CA-C-O	-5.89	114.20	120.92
21	N	646	LYS	N-CA-C	-5.89	103.50	112.99
6	F	74	LEU	CA-C-N	5.89	130.35	121.40
6	F	74	LEU	C-N-CA	5.89	130.35	121.40
16	V	219	GLU	N-CA-C	-5.89	98.72	109.56
21	N	513	ILE	N-CA-CB	5.89	118.55	110.54
21	N	544	GLU	CA-C-N	5.89	128.76	120.28
21	N	544	GLU	C-N-CA	5.89	128.76	120.28
24	Q	21	ASN	CA-C-N	5.89	130.69	120.68
24	Q	21	ASN	C-N-CA	5.89	130.69	120.68
30	K	387	MET	CA-C-N	5.89	128.17	120.28
30	K	387	MET	C-N-CA	5.89	128.17	120.28
14	n	86	ILE	O-C-N	5.89	129.43	123.07
4	D	127	ARG	NE-CZ-NH2	5.89	124.50	119.20
29	I	346	ARG	N-CA-CB	5.89	120.01	110.41
1	a	236	LEU	N-CA-C	-5.89	100.90	110.20
3	c	147	GLN	CA-C-N	5.89	132.27	122.73
3	c	147	GLN	C-N-CA	5.89	132.27	122.73
7	G	153	PRO	N-CA-C	-5.89	106.39	113.98
23	P	300	VAL	N-CA-C	-5.89	104.77	110.72
24	Q	310	SER	N-CA-CB	5.89	120.57	110.68
26	U	192	ASN	CA-CB-CG	5.89	118.49	112.60
31	L	161	ARG	NE-CZ-NH1	5.89	127.39	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	391	LEU	N-CA-CB	5.89	120.00	110.40
2	b	139	HIS	CE1-NE2-CD2	-5.88	103.11	109.00
13	m	39	THR	CA-C-N	5.88	132.78	121.54
13	m	39	THR	C-N-CA	5.88	132.78	121.54
28	H	46	ALA	N-CA-C	5.88	117.77	111.36
28	H	128	ASN	OD1-CG-ND2	-5.88	116.72	122.60
28	H	214	CYS	N-CA-C	-5.88	105.41	112.59
5	e	165	TYR	CA-C-O	-5.88	113.79	120.32
14	n	122	PRO	CA-C-N	5.88	129.25	120.31
14	n	122	PRO	C-N-CA	5.88	129.25	120.31
2	B	52	SER	N-CA-CB	5.88	120.43	110.49
23	P	434	THR	CA-C-O	5.88	126.78	120.55
31	L	426	LYS	CA-CB-CG	5.88	125.86	114.10
21	N	787	MET	N-CA-CB	5.88	120.53	110.77
23	P	14	SER	CA-C-N	5.88	128.16	120.28
23	P	14	SER	C-N-CA	5.88	128.16	120.28
26	U	280	ASN	CA-C-N	5.88	128.64	120.29
26	U	280	ASN	C-N-CA	5.88	128.64	120.29
3	c	123	THR	CA-C-N	5.88	128.43	120.44
3	c	123	THR	C-N-CA	5.88	128.43	120.44
5	e	48	LEU	CB-CA-C	-5.88	100.40	110.16
20	Z	353	VAL	N-CA-CB	5.88	114.20	110.50
22	S	247	VAL	O-C-N	5.88	128.44	121.80
22	S	488	GLN	N-CA-C	-5.88	104.95	111.36
24	Q	127	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
30	K	377	SER	CA-C-N	5.88	130.17	120.94
30	K	377	SER	C-N-CA	5.88	130.17	120.94
31	L	133	ASN	CA-CB-CG	5.88	118.48	112.60
2	B	194	LEU	CA-C-N	5.88	128.15	120.28
2	B	194	LEU	C-N-CA	5.88	128.15	120.28
16	V	216	LEU	N-CA-C	-5.88	103.53	112.99
16	V	301	ASN	CA-CB-CG	-5.88	106.72	112.60
21	N	294	PRO	N-CA-CB	5.88	109.96	103.26
22	S	459	GLN	CA-C-N	5.88	128.76	120.42
22	S	459	GLN	C-N-CA	5.88	128.76	120.42
1	a	115	ASP	CA-C-N	5.88	128.76	120.42
1	a	115	ASP	C-N-CA	5.88	128.76	120.42
21	N	291	SER	N-CA-C	-5.88	104.96	111.36
23	P	176	LYS	O-C-N	5.88	128.35	122.12
4	d	244	GLN	CA-C-N	5.87	128.15	120.28
4	d	244	GLN	C-N-CA	5.87	128.15	120.28
6	f	228	GLU	CA-C-O	5.87	126.43	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	107	ILE	N-CA-C	-5.87	100.02	108.48
2	B	134	LEU	CA-C-O	-5.87	114.50	121.66
16	V	242	LYS	CA-C-N	5.87	128.63	120.29
16	V	242	LYS	C-N-CA	5.87	128.63	120.29
22	S	21	SER	CA-C-N	5.87	128.63	120.29
22	S	21	SER	C-N-CA	5.87	128.63	120.29
25	R	49	PHE	N-CA-CB	5.87	118.75	110.12
7	G	67	ILE	CB-CA-C	-5.87	103.52	111.15
17	T	272	ASN	CA-CB-CG	-5.87	106.73	112.60
21	N	829	LYS	O-C-N	-5.87	117.42	123.29
25	R	106	ASN	CA-C-N	5.87	128.40	120.65
25	R	106	ASN	C-N-CA	5.87	128.40	120.65
3	c	243	GLY	CA-C-N	5.87	128.75	120.42
3	c	243	GLY	C-N-CA	5.87	128.75	120.42
16	V	207	ALA	CA-C-N	5.87	128.42	120.44
16	V	207	ALA	C-N-CA	5.87	128.42	120.44
25	R	112	GLU	N-CA-CB	5.87	118.48	109.91
4	D	112	TYR	CB-CG-CD2	-5.87	112.00	120.80
13	6	159	ASP	CA-CB-CG	-5.87	106.73	112.60
16	V	76	THR	CA-C-N	5.87	129.57	120.00
16	V	76	THR	C-N-CA	5.87	129.57	120.00
33	J	351	ASN	CA-C-O	-5.87	112.69	119.14
22	S	368	LYS	CA-C-N	5.87	128.07	120.44
22	S	368	LYS	C-N-CA	5.87	128.07	120.44
27	O	201	PRO	CA-C-N	5.87	129.44	121.05
27	O	201	PRO	C-N-CA	5.87	129.44	121.05
13	m	85	PHE	CA-CB-CG	5.87	119.67	113.80
11	4	96	ARG	CB-CA-C	5.87	116.68	110.17
13	6	178	LYS	CA-C-O	-5.87	113.94	119.80
18	X	45	PHE	CA-CB-CG	-5.87	107.94	113.80
20	Z	432	GLY	CA-C-N	5.87	128.94	120.38
20	Z	432	GLY	C-N-CA	5.87	128.94	120.38
21	N	190	LEU	CA-C-O	5.87	126.64	120.42
25	R	331	ARG	N-CA-C	5.87	117.35	111.07
26	U	205	LYS	CA-C-O	5.87	126.64	120.42
8	h	88	ALA	CB-CA-C	-5.86	101.63	110.90
9	i	122	HIS	CG-CD2-NE2	5.86	113.06	107.20
1	A	99	ALA	CA-C-N	5.86	128.62	120.29
1	A	99	ALA	C-N-CA	5.86	128.62	120.29
17	T	46	ILE	N-CA-C	-5.86	100.61	108.35
23	P	343	LYS	CA-C-N	5.86	129.22	120.31
23	P	343	LYS	C-N-CA	5.86	129.22	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	236	PHE	CB-CA-C	5.86	120.52	110.79
27	O	219	ILE	CA-C-N	5.86	128.14	120.28
27	O	219	ILE	C-N-CA	5.86	128.14	120.28
30	K	409	GLU	CA-C-O	5.86	126.75	120.24
7	g	228	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
8	1	90	VAL	CA-C-N	5.86	128.13	120.28
8	1	90	VAL	C-N-CA	5.86	128.13	120.28
21	N	165	ILE	CA-C-N	5.86	128.74	120.42
21	N	165	ILE	C-N-CA	5.86	128.74	120.42
2	B	67	LEU	N-CA-CB	5.86	118.93	110.20
2	B	179	TRP	CA-C-O	-5.86	114.73	121.47
9	2	176	THR	N-CA-CB	5.86	118.47	110.38
13	6	147	GLY	CA-C-O	-5.86	113.24	122.27
20	Z	742	GLY	CA-C-N	5.86	128.49	120.46
20	Z	742	GLY	C-N-CA	5.86	128.49	120.46
21	N	398	ARG	CA-C-N	5.86	129.22	120.31
21	N	398	ARG	C-N-CA	5.86	129.22	120.31
21	N	841	THR	O-C-N	-5.86	115.44	120.71
26	U	9	THR	CA-CB-OG1	5.86	118.39	109.60
10	j	39	LYS	CA-C-O	5.86	126.35	118.38
4	D	183	GLU	CA-C-O	5.86	125.53	119.49
23	P	74	ASP	N-CA-C	-5.86	105.62	112.89
24	Q	163	ARG	CD-NE-CZ	-5.86	116.20	124.40
32	M	183	VAL	CA-C-N	5.86	125.55	119.92
32	M	183	VAL	C-N-CA	5.86	125.55	119.92
12	l	82	ARG	CA-C-O	-5.86	114.33	121.36
13	m	164	PHE	CA-CB-CG	-5.86	107.94	113.80
9	2	112	LEU	CA-C-N	5.86	128.13	120.28
9	2	112	LEU	C-N-CA	5.86	128.13	120.28
12	5	99	ASN	CA-CB-CG	-5.86	106.74	112.60
16	V	23	THR	CA-C-N	5.86	129.43	120.82
16	V	23	THR	C-N-CA	5.86	129.43	120.82
21	N	543	ASP	O-C-N	-5.86	115.15	122.24
22	S	252	ASP	O-C-N	5.86	128.33	122.12
23	P	425	HIS	ND1-CE1-NE2	5.86	114.26	108.40
24	Q	268	SER	N-CA-CB	5.86	118.73	110.12
26	U	94	HIS	CG-CD2-NE2	5.86	113.06	107.20
31	L	107	GLU	N-CA-C	-5.86	99.79	108.99
4	D	163	THR	CA-C-O	-5.86	114.26	121.11
14	7	49	TYR	N-CA-CB	5.86	120.47	111.22
22	S	204	ASP	O-C-N	5.86	128.33	122.12
27	O	385	GLU	O-C-N	5.86	128.10	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	332	VAL	CA-C-N	5.85	128.05	120.44
21	N	332	VAL	C-N-CA	5.85	128.05	120.44
33	J	290	ILE	CA-C-N	5.85	129.69	122.37
33	J	290	ILE	C-N-CA	5.85	129.69	122.37
1	a	225	VAL	O-C-N	5.85	129.52	123.20
3	c	108	VAL	CA-C-O	5.85	127.05	120.85
3	c	117	ASP	N-CA-C	5.85	117.66	111.28
4	d	154	GLY	N-CA-C	-5.85	106.66	115.32
12	l	253	TYR	N-CA-CB	-5.85	100.63	111.52
5	E	188	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
15	W	161	VAL	CA-C-N	5.85	129.42	121.05
15	W	161	VAL	C-N-CA	5.85	129.42	121.05
22	S	71	ALA	CA-C-O	5.85	126.75	119.78
33	J	264	GLY	N-CA-C	5.85	121.11	114.67
9	i	97	LEU	CA-C-N	5.85	128.60	120.29
9	i	97	LEU	C-N-CA	5.85	128.60	120.29
4	D	233	VAL	CB-CA-C	-5.85	104.14	112.22
8	1	129	HIS	CA-CB-CG	-5.85	107.95	113.80
17	T	245	TYR	CA-C-N	5.85	128.60	120.29
17	T	245	TYR	C-N-CA	5.85	128.60	120.29
26	U	252	HIS	CB-CG-ND1	5.85	131.48	122.70
1	a	187	LYS	N-CA-C	-5.85	104.82	111.14
1	A	123	ASN	N-CA-C	-5.85	104.98	111.36
14	7	73	GLU	CB-CG-CD	-5.85	102.66	112.60
20	Z	810	ASN	N-CA-C	-5.85	104.98	111.36
26	U	233	PHE	N-CA-C	5.85	117.73	111.36
5	E	194	LYS	CA-C-N	5.85	128.12	120.28
5	E	194	LYS	C-N-CA	5.85	128.12	120.28
10	3	55	GLY	CA-C-N	5.85	129.68	121.02
10	3	55	GLY	C-N-CA	5.85	129.68	121.02
20	Z	258	PRO	N-CA-C	5.85	117.83	110.70
21	N	771	PHE	N-CA-CB	5.85	120.47	111.46
33	J	231	ARG	CA-C-N	5.85	129.20	120.31
33	J	231	ARG	C-N-CA	5.85	129.20	120.31
31	L	324	ILE	N-CA-C	-5.85	99.22	107.75
8	1	42	LYS	CB-CA-C	-5.84	101.55	111.02
28	H	365	LEU	CA-C-N	5.84	128.59	120.29
28	H	365	LEU	C-N-CA	5.84	128.59	120.29
13	6	12	PRO	N-CA-CB	5.84	109.30	102.76
21	N	208	ARG	CA-C-N	5.84	128.11	120.28
21	N	208	ARG	C-N-CA	5.84	128.11	120.28
22	S	63	LEU	CA-C-N	5.84	128.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	63	LEU	C-N-CA	5.84	128.39	120.44
28	H	339	GLN	CG-CD-OE1	-5.84	109.11	120.80
30	K	328	LEU	CA-C-O	5.84	126.11	119.27
31	L	313	ASP	N-CA-CB	5.84	120.63	110.81
8	1	58	ALA	CA-C-N	5.84	128.11	120.28
8	1	58	ALA	C-N-CA	5.84	128.11	120.28
14	7	177	THR	N-CA-CB	5.84	121.71	111.55
17	T	27	LEU	N-CA-C	5.84	121.46	113.16
21	N	434	SER	N-CA-C	-5.84	106.19	113.38
30	K	124	SER	CA-C-O	-5.84	114.92	121.81
30	K	420	THR	N-CA-C	-5.84	105.81	113.17
33	J	249	GLU	N-CA-CB	5.84	119.14	110.49
14	n	177	THR	CA-CB-OG1	5.84	118.36	109.60
26	U	70	HIS	CA-C-N	5.84	128.42	120.54
26	U	70	HIS	C-N-CA	5.84	128.42	120.54
33	J	361	VAL	N-CA-C	-5.84	104.81	110.42
8	1	110	GLY	O-C-N	5.84	129.19	123.76
20	Z	921	GLU	N-CA-C	-5.84	100.78	109.42
21	N	222	TYR	N-CA-C	-5.84	106.13	113.72
21	N	470	LEU	CB-CA-C	-5.84	101.10	110.79
21	N	771	PHE	N-CA-C	-5.84	100.08	108.60
9	i	146	GLY	CA-C-N	5.83	131.33	120.95
9	i	146	GLY	C-N-CA	5.83	131.33	120.95
1	A	225	VAL	CA-C-N	5.83	126.59	122.33
1	A	225	VAL	C-N-CA	5.83	126.59	122.33
3	C	86	ILE	CA-C-O	-5.83	114.88	120.95
7	G	97	ALA	CA-C-N	5.83	128.57	120.29
7	G	97	ALA	C-N-CA	5.83	128.57	120.29
27	O	326	HIS	CG-CD2-NE2	5.83	113.03	107.20
21	N	425	ASN	CA-C-N	5.83	128.70	120.42
21	N	425	ASN	C-N-CA	5.83	128.70	120.42
32	M	343	LEU	N-CA-C	-5.83	99.01	108.52
4	d	13	PRO	CA-C-O	5.83	126.91	118.86
11	k	50	ALA	N-CA-C	5.83	118.79	110.10
3	C	94	HIS	CE1-NE2-CD2	-5.83	103.17	109.00
11	4	26	SER	CA-C-N	5.83	130.57	122.93
11	4	26	SER	C-N-CA	5.83	130.57	122.93
26	U	292	ILE	CA-C-N	5.83	128.09	120.28
26	U	292	ILE	C-N-CA	5.83	128.09	120.28
4	d	48	ARG	N-CA-C	-5.83	97.67	107.99
5	e	245	GLU	CB-CG-CD	-5.83	102.69	112.60
21	N	335	ALA	N-CA-C	5.83	117.31	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	124	VAL	N-CA-C	-5.83	104.83	110.72
23	P	177	ILE	O-C-N	5.83	127.62	121.91
32	M	45	ARG	N-CA-C	-5.83	105.27	112.90
23	P	409	SER	CA-C-N	5.83	128.01	120.44
23	P	409	SER	C-N-CA	5.83	128.01	120.44
10	j	125	ASP	CA-C-N	5.83	128.01	120.44
10	j	125	ASP	C-N-CA	5.83	128.01	120.44
10	j	175	ALA	CA-C-N	5.83	128.09	120.28
10	j	175	ALA	C-N-CA	5.83	128.09	120.28
4	D	221	ILE	CB-CA-C	-5.83	101.83	110.33
21	N	844	LYS	N-CA-C	-5.83	105.54	114.16
28	H	260	ALA	N-CA-C	-5.83	104.89	112.23
30	K	130	LEU	CA-C-N	5.83	128.01	120.44
30	K	130	LEU	C-N-CA	5.83	128.01	120.44
32	M	404	ARG	N-CA-CB	5.83	118.78	110.16
4	d	64	VAL	N-CA-C	-5.82	100.02	108.17
26	U	299	LYS	CA-C-N	5.82	128.08	120.28
26	U	299	LYS	C-N-CA	5.82	128.08	120.28
29	I	323	LYS	N-CA-C	-5.82	99.79	109.46
26	U	222	ASN	CA-C-N	5.82	129.16	120.31
26	U	222	ASN	C-N-CA	5.82	129.16	120.31
5	e	93	ARG	NE-CZ-NH1	5.82	127.32	121.50
2	B	106	PRO	CA-C-N	5.82	128.01	120.44
2	B	106	PRO	C-N-CA	5.82	128.01	120.44
25	R	355	SER	CA-C-O	-5.82	114.25	120.42
15	W	189	PRO	N-CA-C	5.82	120.75	111.26
21	N	216	ASN	N-CA-CB	5.82	119.26	110.30
22	S	66	GLN	CB-CG-CD	5.82	122.49	112.60
31	L	362	LYS	CG-CD-CE	5.82	124.68	111.30
16	V	164	LEU	CA-C-N	5.82	128.43	120.46
16	V	164	LEU	C-N-CA	5.82	128.43	120.46
28	H	155	PHE	O-C-N	5.82	129.88	123.25
30	K	221	MET	CA-C-N	5.82	128.66	120.28
30	K	221	MET	C-N-CA	5.82	128.66	120.28
31	L	364	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
32	M	432	PHE	N-CA-C	-5.82	103.34	110.61
33	J	40	ASN	OD1-CG-ND2	5.82	128.42	122.60
5	e	10	ARG	CA-C-O	-5.82	114.25	120.42
5	E	113	THR	N-CA-C	5.82	117.62	111.28
5	E	248	ALA	CB-CA-C	-5.82	100.96	110.85
24	Q	346	ASN	CA-CB-CG	-5.82	106.78	112.60
25	R	95	ASP	N-CA-C	-5.82	100.47	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	168	ILE	CB-CA-C	-5.82	102.16	110.83
2	b	230	ASP	CA-C-O	5.81	128.54	121.68
22	S	453	ASP	CA-C-N	5.81	131.30	120.95
22	S	453	ASP	C-N-CA	5.81	131.30	120.95
4	d	42	VAL	CA-C-N	-5.81	115.53	123.14
4	d	42	VAL	C-N-CA	-5.81	115.53	123.14
26	U	166	ALA	O-C-N	5.81	128.28	122.12
5	e	100	ASN	N-CA-C	5.81	117.61	111.28
17	T	109	TYR	CA-C-N	5.81	128.07	120.28
17	T	109	TYR	C-N-CA	5.81	128.07	120.28
32	M	371	ASP	CA-CB-CG	-5.81	106.79	112.60
4	d	8	LEU	CA-C-N	5.81	130.42	120.72
4	d	8	LEU	C-N-CA	5.81	130.42	120.72
2	B	133	SER	N-CA-C	-5.81	99.43	108.90
16	V	151	VAL	CB-CA-C	-5.81	103.02	110.98
2	b	101	TYR	CB-CG-CD2	5.81	129.51	120.80
3	c	177	GLN	CA-C-N	5.81	128.53	120.29
3	c	177	GLN	C-N-CA	5.81	128.53	120.29
11	k	70	ARG	CA-C-N	5.81	128.54	120.29
11	k	70	ARG	C-N-CA	5.81	128.54	120.29
4	D	173	GLU	N-CA-CB	5.81	118.66	110.12
5	E	138	PHE	N-CA-C	-5.81	100.24	109.59
16	V	187	ALA	CA-C-N	5.81	127.99	120.44
16	V	187	ALA	C-N-CA	5.81	127.99	120.44
22	S	212	SER	CA-C-N	5.81	128.06	120.28
22	S	212	SER	C-N-CA	5.81	128.06	120.28
23	P	242	GLN	CA-C-N	5.81	127.99	120.44
23	P	242	GLN	C-N-CA	5.81	127.99	120.44
25	R	308	LEU	CA-C-O	5.81	126.90	120.63
27	O	371	VAL	CB-CA-C	-5.81	104.54	111.97
29	I	192	GLN	CA-C-N	5.81	127.99	120.44
29	I	192	GLN	C-N-CA	5.81	127.99	120.44
31	L	357	ARG	N-CA-C	5.81	117.69	111.36
4	d	199	LEU	CA-C-N	5.81	128.06	120.28
4	d	199	LEU	C-N-CA	5.81	128.06	120.28
16	V	216	LEU	CA-C-O	5.81	125.18	119.08
21	N	439	VAL	CA-C-N	5.81	128.34	120.44
21	N	439	VAL	C-N-CA	5.81	128.34	120.44
32	M	35	LYS	CA-C-O	5.81	126.65	119.97
7	G	172	ALA	O-C-N	-5.80	115.53	122.15
15	W	76	LEU	N-CA-CB	5.80	119.28	110.28
17	T	149	ASP	CA-C-N	5.80	127.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	149	ASP	C-N-CA	5.80	127.99	120.44
24	Q	49	LYS	CA-C-N	5.80	128.06	120.28
24	Q	49	LYS	C-N-CA	5.80	128.06	120.28
21	N	267	GLN	CA-C-N	5.80	128.06	120.28
21	N	267	GLN	C-N-CA	5.80	128.06	120.28
24	Q	427	PHE	CA-CB-CG	5.80	119.60	113.80
8	h	12	ILE	N-CA-C	-5.80	100.12	108.42
10	j	126	LEU	N-CA-C	5.80	117.28	111.07
14	n	84	VAL	CA-C-O	-5.80	114.32	120.53
7	G	106	PRO	CA-C-O	-5.80	114.59	121.67
21	N	677	ASP	CA-C-O	5.80	126.68	120.70
25	R	66	LEU	N-CA-C	-5.80	104.96	111.28
29	I	367	SER	CA-C-N	5.80	128.37	120.54
29	I	367	SER	C-N-CA	5.80	128.37	120.54
21	N	37	SER	N-CA-C	5.80	117.68	111.36
23	P	372	THR	N-CA-C	-5.80	101.62	110.14
25	R	403	LEU	N-CA-C	5.80	117.68	111.36
27	O	110	ASP	CA-CB-CG	5.80	118.40	112.60
27	O	374	ASN	CA-C-O	5.80	126.57	120.42
17	T	52	LEU	CA-C-N	5.80	128.52	120.29
17	T	52	LEU	C-N-CA	5.80	128.52	120.29
19	Y	3	THR	N-CA-C	-5.80	99.89	108.99
25	R	226	GLU	CA-C-N	5.80	128.32	120.38
25	R	226	GLU	C-N-CA	5.80	128.32	120.38
7	g	94	GLU	CA-C-O	-5.80	114.28	120.42
9	i	247	VAL	N-CA-C	-5.80	99.95	108.99
10	j	15	MET	O-C-N	-5.80	117.17	123.26
8	1	35	ILE	CB-CA-C	5.80	117.49	111.23
10	3	136	PHE	N-CA-C	-5.80	98.45	110.80
15	W	192	LEU	CA-C-N	5.80	131.52	120.97
15	W	192	LEU	C-N-CA	5.80	131.52	120.97
17	T	18	GLY	CA-C-N	5.80	130.36	122.19
17	T	18	GLY	C-N-CA	5.80	130.36	122.19
22	S	192	GLU	CA-C-O	-5.80	114.28	120.42
27	O	182	LYS	N-CA-C	-5.80	104.93	112.23
32	M	291	PHE	CA-CB-CG	5.80	119.60	113.80
1	a	250	GLU	N-CA-C	-5.79	98.97	108.76
7	G	244	GLN	CA-C-N	5.79	128.04	120.28
7	G	244	GLN	C-N-CA	5.79	128.04	120.28
22	S	423	VAL	CA-C-O	-5.79	114.71	120.85
27	O	34	GLU	N-CA-C	5.79	117.60	111.28
3	c	9	ARG	CA-C-N	5.79	128.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	9	ARG	C-N-CA	5.79	128.04	120.28
11	k	36	ARG	NE-CZ-NH2	5.79	124.42	119.20
13	m	16	ASN	N-CA-C	-5.79	104.73	113.89
16	V	159	ILE	N-CA-C	-5.79	100.00	108.11
17	T	127	GLN	N-CA-C	5.79	117.67	111.36
19	Y	16	LEU	N-CA-C	-5.79	101.16	110.14
27	O	108	GLU	CB-CG-CD	-5.79	102.75	112.60
8	h	134	ALA	N-CA-CB	5.79	121.33	111.66
10	j	157	ASN	OD1-CG-ND2	5.79	128.39	122.60
2	B	45	ILE	N-CA-C	-5.79	99.78	108.12
14	7	105	THR	O-C-N	-5.79	115.98	122.12
22	S	121	VAL	CA-C-N	5.79	127.97	120.44
22	S	121	VAL	C-N-CA	5.79	127.97	120.44
26	U	70	HIS	ND1-CE1-NE2	5.79	114.19	108.40
30	K	192	LEU	CA-C-O	5.79	126.66	120.70
31	L	352	PRO	CA-C-N	5.79	131.95	121.06
31	L	352	PRO	C-N-CA	5.79	131.95	121.06
5	E	120	ALA	CA-C-N	5.79	128.62	120.28
5	E	120	ALA	C-N-CA	5.79	128.62	120.28
12	5	124	ALA	N-CA-C	5.79	117.26	111.07
18	X	86	ILE	CB-CA-C	-5.79	102.20	110.83
18	X	88	ALA	CA-C-O	5.79	126.48	120.40
31	L	129	VAL	CB-CA-C	-5.79	101.75	110.55
10	j	45	HIS	CG-CD2-NE2	5.79	112.99	107.20
13	m	163	ASN	CA-CB-CG	-5.79	106.81	112.60
22	S	459	GLN	OE1-CD-NE2	-5.79	116.81	122.60
24	Q	242	SER	N-CA-C	5.79	118.36	111.71
24	Q	402	THR	CA-C-N	5.79	127.07	119.84
24	Q	402	THR	C-N-CA	5.79	127.07	119.84
26	U	300	LYS	O-C-N	5.79	128.25	122.12
21	N	300	ASN	CA-CB-CG	-5.79	106.81	112.60
21	N	651	PHE	O-C-N	5.79	129.39	122.27
25	R	131	ALA	CA-C-N	5.79	128.03	120.28
25	R	131	ALA	C-N-CA	5.79	128.03	120.28
29	I	327	ALA	CB-CA-C	-5.79	98.97	109.38
30	K	323	THR	CA-C-N	5.79	129.09	120.87
30	K	323	THR	C-N-CA	5.79	129.09	120.87
9	i	46	ASP	N-CA-C	-5.78	102.74	110.55
3	C	14	SER	CB-CA-C	-5.78	98.78	110.17
4	D	22	TYR	N-CA-C	-5.78	104.94	112.23
12	5	254	HIS	CG-CD2-NE2	5.78	112.98	107.20
13	m	44	ASN	CB-CA-C	-5.78	101.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	152	GLY	O-C-N	5.78	127.87	122.90
30	K	166	LYS	N-CA-C	-5.78	102.83	110.40
2	b	230	ASP	CA-CB-CG	5.78	118.38	112.60
6	F	141	GLY	O-C-N	-5.78	117.42	122.91
8	1	12	ILE	N-CA-C	-5.78	99.31	108.90
21	N	669	GLU	CB-CG-CD	-5.78	102.78	112.60
12	l	233	LYS	CA-C-O	5.78	126.54	120.42
9	2	80	ASP	CA-C-O	-5.78	114.43	120.55
22	S	105	PRO	CB-CA-C	5.78	118.57	110.60
22	S	375	ASP	CA-CB-CG	5.78	118.38	112.60
28	H	448	ASP	CA-C-O	-5.78	114.43	120.55
6	f	179	PHE	CB-CG-CD1	5.77	130.52	120.70
23	P	56	LYS	N-CA-CB	5.77	118.61	110.12
22	S	184	TRP	CA-CB-CG	5.77	124.57	113.60
29	I	191	ILE	N-CA-C	-5.77	104.90	113.39
2	b	195	THR	N-CA-C	5.77	117.25	111.07
5	E	114	GLN	O-C-N	5.77	128.24	122.12
21	N	256	GLN	N-CA-C	5.77	117.37	111.14
28	H	61	ALA	CA-C-N	5.77	128.49	120.29
28	H	61	ALA	C-N-CA	5.77	128.49	120.29
28	H	413	ASN	CA-C-O	5.77	127.50	120.92
29	I	319	ARG	CB-CG-CD	5.77	124.57	111.30
2	b	180	ASN	CA-C-N	5.77	128.01	120.28
2	b	180	ASN	C-N-CA	5.77	128.01	120.28
7	g	190	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
9	i	122	HIS	CA-CB-CG	-5.77	108.03	113.80
17	T	142	LEU	N-CA-C	-5.77	106.28	113.38
22	S	472	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
3	c	76	ALA	CB-CA-C	-5.77	99.79	109.48
14	7	142	PRO	O-C-N	5.77	129.63	123.23
16	V	225	LEU	CA-C-N	5.77	128.90	120.71
16	V	225	LEU	C-N-CA	5.77	128.90	120.71
24	Q	102	GLU	CA-C-O	-5.77	114.44	120.55
32	M	239	THR	CA-C-O	-5.77	113.34	119.97
1	A	193	HIS	O-C-N	-5.77	116.17	122.92
31	L	73	GLN	N-CA-CB	5.77	118.98	110.33
33	J	123	HIS	CG-CD2-NE2	5.77	112.97	107.20
8	h	161	VAL	CA-CB-CG2	-5.76	100.60	110.40
8	1	192	VAL	CB-CA-C	5.76	119.16	110.63
12	5	224	SER	N-CA-CB	5.76	119.05	110.29
16	V	255	ILE	CA-C-O	5.76	126.17	119.89
17	T	127	GLN	CA-C-N	5.76	128.00	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	127	GLN	C-N-CA	5.76	128.00	120.28
21	N	125	THR	N-CA-C	-5.76	105.91	113.17
21	N	232	LEU	CA-C-N	5.76	130.83	122.36
21	N	232	LEU	C-N-CA	5.76	130.83	122.36
33	J	367	MET	N-CA-CB	5.76	118.26	110.59
7	G	60	VAL	N-CA-CB	5.76	116.40	110.23
10	3	174	ALA	O-C-N	5.76	128.23	122.12
16	V	194	ARG	CA-C-O	5.76	126.09	119.35
21	N	706	MET	O-C-N	-5.76	116.01	122.12
22	S	374	ASP	CA-C-N	5.76	130.31	122.19
22	S	374	ASP	C-N-CA	5.76	130.31	122.19
23	P	385	ASN	N-CA-CB	5.76	118.59	110.12
25	R	64	LYS	CA-C-N	5.76	128.58	120.28
25	R	64	LYS	C-N-CA	5.76	128.58	120.28
1	A	232	LYS	CA-C-O	-5.76	115.28	121.38
9	2	226	GLU	CA-C-O	-5.76	114.60	120.71
14	7	246	GLN	N-CA-CB	5.76	119.61	110.57
31	L	66	GLU	CA-C-N	5.76	128.00	120.28
31	L	66	GLU	C-N-CA	5.76	128.00	120.28
5	e	15	PHE	CB-CG-CD1	-5.76	110.91	120.70
6	f	226	ASP	CA-C-O	-5.76	114.77	121.10
32	M	42	ARG	CA-C-O	5.76	126.59	119.97
18	X	132	SER	N-CA-C	-5.76	104.00	111.71
19	Y	63	ASN	CA-CB-CG	-5.76	106.84	112.60
28	H	367	ARG	CA-C-N	-5.76	112.64	119.84
28	H	367	ARG	C-N-CA	-5.76	112.64	119.84
1	a	116	VAL	N-CA-C	-5.75	104.91	110.72
13	6	177	LYS	CA-C-N	5.75	128.38	120.67
13	6	177	LYS	C-N-CA	5.75	128.38	120.67
31	L	308	LEU	CB-CA-C	-5.75	101.24	110.79
2	B	119	GLN	OE1-CD-NE2	-5.75	116.85	122.60
16	V	263	GLU	N-CA-C	-5.75	104.91	111.07
21	N	822	GLY	CA-C-N	5.75	125.61	119.28
21	N	822	GLY	C-N-CA	5.75	125.61	119.28
5	e	185	ASN	CA-C-O	5.75	127.02	120.00
13	6	210	LEU	N-CA-C	-5.75	99.04	108.76
14	7	216	VAL	N-CA-CB	5.75	118.36	110.54
22	S	73	THR	O-C-N	-5.75	116.02	122.12
23	P	41	VAL	N-CA-C	-5.75	104.75	110.62
26	U	82	LYS	N-CA-C	5.75	118.01	111.11
32	M	85	VAL	CA-C-N	5.75	128.26	120.44
32	M	85	VAL	C-N-CA	5.75	128.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	246	GLU	N-CA-CB	5.75	118.98	110.53
1	a	25	LEU	N-CA-CB	5.75	119.73	110.65
7	g	239	ALA	CA-C-O	5.75	126.51	120.42
19	Y	80	GLU	CA-C-N	5.75	128.45	120.29
19	Y	80	GLU	C-N-CA	5.75	128.45	120.29
20	Z	24	THR	CA-C-O	-5.75	112.28	120.16
21	N	700	CYS	CA-C-O	-5.75	113.86	120.24
26	U	21	HIS	CA-C-N	5.75	128.45	120.29
26	U	21	HIS	C-N-CA	5.75	128.45	120.29
9	i	65	ARG	NE-CZ-NH2	5.75	124.37	119.20
6	F	119	ASN	CA-CB-CG	5.75	118.35	112.60
21	N	77	SER	CA-C-N	5.75	127.98	120.28
21	N	77	SER	C-N-CA	5.75	127.98	120.28
21	N	738	GLN	N-CA-C	-5.75	105.85	112.92
27	O	265	LYS	CA-C-N	5.75	127.91	120.44
27	O	265	LYS	C-N-CA	5.75	127.91	120.44
2	B	234	ARG	CA-C-N	5.75	129.03	120.87
2	B	234	ARG	C-N-CA	5.75	129.03	120.87
25	R	134	TRP	N-CA-C	-5.75	104.99	112.23
5	e	114	GLN	N-CA-C	-5.74	105.16	111.82
11	4	121	TYR	N-CA-C	5.74	117.54	111.28
12	5	202	PHE	CA-CB-CG	-5.74	108.06	113.80
28	H	384	GLY	CA-C-N	5.74	131.19	121.14
28	H	384	GLY	C-N-CA	5.74	131.19	121.14
33	J	154	THR	N-CA-CB	5.74	118.66	110.16
6	F	119	ASN	N-CA-C	-5.74	106.11	113.23
20	Z	630	LYS	N-CA-CB	5.74	118.56	110.12
23	P	340	ASP	CA-C-N	5.74	129.04	120.31
23	P	340	ASP	C-N-CA	5.74	129.04	120.31
6	F	185	ASN	N-CA-CB	5.74	120.85	110.17
8	1	166	HIS	CG-CD2-NE2	5.74	112.94	107.20
12	5	254	HIS	ND1-CE1-NE2	5.74	114.14	108.40
21	N	726	ASP	N-CA-CB	-5.74	101.45	110.69
23	P	267	PHE	N-CA-C	5.74	119.46	112.23
31	L	261	ARG	CA-C-N	5.74	128.29	120.77
31	L	261	ARG	C-N-CA	5.74	128.29	120.77
2	b	203	GLU	N-CA-C	-5.74	104.03	113.50
4	d	18	PHE	N-CA-C	5.74	118.48	111.82
3	C	116	SER	CA-C-N	5.74	128.44	120.29
3	C	116	SER	C-N-CA	5.74	128.44	120.29
9	2	189	GLN	N-CA-CB	5.74	118.65	110.16
21	N	113	ALA	N-CA-C	5.74	117.54	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	338	TRP	CB-CA-C	-5.74	101.10	110.85
27	O	65	PHE	CA-C-N	5.74	128.32	120.46
27	O	65	PHE	C-N-CA	5.74	128.32	120.46
9	i	128	ILE	N-CA-C	-5.74	100.16	108.36
11	k	27	VAL	CB-CA-C	-5.74	103.64	111.33
31	L	224	PRO	N-CA-C	5.74	120.23	111.11
12	l	206	SER	N-CA-C	-5.74	105.78	112.89
23	P	436	GLU	CA-CB-CG	-5.74	102.63	114.10
7	G	134	VAL	N-CA-C	-5.73	100.22	108.42
13	6	208	ASP	CA-C-N	5.73	129.46	121.09
13	6	208	ASP	C-N-CA	5.73	129.46	121.09
5	E	82	THR	CA-C-N	5.73	127.89	120.44
5	E	82	THR	C-N-CA	5.73	127.89	120.44
24	Q	105	GLU	CA-C-N	5.73	127.89	120.44
24	Q	105	GLU	C-N-CA	5.73	127.89	120.44
24	Q	241	GLU	N-CA-CB	5.73	118.64	110.16
33	J	45	GLU	CA-C-N	5.73	127.89	120.44
33	J	45	GLU	C-N-CA	5.73	127.89	120.44
4	D	184	PRO	N-CA-C	-5.73	103.71	110.70
4	d	208	LYS	CA-C-O	5.73	126.35	119.59
5	e	210	GLU	N-CA-CB	5.73	120.17	110.49
11	k	55	GLN	CA-C-N	5.73	128.42	120.29
11	k	55	GLN	C-N-CA	5.73	128.42	120.29
23	P	136	ARG	CA-C-O	5.73	126.62	120.55
23	P	425	HIS	CG-CD2-NE2	5.73	112.93	107.20
29	I	83	LYS	CB-CA-C	-5.73	101.11	112.05
32	M	17	GLU	CA-C-N	5.73	132.74	122.09
32	M	17	GLU	C-N-CA	5.73	132.74	122.09
7	G	224	THR	CA-C-N	5.73	130.71	122.35
7	G	224	THR	C-N-CA	5.73	130.71	122.35
8	1	65	ALA	CA-C-N	5.73	128.42	120.29
8	1	65	ALA	C-N-CA	5.73	128.42	120.29
1	A	102	ALA	CA-C-N	5.72	128.22	120.44
1	A	102	ALA	C-N-CA	5.72	128.22	120.44
6	F	120	THR	N-CA-C	-5.72	104.42	111.40
11	4	107	TYR	CB-CG-CD1	5.72	129.39	120.80
16	V	292	ILE	N-CA-C	-5.72	104.94	110.72
21	N	816	LYS	CA-C-N	5.72	127.95	120.28
21	N	816	LYS	C-N-CA	5.72	127.95	120.28
24	Q	336	ASN	O-C-N	5.72	128.68	122.15
12	5	111	GLU	N-CA-CB	5.72	118.88	110.35
25	R	134	TRP	CA-C-O	-5.72	113.04	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	239	THR	O-C-N	5.72	129.31	122.27
1	A	14	ARG	CG-CD-NE	-5.72	99.41	112.00
33	J	185	VAL	O-C-N	-5.72	117.14	123.03
13	6	28	PHE	CB-CG-CD2	-5.72	110.98	120.70
15	W	192	LEU	CA-C-O	5.72	126.70	119.95
17	T	218	GLU	CA-C-N	5.72	130.36	120.58
17	T	218	GLU	C-N-CA	5.72	130.36	120.58
20	Z	444	GLU	CA-C-N	5.72	125.39	119.56
20	Z	444	GLU	C-N-CA	5.72	125.39	119.56
30	K	424	PHE	N-CA-C	-5.72	104.15	113.19
33	J	186	ILE	N-CA-CB	5.72	117.52	111.00
21	N	908	ARG	N-CA-CB	5.72	118.36	110.07
22	S	330	LEU	N-CA-CB	5.72	119.14	110.28
28	H	120	ASN	CA-C-O	5.72	126.12	119.32
30	K	243	VAL	O-C-N	5.72	128.50	122.67
3	c	184	MET	CG-SD-CE	-5.72	88.33	100.90
5	e	20	ARG	N-CA-C	-5.72	99.69	109.24
11	k	54	VAL	CA-C-N	5.72	127.94	120.28
11	k	54	VAL	C-N-CA	5.72	127.94	120.28
2	B	140	ASP	N-CA-CB	5.72	120.59	111.56
14	7	76	ILE	O-C-N	-5.72	114.99	120.59
23	P	407	ASN	N-CA-CB	5.72	118.43	110.26
28	H	358	PRO	CB-CA-C	5.72	116.21	109.92
29	I	148	LEU	N-CA-CB	5.72	119.53	110.55
33	J	125	VAL	N-CA-C	-5.72	103.75	110.21
13	m	59	VAL	CG1-CB-CG2	-5.71	98.23	110.80
3	C	129	ARG	CA-C-O	-5.71	114.08	120.25
23	P	161	CYS	N-CA-C	5.71	117.51	111.28
4	d	89	ALA	CA-C-N	5.71	127.94	120.28
4	d	89	ALA	C-N-CA	5.71	127.94	120.28
4	d	229	ILE	CB-CA-C	-5.71	104.34	112.22
5	E	27	SER	CA-C-N	5.71	128.99	120.31
5	E	27	SER	C-N-CA	5.71	128.99	120.31
9	2	237	GLY	CA-C-O	5.71	125.46	119.06
13	6	155	MET	O-C-N	-5.71	115.34	120.71
3	c	244	ILE	CB-CA-C	5.71	120.10	112.22
12	l	83	PHE	CA-CB-CG	5.71	119.51	113.80
2	B	92	VAL	CA-CB-CG1	5.71	120.11	110.40
5	E	150	ASP	CA-CB-CG	-5.71	106.89	112.60
22	S	164	ILE	CA-C-O	-5.71	112.30	119.95
22	S	447	GLU	O-C-N	-5.71	115.87	122.95
24	Q	373	VAL	N-CA-CB	5.71	117.23	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	274	ILE	CA-C-N	5.71	127.86	120.44
27	O	274	ILE	C-N-CA	5.71	127.86	120.44
32	M	157	ASP	CA-C-O	5.71	127.43	121.38
32	M	316	SER	CA-C-N	5.71	132.45	121.54
32	M	316	SER	C-N-CA	5.71	132.45	121.54
33	J	345	LYS	CA-C-O	5.71	126.60	120.55
1	A	129	THR	CA-C-O	5.71	125.95	119.27
10	3	137	ILE	CA-C-N	5.71	131.03	122.58
10	3	137	ILE	C-N-CA	5.71	131.03	122.58
27	O	304	ASN	CA-CB-CG	-5.71	106.89	112.60
30	K	137	VAL	CB-CA-C	5.71	119.45	111.40
31	L	265	GLU	CA-C-N	5.71	130.34	120.58
31	L	265	GLU	C-N-CA	5.71	130.34	120.58
32	M	231	LEU	CA-C-N	5.71	127.86	120.44
32	M	231	LEU	C-N-CA	5.71	127.86	120.44
1	A	209	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
7	g	54	ILE	N-CA-CB	5.71	118.65	111.46
16	V	295	VAL	N-CA-C	5.71	116.44	110.62
31	L	81	ILE	CB-CA-C	-5.71	104.35	112.22
9	i	116	LEU	CA-C-N	5.70	127.92	120.28
9	i	116	LEU	C-N-CA	5.70	127.92	120.28
26	U	94	HIS	CE1-NE2-CD2	-5.70	103.30	109.00
30	K	230	THR	N-CA-CB	5.70	119.34	110.44
33	J	291	ILE	CB-CA-C	-5.70	104.06	110.96
29	I	163	ASP	CA-CB-CG	-5.70	106.90	112.60
9	i	57	ASP	CA-CB-CG	-5.70	106.90	112.60
2	B	47	THR	N-CA-C	-5.70	100.28	108.60
21	N	394	ARG	N-CA-C	-5.70	100.49	109.50
8	h	60	ASP	N-CA-CB	5.70	118.69	110.20
9	i	168	GLU	N-CA-C	5.70	117.49	111.28
9	2	35	VAL	N-CA-C	-5.70	99.34	107.77
22	S	60	LEU	N-CA-C	5.70	117.49	111.28
22	S	84	ASP	O-C-N	5.70	130.17	122.59
24	Q	29	SER	CA-CB-OG	5.70	122.50	111.10
1	a	244	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	a	249	ALA	CB-CA-C	-5.70	101.16	110.85
2	b	214	ILE	CA-C-O	5.70	126.49	120.51
3	c	62	SER	N-CA-C	-5.70	100.65	109.14
22	S	25	TYR	N-CA-C	-5.70	105.15	111.36
29	I	432	LEU	N-CA-C	-5.70	104.69	111.69
8	1	100	ASP	N-CA-C	-5.69	106.00	113.17
23	P	91	LEU	N-CA-CB	5.69	118.56	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	75	PHE	CA-C-O	-5.69	114.97	121.40
19	Y	81	LEU	N-CA-C	5.69	117.56	111.36
20	Z	806	GLU	CA-C-N	5.69	128.50	120.42
20	Z	806	GLU	C-N-CA	5.69	128.50	120.42
28	H	187	LEU	CA-C-O	-5.69	112.36	120.16
13	6	65	PHE	O-C-N	5.69	130.02	123.02
22	S	149	SER	N-CA-C	-5.69	105.00	111.14
29	I	169	SER	CA-C-N	5.69	127.73	120.56
29	I	169	SER	C-N-CA	5.69	127.73	120.56
4	d	184	PRO	CA-C-N	5.69	126.95	119.84
4	d	184	PRO	C-N-CA	5.69	126.95	119.84
19	Y	71	ASP	CA-CB-CG	-5.69	106.91	112.60
22	S	54	TRP	CE2-CD2-CE3	5.69	124.49	118.80
24	Q	166	LYS	N-CA-C	-5.69	105.45	112.90
28	H	64	LYS	CA-C-N	5.69	127.90	120.28
28	H	64	LYS	C-N-CA	5.69	127.90	120.28
4	d	241	GLN	CG-CD-NE2	5.69	124.93	116.40
6	f	167	GLY	N-CA-C	5.69	121.04	114.16
11	k	128	LEU	O-C-N	-5.69	116.26	122.06
11	4	170	LYS	O-C-N	5.69	128.63	122.15
17	T	117	ASN	OD1-CG-ND2	5.69	128.29	122.60
27	O	190	TYR	CA-C-N	5.69	127.90	120.28
27	O	190	TYR	C-N-CA	5.69	127.90	120.28
28	H	172	MET	CA-C-O	5.69	126.74	120.71
3	c	128	LEU	CA-C-N	5.68	129.32	120.68
3	c	128	LEU	C-N-CA	5.68	129.32	120.68
2	B	127	VAL	N-CA-CB	5.68	119.38	112.10
15	W	139	VAL	CB-CA-C	5.68	118.63	110.33
22	S	70	ASN	CA-CB-CG	5.68	118.28	112.60
25	R	203	ASP	N-CA-C	5.68	119.51	109.96
5	E	45	GLY	CA-C-N	5.68	130.90	123.06
5	E	45	GLY	C-N-CA	5.68	130.90	123.06
7	G	29	LYS	CA-C-N	5.68	127.89	120.28
7	G	29	LYS	C-N-CA	5.68	127.89	120.28
24	Q	221	MET	CA-C-N	5.68	127.83	120.44
24	Q	221	MET	C-N-CA	5.68	127.83	120.44
27	O	323	ASN	CA-C-O	5.68	125.94	119.18
30	K	107	THR	N-CA-CB	5.68	120.36	110.81
1	A	119	LYS	N-CA-C	-5.68	105.17	111.36
5	E	205	LYS	CA-C-N	5.68	128.94	120.31
5	E	205	LYS	C-N-CA	5.68	128.94	120.31
17	T	212	ASN	CA-CB-CG	-5.68	106.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	814	ALA	CA-C-N	5.68	127.89	120.28
21	N	814	ALA	C-N-CA	5.68	127.89	120.28
23	P	366	ASN	CB-CA-C	-5.68	101.36	110.79
25	R	275	GLU	CA-C-N	5.68	128.17	120.44
25	R	275	GLU	C-N-CA	5.68	128.17	120.44
4	d	200	LEU	CA-C-N	5.68	127.89	120.28
4	d	200	LEU	C-N-CA	5.68	127.89	120.28
16	V	300	VAL	CA-CB-CG1	5.68	120.06	110.40
9	i	87	LEU	CA-C-N	5.68	129.63	120.55
9	i	87	LEU	C-N-CA	5.68	129.63	120.55
14	7	164	ASN	CA-C-O	5.68	127.38	121.31
16	V	114	PHE	O-C-N	-5.68	116.38	122.85
12	5	89	VAL	O-C-N	-5.67	117.35	123.14
25	R	217	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
27	O	165	LEU	N-CA-C	5.67	117.92	111.11
30	K	49	PHE	CA-C-N	5.67	128.16	120.44
30	K	49	PHE	C-N-CA	5.67	128.16	120.44
24	Q	214	THR	CA-C-N	5.67	128.48	120.42
24	Q	214	THR	C-N-CA	5.67	128.48	120.42
14	n	204	GLN	N-CA-CB	5.67	118.23	110.01
1	A	184	ASN	OD1-CG-ND2	5.67	128.27	122.60
5	E	130	GLU	N-CA-C	-5.67	100.45	109.07
13	6	214	ILE	O-C-N	5.67	129.38	123.26
25	R	149	ASN	CA-C-N	5.67	128.15	120.44
25	R	149	ASN	C-N-CA	5.67	128.15	120.44
25	R	343	GLU	N-CA-C	-5.67	105.00	111.07
26	U	265	LEU	CA-C-O	-5.67	113.45	119.97
28	H	251	PRO	N-CA-CB	5.67	108.58	103.08
29	I	228	GLY	CA-C-N	5.67	127.88	120.28
29	I	228	GLY	C-N-CA	5.67	127.88	120.28
32	M	425	ARG	N-CA-C	-5.67	100.69	109.14
3	c	121	GLY	N-CA-C	5.67	120.67	113.24
6	f	86	ASN	N-CA-CB	5.67	118.45	110.12
13	m	55	GLY	N-CA-C	-5.67	106.56	111.95
6	F	195	GLU	CB-CA-C	-5.67	101.38	110.79
9	2	58	LYS	N-CA-C	-5.67	105.47	112.90
16	V	125	THR	CA-C-O	5.67	126.54	120.70
17	T	130	ASP	CA-C-N	5.67	128.93	120.31
17	T	130	ASP	C-N-CA	5.67	128.93	120.31
29	I	190	GLN	CB-CA-C	-5.67	100.59	110.17
8	h	147	CYS	O-C-N	5.67	128.61	122.15
8	1	62	GLN	CG-CD-NE2	5.67	124.90	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	138	PHE	N-CA-CB	5.67	119.28	110.44
32	M	26	SER	N-CA-C	-5.67	100.51	108.96
4	d	204	GLN	N-CA-CB	5.67	120.07	110.49
21	N	69	TYR	CA-C-N	5.67	127.81	120.44
21	N	69	TYR	C-N-CA	5.67	127.81	120.44
26	U	265	LEU	O-C-N	5.67	129.24	122.27
33	J	2	THR	CA-CB-OG1	5.67	118.10	109.60
6	f	54	ASP	N-CA-C	-5.67	98.73	110.80
13	m	147	GLY	N-CA-C	-5.67	102.82	112.51
4	D	151	GLU	CA-C-O	-5.67	115.22	120.94
13	6	15	ASP	N-CA-C	-5.67	99.06	108.75
21	N	436	ASP	N-CA-CB	5.67	119.63	110.51
5	e	181	ALA	CA-C-N	5.66	127.87	120.28
5	e	181	ALA	C-N-CA	5.66	127.87	120.28
1	A	203	VAL	N-CA-C	-5.66	104.84	110.62
3	C	160	TRP	CB-CG-CD2	-5.66	118.87	126.80
8	1	69	GLN	CA-C-N	5.66	128.33	120.29
8	1	69	GLN	C-N-CA	5.66	128.33	120.29
9	2	234	PHE	CA-C-N	5.66	126.92	119.84
9	2	234	PHE	C-N-CA	5.66	126.92	119.84
11	4	71	GLU	CA-C-N	5.66	130.17	122.07
11	4	71	GLU	C-N-CA	5.66	130.17	122.07
23	P	182	GLU	CA-C-N	5.66	127.87	120.28
23	P	182	GLU	C-N-CA	5.66	127.87	120.28
24	Q	54	GLN	OE1-CD-NE2	-5.66	116.94	122.60
26	U	202	SER	N-CA-C	5.66	117.53	111.36
7	g	102	LEU	O-C-N	5.66	128.60	122.15
13	6	132	SER	CA-C-O	-5.66	114.71	121.11
22	S	311	GLN	CA-C-N	5.66	127.87	120.28
22	S	311	GLN	C-N-CA	5.66	127.87	120.28
5	E	52	LYS	CA-C-O	5.66	126.60	120.32
21	N	244	LYS	CA-C-O	5.66	126.55	120.55
23	P	277	GLN	N-CA-CB	5.66	118.54	110.16
25	R	51	LEU	CA-C-N	5.66	127.87	120.28
25	R	51	LEU	C-N-CA	5.66	127.87	120.28
25	R	201	GLY	CA-C-N	5.66	132.01	120.80
25	R	201	GLY	C-N-CA	5.66	132.01	120.80
29	I	125	MET	N-CA-CB	5.66	120.44	110.37
13	6	148	GLY	CA-C-N	5.66	127.86	120.28
13	6	148	GLY	C-N-CA	5.66	127.86	120.28
33	J	393	ASN	CA-CB-CG	-5.66	106.94	112.60
32	M	48	LEU	CA-C-O	5.66	126.55	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	98	ARG	CA-C-O	-5.66	113.96	120.24
5	E	81	LEU	N-CA-C	-5.66	100.60	109.25
11	4	20	ALA	N-CA-C	5.66	118.65	110.28
16	V	202	ASP	CB-CA-C	-5.66	98.69	109.66
21	N	772	GLN	N-CA-C	-5.66	100.18	109.40
22	S	367	TYR	CA-C-N	5.66	127.79	120.44
22	S	367	TYR	C-N-CA	5.66	127.79	120.44
25	R	247	GLU	CA-C-N	5.66	128.32	120.29
25	R	247	GLU	C-N-CA	5.66	128.32	120.29
31	L	273	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	a	84	ASN	N-CA-CB	5.65	120.67	110.83
11	k	154	THR	CA-C-O	5.65	126.54	120.55
7	G	234	ASP	CB-CA-C	-5.65	101.41	110.79
26	U	203	LYS	CA-C-N	5.65	127.86	120.28
26	U	203	LYS	C-N-CA	5.65	127.86	120.28
1	a	132	ALA	N-CA-C	-5.65	106.37	113.72
2	b	99	ARG	CD-NE-CZ	-5.65	116.49	124.40
1	A	140	ILE	CA-CB-CG1	-5.65	100.79	110.40
12	5	214	VAL	CB-CA-C	-5.65	104.51	112.14
12	5	279	GLU	N-CA-C	-5.65	106.43	113.38
24	Q	104	PHE	CA-C-O	-5.65	113.47	119.97
32	M	259	GLY	CA-C-N	5.65	130.29	120.68
32	M	259	GLY	C-N-CA	5.65	130.29	120.68
2	b	105	PRO	N-CA-CB	5.65	106.16	103.22
2	B	246	ARG	NE-CZ-NH1	-5.65	115.85	121.50
18	X	129	LEU	CA-C-O	-5.65	114.43	120.42
27	O	318	HIS	N-CA-CB	5.65	121.33	112.46
29	I	239	GLN	CB-CG-CD	-5.65	102.99	112.60
3	C	58	GLU	CA-C-O	-5.65	114.25	120.69
14	7	202	THR	CA-C-N	5.65	128.20	120.46
14	7	202	THR	C-N-CA	5.65	128.20	120.46
31	L	124	GLY	CA-C-O	-5.65	113.44	121.52
7	g	121	GLN	CA-C-O	5.65	126.45	119.79
3	C	52	VAL	N-CA-CB	5.65	120.55	111.23
17	T	35	ILE	CA-C-O	5.65	126.84	120.85
33	J	136	LEU	N-CA-CB	5.65	118.52	110.16
20	Z	241	THR	CA-C-N	5.65	127.85	120.28
20	Z	241	THR	C-N-CA	5.65	127.85	120.28
20	Z	470	ALA	CA-C-N	5.65	128.16	120.54
20	Z	470	ALA	C-N-CA	5.65	128.16	120.54
20	Z	631	GLY	CA-C-N	5.65	127.78	120.44
20	Z	631	GLY	C-N-CA	5.65	127.78	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	306	MET	CA-C-O	-5.65	114.44	120.42
32	M	339	ARG	N-CA-CB	5.65	120.03	110.49
4	d	182	LYS	N-CA-CB	5.64	119.25	110.44
11	k	19	LYS	N-CA-C	-5.64	104.97	113.89
20	Z	151	HIS	N-CA-C	-5.64	107.04	114.04
5	e	234	GLU	CA-C-N	5.64	127.78	120.44
5	e	234	GLU	C-N-CA	5.64	127.78	120.44
10	j	97	GLU	CB-CA-C	-5.64	102.02	110.88
13	m	181	LYS	N-CA-CB	5.64	119.63	110.77
7	G	195	GLN	O-C-N	5.64	128.10	122.12
28	H	251	PRO	CA-C-N	5.64	125.40	119.76
28	H	251	PRO	C-N-CA	5.64	125.40	119.76
2	b	21	ILE	CA-C-N	5.64	127.84	120.28
2	b	21	ILE	C-N-CA	5.64	127.84	120.28
4	d	78	LEU	O-C-N	5.64	130.07	122.96
8	1	177	SER	CA-C-N	5.64	130.14	122.19
8	1	177	SER	C-N-CA	5.64	130.14	122.19
1	a	12	TYR	CB-CA-C	-5.64	100.72	109.80
1	a	75	ILE	CB-CA-C	-5.64	104.83	111.94
1	a	246	VAL	CA-C-N	5.64	128.88	120.31
1	a	246	VAL	C-N-CA	5.64	128.88	120.31
14	n	216	VAL	N-CA-CB	-5.64	103.95	110.55
21	N	216	ASN	O-C-N	-5.64	114.77	122.33
25	R	381	ILE	CA-C-O	5.64	125.84	120.31
7	g	171	SER	CA-C-O	-5.64	114.44	120.42
9	i	93	GLU	CA-C-N	5.64	127.83	120.28
9	i	93	GLU	C-N-CA	5.64	127.83	120.28
26	U	24	ARG	N-CA-CB	5.64	119.12	110.61
27	O	185	PHE	N-CA-C	5.64	118.28	111.40
29	I	204	HIS	CA-CB-CG	-5.64	108.16	113.80
4	D	144	GLU	CA-C-N	5.64	125.40	119.76
4	D	144	GLU	C-N-CA	5.64	125.40	119.76
5	E	32	LYS	N-CA-C	5.64	118.36	111.82
6	F	128	TYR	CA-C-N	5.64	132.46	121.41
6	F	128	TYR	C-N-CA	5.64	132.46	121.41
7	G	130	ARG	CB-CA-C	-5.64	100.28	109.41
13	6	56	ASP	CA-CB-CG	-5.64	106.96	112.60
13	6	87	HIS	N-CA-C	-5.64	104.20	113.50
23	P	276	LEU	O-C-N	5.64	128.09	122.12
23	P	413	ASN	N-CA-CB	5.64	118.50	110.16
24	Q	313	ASP	N-CA-C	-5.64	105.14	111.28
30	K	62	THR	CA-C-N	5.64	127.83	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	62	THR	C-N-CA	5.64	127.83	120.28
2	b	158	PRO	O-C-N	5.63	130.60	123.05
2	b	224	TYR	N-CA-CB	5.63	120.30	111.56
5	E	73	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
16	V	282	GLU	N-CA-CB	5.63	118.40	110.12
22	S	325	GLY	CA-C-N	5.63	128.10	120.44
22	S	325	GLY	C-N-CA	5.63	128.10	120.44
23	P	429	ILE	O-C-N	-5.63	116.40	121.87
26	U	238	ASN	N-CA-C	-5.63	100.73	109.24
27	O	350	ILE	CA-C-O	-5.63	113.86	121.02
28	H	340	LEU	N-CA-C	5.63	117.89	111.02
29	I	230	THR	CA-C-O	5.63	126.39	120.42
3	c	94	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
1	A	139	VAL	N-CA-C	5.63	116.87	109.21
28	H	140	ASP	CA-C-O	-5.63	115.20	121.23
2	b	69	PRO	N-CA-C	5.63	121.16	113.84
2	b	97	TYR	N-CA-C	5.63	117.05	110.41
6	f	9	ASP	CA-CB-CG	-5.63	106.97	112.60
17	T	241	GLU	CB-CG-CD	-5.63	103.03	112.60
31	L	62	ARG	NE-CZ-NH1	-5.63	115.87	121.50
33	J	57	PHE	CA-C-N	5.63	128.17	120.46
33	J	57	PHE	C-N-CA	5.63	128.17	120.46
5	E	223	THR	CA-C-O	5.63	126.57	120.32
15	W	179	ARG	CA-C-N	5.63	132.29	121.54
15	W	179	ARG	C-N-CA	5.63	132.29	121.54
21	N	570	ARG	CA-C-N	5.63	127.82	120.28
21	N	570	ARG	C-N-CA	5.63	127.82	120.28
32	M	320	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	a	180	THR	N-CA-CB	5.63	118.39	110.12
14	n	92	ASP	CA-CB-CG	-5.63	106.97	112.60
16	V	19	GLY	N-CA-C	-5.63	99.84	113.18
21	N	856	PHE	N-CA-C	-5.63	100.51	109.23
22	S	485	LYS	CA-C-N	5.63	127.82	120.28
22	S	485	LYS	C-N-CA	5.63	127.82	120.28
30	K	134	SER	N-CA-CB	5.63	118.51	109.28
30	K	369	ASP	CA-C-O	5.63	126.23	119.59
20	Z	151	HIS	CA-C-N	5.63	128.28	120.29
20	Z	151	HIS	C-N-CA	5.63	128.28	120.29
24	Q	308	ASN	O-C-N	5.63	128.08	122.12
23	P	97	ILE	CA-C-O	-5.62	115.10	120.95
9	i	236	ARG	N-CA-CB	5.62	118.29	109.69
14	n	174	THR	CB-CA-C	5.62	120.11	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	329	GLU	CA-C-N	5.62	128.86	120.31
22	S	329	GLU	C-N-CA	5.62	128.86	120.31
23	P	9	ALA	O-C-N	5.62	127.86	122.07
23	P	275	ASN	N-CA-C	-5.62	105.53	112.90
24	Q	309	ARG	N-CA-CB	5.62	121.29	112.46
26	U	180	ASP	O-C-N	5.62	127.64	121.85
21	N	388	PRO	CA-C-O	-5.62	112.27	118.68
22	S	140	LEU	CA-C-N	5.62	127.75	120.44
22	S	140	LEU	C-N-CA	5.62	127.75	120.44
11	k	9	VAL	N-CA-C	-5.62	97.65	109.34
21	N	654	GLN	N-CA-CB	5.62	118.16	110.01
28	H	365	LEU	N-CA-C	-5.62	106.47	113.55
33	J	121	MET	CA-C-O	5.62	126.89	120.54
11	k	79	ALA	CA-C-O	-5.62	114.00	120.24
11	k	137	GLY	N-CA-C	-5.62	107.36	114.16
2	B	142	PHE	CA-CB-CG	-5.62	108.18	113.80
12	5	170	LEU	CA-C-O	-5.62	114.52	120.92
33	J	258	VAL	CA-C-O	-5.62	114.89	120.85
2	B	139	HIS	ND1-CE1-NE2	5.62	114.02	108.40
5	E	179	ALA	CA-C-N	5.62	128.27	120.29
5	E	179	ALA	C-N-CA	5.62	128.27	120.29
32	M	361	LEU	O-C-N	5.62	128.07	122.12
2	b	7	PHE	N-CA-CB	5.62	119.98	110.49
6	f	175	THR	N-CA-C	-5.62	106.32	112.72
8	h	171	ALA	CA-C-N	5.62	128.39	120.42
8	h	171	ALA	C-N-CA	5.62	128.39	120.42
6	F	101	ARG	CA-C-O	5.62	127.45	120.54
12	5	102	ALA	N-CA-CB	-5.62	101.85	110.16
26	U	184	GLY	CA-C-N	5.62	129.57	121.54
26	U	184	GLY	C-N-CA	5.62	129.57	121.54
29	I	333	THR	CA-C-N	5.62	128.82	120.90
29	I	333	THR	C-N-CA	5.62	128.82	120.90
29	I	352	ASN	CA-C-O	-5.62	112.47	120.16
32	M	371	ASP	N-CA-C	-5.62	100.98	109.85
17	T	42	PRO	N-CA-CB	5.61	109.05	102.76
24	Q	130	ARG	CA-C-O	-5.61	115.70	121.87
30	K	189	GLU	O-C-N	-5.61	115.75	122.15
32	M	417	GLU	CA-C-N	5.61	127.35	120.22
32	M	417	GLU	C-N-CA	5.61	127.35	120.22
8	h	92	LYS	N-CA-C	5.61	117.84	111.11
12	l	285	VAL	N-CA-C	-5.61	100.34	108.36
13	m	58	ILE	N-CA-C	-5.61	99.47	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	223	LEU	CA-C-O	5.61	127.05	120.43
21	N	442	LEU	CA-C-N	5.61	128.84	120.31
21	N	442	LEU	C-N-CA	5.61	128.84	120.31
23	P	336	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
29	I	203	THR	CA-C-O	-5.61	114.92	120.70
19	Y	42	THR	CA-CB-OG1	5.61	118.01	109.60
21	N	495	PRO	N-CA-CB	5.61	109.14	103.25
27	O	154	GLU	N-CA-CB	5.61	118.46	110.16
29	I	140	LEU	N-CA-C	-5.61	106.44	113.28
31	L	78	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	b	169	VAL	CA-C-O	5.61	126.79	120.85
9	i	141	SER	N-CA-C	-5.61	100.75	109.72
1	A	181	ASN	CB-CA-C	-5.61	101.48	110.79
17	T	206	LYS	CA-C-N	5.61	128.07	120.44
17	T	206	LYS	C-N-CA	5.61	128.07	120.44
25	R	412	THR	N-CA-C	-5.61	105.08	111.14
3	c	179	ASP	CA-CB-CG	-5.61	106.99	112.60
3	C	205	ALA	N-CA-C	-5.61	101.04	109.95
11	4	153	THR	CA-C-N	5.61	128.35	120.28
11	4	153	THR	C-N-CA	5.61	128.35	120.28
24	Q	283	ASN	CA-CB-CG	5.61	118.21	112.60
25	R	374	ASN	CA-CB-CG	5.61	118.20	112.60
26	U	156	HIS	CG-CD2-NE2	5.61	112.81	107.20
1	a	209	HIS	CE1-NE2-CD2	-5.60	103.40	109.00
4	d	89	ALA	CB-CA-C	-5.60	102.08	110.88
27	O	149	LEU	CA-C-O	-5.60	113.53	119.97
14	n	234	ASP	N-CA-C	-5.60	100.84	109.52
6	f	97	LEU	O-C-N	5.60	128.14	122.09
6	f	173	GLU	CB-CG-CD	-5.60	103.08	112.60
9	i	179	GLU	N-CA-C	-5.60	105.18	111.28
11	k	63	ASN	CA-CB-CG	-5.60	107.00	112.60
6	F	118	LYS	O-C-N	-5.60	116.19	122.12
24	Q	198	LEU	N-CA-C	-5.60	105.26	111.36
29	I	159	VAL	CA-C-N	5.60	130.36	121.18
29	I	159	VAL	C-N-CA	5.60	130.36	121.18
31	L	393	ASN	CA-CB-CG	5.60	118.20	112.60
32	M	369	THR	CA-C-O	5.60	127.31	121.15
7	g	83	PRO	CA-C-N	5.60	128.24	120.29
7	g	83	PRO	C-N-CA	5.60	128.24	120.29
5	E	232	ASP	N-CA-CB	5.60	118.93	110.42
9	2	247	VAL	CA-C-O	-5.60	113.93	121.32
11	4	151	ASP	N-CA-CB	5.60	120.07	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	227	PRO	CA-C-N	5.60	129.48	122.43
17	T	227	PRO	C-N-CA	5.60	129.48	122.43
18	X	27	ILE	N-CA-C	-5.60	96.79	108.88
22	S	444	GLU	CA-C-O	5.60	126.17	120.24
24	Q	32	ASP	CA-CB-CG	-5.60	107.00	112.60
27	O	274	ILE	CA-C-O	-5.60	114.42	120.47
32	M	378	GLU	N-CA-C	5.60	117.06	111.07
33	J	332	SER	O-C-N	5.60	128.77	122.22
13	m	229	ARG	NE-CZ-NH2	5.60	124.24	119.20
13	m	103	HIS	O-C-N	-5.59	115.39	122.27
2	B	11	THR	CA-C-N	5.59	131.64	122.07
2	B	11	THR	C-N-CA	5.59	131.64	122.07
3	C	144	TYR	CA-CB-CG	-5.59	103.83	113.90
10	3	114	SER	O-C-N	-5.59	115.38	122.26
21	N	773	MET	N-CA-C	-5.59	100.77	109.72
28	H	433	ALA	CA-C-O	-5.59	112.50	119.38
32	M	343	LEU	CA-C-O	-5.59	114.17	120.32
10	j	138	VAL	CA-C-O	-5.59	115.80	121.67
13	m	71	ALA	CA-C-N	5.59	127.77	120.28
13	m	71	ALA	C-N-CA	5.59	127.77	120.28
1	A	198	SER	N-CA-CB	5.59	121.18	111.39
14	n	157	ASP	CA-CB-CG	-5.59	107.01	112.60
16	V	291	ASN	CB-CG-ND2	-5.59	108.01	116.40
17	T	76	ASP	CB-CA-C	-5.59	102.10	110.88
33	J	243	SER	CA-C-O	5.59	127.37	121.33
9	i	195	ASP	N-CA-C	-5.59	100.07	109.07
14	7	141	ASN	OD1-CG-ND2	5.59	128.19	122.60
20	Z	736	LEU	CA-C-N	5.59	128.33	120.28
20	Z	736	LEU	C-N-CA	5.59	128.33	120.28
21	N	376	LYS	CA-C-O	-5.59	115.40	121.44
23	P	431	HIS	CB-CG-ND1	5.59	131.08	122.70
24	Q	30	LEU	N-CA-CB	5.59	118.11	110.01
9	2	80	ASP	CA-CB-CG	-5.59	107.01	112.60
23	P	194	SER	N-CA-CB	5.59	118.43	110.16
7	g	221	LEU	CA-C-O	-5.59	114.63	120.55
11	k	21	VAL	N-CA-C	-5.59	99.59	107.75
5	E	50	VAL	CA-C-N	5.59	131.03	122.93
5	E	50	VAL	C-N-CA	5.59	131.03	122.93
11	4	85	ARG	CD-NE-CZ	-5.59	116.58	124.40
15	W	106	GLN	N-CA-CB	5.59	118.26	109.83
21	N	573	HIS	CB-CA-C	-5.59	102.11	110.88
21	N	657	MET	CA-C-N	5.59	128.35	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	657	MET	C-N-CA	5.59	128.35	120.42
21	N	796	VAL	CA-C-N	5.59	127.77	120.28
21	N	796	VAL	C-N-CA	5.59	127.77	120.28
22	S	47	THR	CB-CA-C	5.59	121.54	110.42
27	O	193	LEU	CA-C-N	5.59	127.77	120.28
27	O	193	LEU	C-N-CA	5.59	127.77	120.28
31	L	394	CYS	CA-C-N	5.59	128.22	120.29
31	L	394	CYS	C-N-CA	5.59	128.22	120.29
3	c	183	ASP	CA-C-N	5.58	132.21	121.54
3	c	183	ASP	C-N-CA	5.58	132.21	121.54
21	N	690	HIS	CA-CB-CG	-5.58	108.22	113.80
23	P	156	ALA	O-C-N	5.58	128.75	122.22
26	U	145	ASP	N-CA-C	-5.58	106.13	113.17
4	D	201	GLU	N-CA-CB	5.58	118.33	110.12
24	Q	65	TYR	CA-C-O	5.58	126.68	120.82
27	O	235	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
13	6	144	CYS	N-CA-C	-5.58	98.81	108.69
22	S	129	GLU	N-CA-C	-5.58	98.72	107.93
29	I	110	GLU	CB-CG-CD	-5.58	103.11	112.60
16	V	244	MET	CG-SD-CE	-5.58	88.62	100.90
26	U	225	ILE	N-CA-C	5.58	116.23	110.82
3	c	9	ARG	CG-CD-NE	-5.58	99.73	112.00
16	V	211	LYS	CA-C-O	-5.58	114.51	120.42
32	M	88	MET	CG-SD-CE	-5.58	88.63	100.90
6	f	218	LYS	CA-CB-CG	5.58	125.25	114.10
12	l	261	ILE	O-C-N	-5.58	117.24	123.26
21	N	62	ALA	CA-C-N	5.58	127.75	120.28
21	N	62	ALA	C-N-CA	5.58	127.75	120.28
26	U	27	THR	N-CA-CB	5.58	118.16	109.85
30	K	49	PHE	CA-CB-CG	-5.58	108.22	113.80
30	K	398	ASN	N-CA-CB	5.58	119.92	110.49
33	J	72	VAL	CB-CA-C	-5.58	103.74	110.99
2	B	100	ILE	N-CA-CB	-5.58	106.05	111.57
4	D	81	ASP	CA-C-N	5.58	127.75	120.28
4	D	81	ASP	C-N-CA	5.58	127.75	120.28
11	4	22	THR	CA-C-O	5.58	126.67	120.43
11	4	52	ASP	CA-CB-CG	-5.58	107.03	112.60
17	T	193	THR	CA-CB-OG1	5.58	117.96	109.60
22	S	400	LYS	O-C-N	-5.58	116.23	122.03
3	c	99	LEU	CB-CA-C	5.57	119.63	110.88
3	c	57	LEU	CA-C-O	5.57	126.98	120.80
1	A	103	GLU	N-CA-C	-5.57	105.12	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	421	GLU	CA-C-O	-5.57	113.56	119.97
12	l	285	VAL	N-CA-CB	5.57	117.67	110.99
14	n	44	VAL	O-C-N	-5.57	117.05	123.07
16	V	154	ASP	N-CA-CB	5.57	120.96	111.66
30	K	325	ASP	CA-CB-CG	-5.57	107.03	112.60
3	c	180	TYR	N-CA-C	-5.57	101.61	109.96
9	2	85	THR	CA-C-O	5.57	126.32	120.42
14	7	246	GLN	OE1-CD-NE2	-5.57	117.03	122.60
24	Q	373	VAL	CA-CB-CG1	5.57	119.87	110.40
28	H	349	ILE	N-CA-C	-5.57	99.62	107.75
9	i	234	PHE	CA-CB-CG	-5.57	108.23	113.80
14	n	87	SER	N-CA-CB	5.57	119.40	111.05
11	4	69	ILE	N-CA-C	-5.57	104.93	111.00
21	N	137	PHE	N-CA-CB	-5.57	101.94	110.01
21	N	218	PRO	CA-C-O	-5.57	112.19	118.98
21	N	246	LYS	CA-C-N	5.57	128.20	120.29
21	N	246	LYS	C-N-CA	5.57	128.20	120.29
22	S	261	HIS	ND1-CE1-NE2	5.57	113.97	108.40
23	P	153	ILE	CA-CB-CG1	5.57	119.86	110.40
22	S	446	THR	CB-CA-C	5.56	118.73	109.38
29	I	241	SER	N-CA-C	-5.56	103.60	111.56
7	G	98	SER	CA-C-O	-5.56	114.52	120.42
17	T	86	LYS	CA-C-N	5.56	125.66	119.32
17	T	86	LYS	C-N-CA	5.56	125.66	119.32
30	K	373	ILE	CB-CA-C	-5.56	105.20	110.65
1	A	134	MET	N-CA-CB	5.56	120.63	111.62
3	C	136	ILE	CA-CB-CG2	-5.56	101.05	110.50
5	E	200	VAL	CA-C-N	5.56	128.19	120.29
5	E	200	VAL	C-N-CA	5.56	128.19	120.29
2	B	157	PHE	CA-C-O	-5.56	113.50	120.23
16	V	131	GLN	CA-C-O	-5.56	114.98	120.82
8	h	129	HIS	ND1-CE1-NE2	5.56	113.96	108.40
9	i	58	LYS	N-CA-C	-5.56	105.30	111.36
21	N	85	ALA	CA-C-N	5.56	132.15	121.54
21	N	85	ALA	C-N-CA	5.56	132.15	121.54
26	U	14	VAL	CB-CA-C	-5.56	104.64	112.14
27	O	329	MET	CB-CA-C	-5.56	101.57	110.79
31	L	99	GLN	OE1-CD-NE2	5.56	128.16	122.60
7	g	182	HIS	O-C-N	-5.56	115.82	122.15
8	h	46	VAL	CA-C-O	5.56	123.98	118.98
29	I	259	ASP	N-CA-C	-5.56	106.67	113.50
2	b	183	LEU	CA-C-O	-5.55	114.62	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	34	LYS	O-C-N	-5.55	116.68	121.85
13	m	118	ILE	N-CA-C	-5.55	100.06	108.17
1	A	33	LYS	N-CA-C	-5.55	105.11	112.94
3	C	95	ALA	CB-CA-C	-5.55	101.57	110.79
8	1	153	GLU	CA-C-N	5.55	130.63	122.63
8	1	153	GLU	C-N-CA	5.55	130.63	122.63
12	5	266	HIS	CA-C-O	-5.55	114.35	120.24
14	7	63	TYR	CA-CB-CG	5.55	123.90	113.90
21	N	808	ALA	CA-C-N	5.55	127.72	120.28
21	N	808	ALA	C-N-CA	5.55	127.72	120.28
22	S	148	ASP	CA-C-O	5.55	126.44	120.55
23	P	373	GLU	CA-C-N	5.55	127.66	120.44
23	P	373	GLU	C-N-CA	5.55	127.66	120.44
27	O	23	HIS	CG-CD2-NE2	5.55	112.75	107.20
31	L	107	GLU	N-CA-CB	5.55	121.85	111.52
31	L	172	SER	N-CA-C	-5.55	106.27	113.16
10	j	59	ASP	CA-CB-CG	-5.55	107.05	112.60
20	Z	800	SER	CA-C-N	5.55	128.04	120.54
20	Z	800	SER	C-N-CA	5.55	128.04	120.54
28	H	327	ASN	CB-CA-C	-5.55	101.41	110.85
7	g	83	PRO	N-CA-CB	5.55	108.62	103.46
11	k	151	ASP	N-CA-C	-5.55	100.13	109.07
1	A	15	HIS	CA-CB-CG	-5.55	108.25	113.80
8	1	152	ARG	NE-CZ-NH1	-5.55	115.95	121.50
12	5	153	ALA	CB-CA-C	-5.55	101.57	110.79
18	X	19	GLU	O-C-N	-5.55	115.21	122.59
19	Y	71	ASP	N-CA-C	-5.55	105.86	113.30
22	S	65	ASN	CB-CA-C	-5.55	101.57	110.79
25	R	182	ASN	CA-C-N	5.55	130.80	122.47
25	R	182	ASN	C-N-CA	5.55	130.80	122.47
28	H	49	LEU	N-CA-CB	5.55	118.38	110.16
28	H	120	ASN	CB-CA-C	-5.55	100.79	110.17
9	i	172	LYS	CG-CD-CE	5.55	124.06	111.30
12	l	266	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
6	F	67	ASP	N-CA-C	-5.55	100.05	107.88
29	I	333	THR	N-CA-C	-5.55	104.05	112.04
4	D	235	GLN	CG-CD-OE1	-5.55	109.70	120.80
5	E	121	LEU	CB-CA-C	-5.55	100.37	110.63
5	E	188	HIS	N-CA-C	-5.55	100.31	108.79
23	P	263	HIS	CG-CD2-NE2	5.55	112.75	107.20
24	Q	132	PHE	CB-CG-CD2	5.55	130.13	120.70
30	K	122	ILE	N-CA-CB	5.55	118.89	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	57	ALA	N-CA-CB	5.54	118.38	110.06
21	N	295	THR	N-CA-CB	5.54	118.88	110.28
32	M	398	ALA	N-CA-C	-5.54	105.39	111.82
6	f	148	GLN	CA-C-N	5.54	125.64	119.32
6	f	148	GLN	C-N-CA	5.54	125.64	119.32
7	g	158	TRP	CA-C-N	5.54	125.61	120.34
7	g	158	TRP	C-N-CA	5.54	125.61	120.34
8	1	62	GLN	CA-C-N	5.54	128.16	120.29
8	1	62	GLN	C-N-CA	5.54	128.16	120.29
21	N	228	VAL	CB-CA-C	-5.54	104.87	111.97
1	a	82	VAL	CB-CA-C	5.54	118.88	110.62
3	C	19	LEU	CA-C-O	5.54	126.30	120.54
6	F	171	TYR	N-CA-CB	5.54	118.04	110.01
11	4	153	THR	N-CA-CB	5.54	118.28	110.36
12	5	218	ASN	CA-CB-CG	-5.54	107.06	112.60
21	N	24	ALA	CA-C-O	-5.54	114.55	120.42
23	P	434	THR	O-C-N	-5.54	116.25	122.12
26	U	139	ALA	CA-C-N	5.54	130.64	122.94
26	U	139	ALA	C-N-CA	5.54	130.64	122.94
27	O	184	ASP	N-CA-C	-5.54	100.15	108.96
27	O	206	THR	CA-C-N	5.54	128.73	120.31
27	O	206	THR	C-N-CA	5.54	128.73	120.31
28	H	87	ASP	N-CA-C	-5.54	105.25	112.23
28	H	106	ILE	N-CA-CB	5.54	118.65	111.67
9	i	174	ASP	CA-CB-CG	-5.54	107.06	112.60
3	C	240	VAL	CA-C-O	5.54	126.72	120.85
11	4	77	PRO	CA-C-N	5.54	127.70	120.28
11	4	77	PRO	C-N-CA	5.54	127.70	120.28
24	Q	77	PHE	CA-CB-CG	5.54	119.34	113.80
30	K	326	PRO	CA-C-N	5.54	133.44	121.64
30	K	326	PRO	C-N-CA	5.54	133.44	121.64
5	e	174	SER	N-CA-C	-5.54	104.88	111.69
10	j	56	LEU	CA-C-N	5.54	127.97	120.38
10	j	56	LEU	C-N-CA	5.54	127.97	120.38
13	m	225	TYR	N-CA-CB	5.54	121.02	111.00
15	W	2	VAL	CA-C-N	5.54	130.04	122.34
15	W	2	VAL	C-N-CA	5.54	130.04	122.34
27	O	87	LYS	O-C-N	5.54	128.07	122.09
27	O	122	HIS	ND1-CE1-NE2	5.54	113.94	108.40
27	O	310	PHE	CB-CG-CD1	-5.54	111.28	120.70
28	H	319	PHE	CA-C-O	5.54	127.19	120.99
30	K	70	ASP	N-CA-CB	5.54	118.83	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	67	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
7	g	199	ILE	CA-C-N	5.54	128.28	120.42
7	g	199	ILE	C-N-CA	5.54	128.28	120.42
9	i	60	CYS	N-CA-CB	5.54	119.96	110.77
9	i	117	PHE	CA-C-O	-5.54	114.68	120.55
2	B	152	PRO	CA-C-O	-5.54	111.68	118.99
25	R	40	ILE	CA-C-O	-5.54	115.30	121.17
21	N	190	LEU	CB-CA-C	-5.54	101.44	110.85
23	P	295	SER	CA-C-O	-5.54	114.55	120.42
28	H	51	GLN	CA-C-N	5.54	127.70	120.28
28	H	51	GLN	C-N-CA	5.54	127.70	120.28
31	L	105	ILE	CA-C-O	-5.54	114.65	120.57
7	g	74	ILE	CA-CB-CG1	5.53	119.81	110.40
3	C	113	ARG	CA-C-O	-5.53	114.68	120.55
20	Z	369	PHE	CA-CB-CG	-5.53	108.27	113.80
21	N	576	VAL	CA-CB-CG1	5.53	119.81	110.40
23	P	255	ALA	CB-CA-C	-5.53	101.44	110.85
26	U	42	ASN	CA-C-N	5.53	131.42	122.29
26	U	42	ASN	C-N-CA	5.53	131.42	122.29
30	K	363	ALA	CA-C-O	-5.53	115.35	120.94
32	M	104	GLY	CA-C-N	5.53	129.10	120.75
32	M	104	GLY	C-N-CA	5.53	129.10	120.75
26	U	277	TYR	CA-C-O	-5.53	114.66	120.63
30	K	42	ASN	CA-CB-CG	5.53	118.13	112.60
30	K	384	ALA	CA-C-N	5.53	127.96	120.44
30	K	384	ALA	C-N-CA	5.53	127.96	120.44
5	e	168	ASN	N-CA-CB	5.53	118.78	110.65
12	l	179	TYR	O-C-N	5.53	129.69	123.27
14	n	145	ASN	OD1-CG-ND2	5.53	128.13	122.60
1	A	67	THR	O-C-N	5.53	130.00	122.37
3	C	187	ASP	CA-C-O	5.53	126.28	120.42
10	3	112	ILE	N-CA-C	-5.53	100.09	108.17
13	6	213	LEU	N-CA-C	-5.53	100.69	109.59
7	g	70	VAL	N-CA-C	-5.53	99.59	107.77
12	l	113	ASN	CA-C-O	-5.53	112.58	120.16
15	W	87	MET	O-C-N	-5.53	115.85	122.15
22	S	289	ALA	CA-C-N	5.53	128.14	120.29
22	S	289	ALA	C-N-CA	5.53	128.14	120.29
6	f	202	ARG	NE-CZ-NH1	-5.53	115.97	121.50
14	n	155	ASN	OD1-CG-ND2	-5.53	117.07	122.60
4	D	193	LYS	CA-C-O	-5.53	113.86	120.10
21	N	789	GLU	CA-C-N	5.53	132.10	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	789	GLU	C-N-CA	5.53	132.10	121.54
25	R	350	LEU	O-C-N	5.53	128.69	122.22
28	H	278	GLU	N-CA-C	-5.53	105.89	113.30
2	b	234	ARG	N-CA-C	-5.53	105.17	111.14
7	G	108	PRO	CA-C-O	-5.53	114.93	121.67
15	W	8	LEU	CD1-CG-CD2	5.53	122.96	110.80
22	S	29	ASP	CA-C-N	5.53	127.69	120.28
22	S	29	ASP	C-N-CA	5.53	127.69	120.28
23	P	278	ASN	N-CA-CB	5.53	118.22	109.82
23	P	373	GLU	N-CA-C	5.53	117.30	111.28
25	R	146	ASP	N-CA-C	-5.53	99.28	108.34
28	H	45	TYR	N-CA-C	-5.53	106.90	113.97
32	M	15	ASP	N-CA-C	-5.53	98.91	108.69
12	l	261	ILE	N-CA-C	-5.52	100.38	108.11
24	Q	290	THR	CA-C-N	5.52	131.13	123.07
24	Q	290	THR	C-N-CA	5.52	131.13	123.07
2	b	39	ALA	N-CA-C	-5.52	101.23	109.96
14	n	96	ILE	CA-CB-CG2	5.52	119.89	110.50
16	V	161	THR	CA-C-N	5.52	126.22	120.03
16	V	161	THR	C-N-CA	5.52	126.22	120.03
21	N	187	ASN	CA-C-O	-5.52	114.69	120.55
21	N	451	GLY	CA-C-N	5.52	127.68	120.28
21	N	451	GLY	C-N-CA	5.52	127.68	120.28
22	S	177	ASN	OD1-CG-ND2	5.52	128.12	122.60
27	O	11	LEU	N-CA-C	-5.52	105.16	111.07
17	T	248	GLU	CB-CA-C	-5.52	101.62	110.79
24	Q	280	ASN	N-CA-C	5.52	117.38	111.36
30	K	427	TYR	N-CA-C	-5.52	106.75	112.93
5	e	117	CYS	CA-C-O	5.52	126.15	119.31
14	n	234	ASP	CA-C-N	5.52	131.65	122.54
14	n	234	ASP	C-N-CA	5.52	131.65	122.54
5	E	157	HIS	ND1-CE1-NE2	5.52	113.92	108.40
12	5	80	ALA	N-CA-C	-5.52	100.33	108.99
13	6	219	GLY	N-CA-C	-5.52	105.28	111.63
23	P	130	ILE	CB-CG1-CD1	5.52	125.39	113.80
23	P	413	ASN	CB-CA-C	-5.52	101.47	110.85
27	O	8	ASP	N-CA-C	-5.52	105.42	111.82
30	K	197	LEU	N-CA-C	5.52	117.38	111.36
33	J	304	LEU	N-CA-C	-5.52	106.59	113.38
14	n	125	ILE	O-C-N	5.52	127.32	121.91
17	T	38	ASN	CA-CB-CG	-5.52	107.08	112.60
20	Z	728	LYS	CA-C-O	-5.52	112.62	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	334	HIS	CE1-NE2-CD2	-5.52	103.48	109.00
25	R	74	ASN	OD1-CG-ND2	-5.52	117.08	122.60
26	U	99	LEU	N-CA-CB	-5.52	102.22	110.17
27	O	176	SER	N-CA-CB	5.52	118.33	110.16
1	A	91	ARG	CG-CD-NE	-5.52	99.87	112.00
6	F	16	THR	CA-CB-OG1	5.52	117.87	109.60
25	R	223	ASN	N-CA-CB	5.52	119.69	110.53
4	d	170	THR	CA-C-N	5.51	127.62	120.56
4	d	170	THR	C-N-CA	5.51	127.62	120.56
8	h	107	ILE	N-CA-CB	5.51	120.99	111.39
13	m	82	TRP	N-CA-CB	5.51	119.67	110.41
1	A	140	ILE	N-CA-CB	5.51	117.61	110.99
14	7	223	ARG	CA-C-O	5.51	127.18	120.62
21	N	106	ILE	N-CA-C	-5.51	105.35	110.53
22	S	416	GLU	CA-C-O	5.51	126.40	120.55
24	Q	159	ASN	OD1-CG-ND2	-5.51	117.08	122.60
25	R	140	TYR	O-C-N	5.51	128.44	122.15
25	R	274	PRO	CA-C-N	5.51	127.67	120.28
25	R	274	PRO	C-N-CA	5.51	127.67	120.28
33	J	318	PRO	N-CA-CB	5.51	108.43	103.08
13	m	146	ALA	O-C-N	5.51	129.80	123.29
23	P	52	LEU	O-C-N	-5.51	116.28	122.12
8	h	140	SER	N-CA-C	-5.51	105.68	112.90
14	n	149	VAL	N-CA-CB	5.51	117.66	111.21
1	A	112	MET	CA-C-O	-5.51	112.59	119.54
6	F	49	LEU	CB-CA-C	-5.51	101.25	110.29
15	W	14	GLU	N-CA-C	-5.51	106.33	113.16
16	V	38	LEU	CA-C-N	5.51	127.61	120.44
16	V	38	LEU	C-N-CA	5.51	127.61	120.44
30	K	128	ARG	N-CA-C	-5.51	104.48	113.19
3	c	51	LYS	N-CA-C	5.51	120.00	113.28
12	l	260	TRP	CA-C-O	-5.51	114.99	121.16
12	5	99	ASN	N-CA-C	-5.51	104.10	111.87
13	6	177	LYS	CA-C-O	5.51	127.68	121.51
16	V	48	GLU	N-CA-C	-5.51	101.50	110.20
28	H	215	LYS	N-CA-C	5.51	118.80	110.64
28	H	432	ARG	N-CA-C	5.51	118.21	111.82
33	J	42	ARG	CA-C-N	5.51	127.66	120.28
33	J	42	ARG	C-N-CA	5.51	127.66	120.28
11	4	55	GLN	CA-C-N	5.51	127.66	120.28
11	4	55	GLN	C-N-CA	5.51	127.66	120.28
27	O	244	ASN	CA-CB-CG	5.51	118.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	19	LEU	N-CA-C	-5.51	98.57	108.48
4	d	213	THR	O-C-N	-5.51	116.88	123.27
22	S	298	ARG	N-CA-C	5.51	118.04	111.71
24	Q	331	THR	N-CA-C	5.51	117.36	111.36
25	R	244	THR	CA-C-N	5.51	129.06	120.75
25	R	244	THR	C-N-CA	5.51	129.06	120.75
31	L	202	LYS	N-CA-CB	5.51	118.05	110.07
32	M	52	SER	CB-CA-C	-5.51	102.20	110.90
16	V	281	SER	CA-C-O	-5.50	114.71	120.55
31	L	379	ALA	CA-C-N	5.50	128.24	120.42
31	L	379	ALA	C-N-CA	5.50	128.24	120.42
32	M	427	SER	N-CA-CB	5.50	119.79	110.49
4	D	39	LYS	O-C-N	5.50	128.09	122.09
9	2	138	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
25	R	96	GLN	CB-CG-CD	5.50	121.96	112.60
32	M	332	VAL	CB-CA-C	-5.50	104.88	110.93
2	B	27	ALA	CA-C-N	5.50	128.00	120.46
2	B	27	ALA	C-N-CA	5.50	128.00	120.46
21	N	133	LEU	CA-C-N	5.50	127.65	120.28
21	N	133	LEU	C-N-CA	5.50	127.65	120.28
21	N	832	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
25	R	325	HIS	N-CA-C	-5.50	105.78	112.88
30	K	224	LYS	CA-C-N	5.50	127.59	120.44
30	K	224	LYS	C-N-CA	5.50	127.59	120.44
31	L	301	ILE	CB-CA-C	-5.50	104.84	111.88
33	J	179	ILE	CA-C-O	5.50	127.61	120.95
12	l	279	GLU	CA-C-O	5.50	126.25	120.42
5	E	124	GLY	CA-C-N	5.50	129.41	120.23
5	E	124	GLY	C-N-CA	5.50	129.41	120.23
24	Q	280	ASN	CB-CA-C	-5.50	101.50	110.85
29	I	228	GLY	CA-C-O	5.50	124.90	118.96
3	c	221	ASN	OD1-CG-ND2	5.50	128.10	122.60
12	l	239	ALA	CA-C-N	5.50	127.65	120.28
12	l	239	ALA	C-N-CA	5.50	127.65	120.28
13	m	9	GLN	CB-CG-CD	-5.50	103.25	112.60
1	A	199	TRP	CD2-CE2-CZ2	-5.50	116.90	122.40
8	1	84	THR	CA-C-N	5.50	127.59	120.44
8	1	84	THR	C-N-CA	5.50	127.59	120.44
12	5	125	ALA	N-CA-C	5.50	117.71	111.11
16	V	79	SER	N-CA-C	-5.50	100.96	108.38
19	Y	79	ALA	CB-CA-C	-5.50	102.21	110.90
21	N	298	TYR	O-C-N	5.50	127.95	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	192	GLU	CA-C-N	5.50	128.67	120.31
25	R	192	GLU	C-N-CA	5.50	128.67	120.31
10	j	44	PHE	N-CA-C	-5.50	101.38	109.18
11	4	24	GLY	CA-C-O	-5.50	114.75	121.68
24	Q	130	ARG	N-CA-C	5.50	117.63	110.43
32	M	129	LEU	CA-C-N	5.50	126.36	119.98
32	M	129	LEU	C-N-CA	5.50	126.36	119.98
33	J	318	PRO	N-CA-C	-5.50	103.99	110.70
9	i	100	SER	N-CA-CB	5.50	120.65	112.30
17	T	132	HIS	CA-C-N	5.50	129.42	121.18
17	T	132	HIS	C-N-CA	5.50	129.42	121.18
24	Q	42	ALA	CA-C-O	5.50	128.37	120.51
6	f	9	ASP	N-CA-C	-5.49	99.36	108.75
6	f	82	ARG	CA-C-N	5.49	128.22	120.42
6	f	82	ARG	C-N-CA	5.49	128.22	120.42
14	n	118	GLU	N-CA-C	-5.49	102.01	109.54
14	n	211	VAL	CA-CB-CG2	-5.49	101.06	110.40
15	W	100	HIS	N-CA-C	-5.49	98.68	108.13
17	T	24	GLU	CA-C-N	5.49	127.64	120.28
17	T	24	GLU	C-N-CA	5.49	127.64	120.28
23	P	96	MET	CB-CA-C	-5.49	102.25	110.88
30	K	198	TYR	CB-CA-C	-5.49	102.25	110.88
8	1	92	LYS	N-CA-C	-5.49	105.37	111.36
25	R	241	ILE	N-CA-CB	5.49	118.06	111.31
1	a	244	ARG	NH1-CZ-NH2	-5.49	112.16	119.30
1	A	14	ARG	NE-CZ-NH1	-5.49	116.01	121.50
4	D	88	LYS	CB-CG-CD	5.49	123.93	111.30
10	3	36	VAL	N-CA-C	-5.49	106.32	111.48
24	Q	339	TYR	CA-C-N	5.49	128.09	120.29
24	Q	339	TYR	C-N-CA	5.49	128.09	120.29
28	H	262	ALA	O-C-N	-5.49	115.89	122.15
7	g	21	ASN	CA-C-N	5.49	127.89	120.65
7	g	21	ASN	C-N-CA	5.49	127.89	120.65
2	B	101	TYR	N-CA-C	-5.49	104.94	111.69
8	1	75	TYR	CA-C-N	5.49	128.08	120.29
8	1	75	TYR	C-N-CA	5.49	128.08	120.29
9	2	93	GLU	N-CA-C	-5.49	105.45	111.82
16	V	255	ILE	CA-CB-CG2	-5.49	101.17	110.50
22	S	61	SER	N-CA-CB	5.49	118.19	110.12
22	S	171	TYR	CA-C-O	5.49	126.74	120.54
23	P	337	HIS	N-CA-C	-5.49	106.95	113.97
26	U	211	LEU	N-CA-C	-5.49	105.38	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	241	SER	CB-CA-C	5.49	118.85	111.82
2	b	142	PHE	N-CA-C	-5.49	107.59	114.56
22	S	428	ARG	NE-CZ-NH1	-5.49	116.01	121.50
2	b	236	ARG	NE-CZ-NH2	-5.49	114.26	119.20
4	d	183	GLU	O-C-N	-5.49	115.01	121.32
10	j	87	PHE	CA-CB-CG	5.49	119.28	113.80
12	5	126	ASP	CB-CA-C	-5.49	101.69	110.79
14	7	89	ASP	CA-CB-CG	-5.49	107.11	112.60
20	Z	285	ALA	CA-C-N	5.49	127.97	120.46
20	Z	285	ALA	C-N-CA	5.49	127.97	120.46
21	N	266	SER	CA-C-N	5.49	127.63	120.28
21	N	266	SER	C-N-CA	5.49	127.63	120.28
21	N	420	THR	CA-C-N	5.49	127.63	120.28
21	N	420	THR	C-N-CA	5.49	127.63	120.28
30	K	121	ARG	N-CA-C	-5.49	102.36	110.48
4	d	24	LEU	N-CA-C	5.48	117.33	111.36
3	C	32	ALA	N-CA-CB	5.48	120.82	111.66
8	1	197	PHE	N-CA-C	-5.48	100.97	109.14
9	2	238	THR	CA-C-N	5.48	130.50	122.39
9	2	238	THR	C-N-CA	5.48	130.50	122.39
21	N	554	THR	CA-C-N	5.48	128.20	120.42
21	N	554	THR	C-N-CA	5.48	128.20	120.42
22	S	372	LEU	N-CA-C	5.48	118.18	111.82
25	R	403	LEU	CA-C-N	5.48	129.29	120.30
25	R	403	LEU	C-N-CA	5.48	129.29	120.30
26	U	45	THR	CB-CA-C	5.48	118.78	109.84
28	H	249	TYR	CA-C-O	5.48	126.92	120.89
3	C	138	ALA	N-CA-CB	5.48	120.28	110.80
7	G	241	ASP	CA-C-N	5.48	127.89	120.44
7	G	241	ASP	C-N-CA	5.48	127.89	120.44
14	7	111	ASN	CA-C-N	5.48	125.09	119.56
14	7	111	ASN	C-N-CA	5.48	125.09	119.56
16	V	83	VAL	N-CA-C	5.48	116.11	110.36
16	V	273	ARG	N-CA-C	5.48	118.18	110.23
21	N	778	LYS	CA-C-N	5.48	127.89	120.38
21	N	778	LYS	C-N-CA	5.48	127.89	120.38
23	P	349	ASN	O-C-N	-5.48	116.31	122.12
27	O	241	THR	CA-CB-OG1	5.48	117.82	109.60
4	d	67	ILE	CB-CA-C	-5.48	104.96	111.97
12	l	120	MET	N-CA-C	-5.48	98.27	108.02
5	E	96	ALA	CA-C-O	5.48	126.36	120.55
12	5	242	ARG	O-C-N	-5.48	114.90	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	79	LEU	CA-C-O	5.48	125.70	119.18
8	h	143	ILE	CA-C-N	5.48	127.56	120.44
8	h	143	ILE	C-N-CA	5.48	127.56	120.44
14	n	215	ARG	NE-CZ-NH1	-5.48	116.02	121.50
4	D	229	ILE	CA-C-N	5.48	127.62	120.28
4	D	229	ILE	C-N-CA	5.48	127.62	120.28
9	2	87	LEU	CA-C-O	5.48	126.36	120.55
22	S	298	ARG	NE-CZ-NH2	5.48	124.13	119.20
28	H	345	PRO	CA-C-N	5.48	133.08	122.07
28	H	345	PRO	C-N-CA	5.48	133.08	122.07
33	J	49	ASN	CB-CG-ND2	-5.48	108.19	116.40
33	J	343	LEU	CA-C-O	5.48	126.23	120.42
1	a	241	ILE	O-C-N	5.48	127.18	121.87
32	M	223	PRO	CA-C-N	5.48	125.42	119.78
32	M	223	PRO	C-N-CA	5.48	125.42	119.78
33	J	308	GLY	N-CA-C	-5.48	107.69	115.30
3	C	19	LEU	N-CA-C	-5.47	98.84	108.20
13	6	203	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
17	T	205	ILE	CA-C-N	5.47	127.62	120.28
17	T	205	ILE	C-N-CA	5.47	127.62	120.28
22	S	378	GLN	CA-C-N	5.47	128.06	120.29
22	S	378	GLN	C-N-CA	5.47	128.06	120.29
28	H	467	ASN	CA-CB-CG	-5.47	107.13	112.60
30	K	51	LEU	N-CA-CB	5.47	118.76	110.28
31	L	233	LYS	N-CA-CB	5.47	118.58	110.53
33	J	163	VAL	CB-CA-C	-5.47	104.00	110.84
6	f	60	GLN	O-C-N	5.47	129.71	123.31
8	h	153	GLU	CA-C-O	5.47	127.29	121.05
14	n	100	LEU	N-CA-C	5.47	117.33	111.36
17	T	73	PHE	CA-C-O	5.47	128.05	121.65
23	P	272	PRO	N-CA-CB	5.47	108.19	103.27
5	E	132	ARG	CA-C-O	5.47	126.93	120.69
15	W	36	ILE	N-CA-C	-5.47	105.04	110.62
22	S	43	LYS	CA-C-N	5.47	131.99	121.54
22	S	43	LYS	C-N-CA	5.47	131.99	121.54
27	O	122	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
29	I	73	GLU	N-CA-C	5.47	116.92	111.07
2	b	29	LYS	N-CA-CB	5.47	119.60	110.41
5	e	50	VAL	N-CA-CB	5.47	120.81	112.06
5	e	112	LEU	CA-C-N	5.47	128.06	120.29
5	e	112	LEU	C-N-CA	5.47	128.06	120.29
7	g	127	ASN	CA-CB-CG	-5.47	107.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	8	SER	O-C-N	-5.47	117.02	123.25
4	D	66	LYS	N-CA-CB	5.47	118.13	109.71
12	5	99	ASN	OD1-CG-ND2	5.47	128.07	122.60
20	Z	64	TYR	N-CA-C	-5.47	106.54	113.43
25	R	62	TYR	N-CA-C	-5.47	106.11	112.89
32	M	320	ARG	NH1-CZ-NH2	-5.47	112.19	119.30
1	a	211	ILE	CA-C-N	5.47	127.88	120.44
1	a	211	ILE	C-N-CA	5.47	127.88	120.44
9	i	131	GLY	CA-C-O	-5.47	115.64	121.38
16	V	211	LYS	CA-C-N	5.47	127.61	120.28
16	V	211	LYS	C-N-CA	5.47	127.61	120.28
12	l	228	ALA	CA-C-N	5.47	128.05	120.29
12	l	228	ALA	C-N-CA	5.47	128.05	120.29
13	6	77	LYS	N-CA-CB	5.47	118.16	110.12
19	Y	72	ASP	CA-C-N	5.47	127.88	120.44
19	Y	72	ASP	C-N-CA	5.47	127.88	120.44
20	Z	740	VAL	CB-CA-C	-5.47	104.68	112.22
24	Q	36	SER	CA-C-N	5.47	127.55	120.44
24	Q	36	SER	C-N-CA	5.47	127.55	120.44
27	O	263	PHE	CA-C-O	5.47	126.00	119.60
30	K	374	ARG	N-CA-C	-5.47	104.73	111.40
32	M	291	PHE	N-CA-C	-5.47	105.56	113.21
7	g	66	LYS	N-CA-C	-5.46	105.83	112.88
7	g	171	SER	CB-CA-C	-5.46	101.56	110.85
8	h	81	THR	CA-C-O	-5.46	114.52	120.69
13	m	152	SER	N-CA-C	5.46	117.24	111.28
14	7	221	ASP	CA-CB-CG	5.46	118.06	112.60
24	Q	383	ASP	O-C-N	5.46	128.61	122.22
27	O	294	MET	CB-CA-C	-5.46	101.56	110.85
28	H	185	LEU	CA-C-N	5.46	125.44	120.03
28	H	185	LEU	C-N-CA	5.46	125.44	120.03
31	L	75	LYS	N-CA-CB	5.46	118.75	110.28
31	L	85	GLU	CA-C-N	5.46	127.60	120.28
31	L	85	GLU	C-N-CA	5.46	127.60	120.28
33	J	385	ALA	CA-C-N	5.46	128.18	120.42
33	J	385	ALA	C-N-CA	5.46	128.18	120.42
9	2	236	ARG	NE-CZ-NH2	-5.46	114.28	119.20
12	5	92	ASP	CA-C-O	5.46	126.56	120.77
10	j	3	ASP	N-CA-CB	5.46	117.41	110.04
10	j	120	PHE	O-C-N	5.46	129.80	123.41
17	T	36	LYS	CA-C-N	5.46	127.60	120.28
17	T	36	LYS	C-N-CA	5.46	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	328	PHE	CA-CB-CG	5.46	119.26	113.80
21	N	400	ILE	CA-C-N	5.46	127.60	120.28
21	N	400	ILE	C-N-CA	5.46	127.60	120.28
24	Q	402	THR	N-CA-CB	5.46	118.65	110.02
30	K	290	ARG	NE-CZ-NH2	5.46	124.12	119.20
6	F	163	ALA	CB-CA-C	-5.46	102.07	110.26
11	4	10	GLN	N-CA-C	5.46	117.23	111.28
23	P	350	LEU	O-C-N	-5.46	116.33	122.12
24	Q	390	LEU	O-C-N	5.46	129.71	123.27
25	R	325	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
31	L	386	PHE	O-C-N	5.46	129.31	122.92
4	d	19	GLN	CA-C-N	5.46	128.17	120.42
4	d	19	GLN	C-N-CA	5.46	128.17	120.42
5	e	13	SER	N-CA-C	-5.46	104.57	113.19
10	3	76	LEU	CA-C-N	5.46	128.04	120.29
10	3	76	LEU	C-N-CA	5.46	128.04	120.29
19	Y	3	THR	OG1-CB-CG2	5.46	120.22	109.30
29	I	83	LYS	N-CA-CB	5.46	118.89	110.43
29	I	314	ASP	N-CA-CB	5.46	119.72	110.49
29	I	418	GLN	N-CA-CB	5.46	118.14	110.12
4	d	207	ALA	N-CA-C	-5.46	104.50	113.50
22	S	198	SER	N-CA-C	-5.46	100.44	108.79
23	P	111	ASP	CA-CB-CG	5.46	118.06	112.60
23	P	366	ASN	CA-C-N	5.46	127.59	120.28
23	P	366	ASN	C-N-CA	5.46	127.59	120.28
29	I	119	ILE	N-CA-CB	5.46	118.33	111.46
1	a	171	THR	N-CA-C	-5.45	100.78	109.23
3	C	32	ALA	CA-C-O	-5.45	115.44	121.33
4	D	26	ALA	CA-C-N	5.45	129.09	120.47
4	D	26	ALA	C-N-CA	5.45	129.09	120.47
6	F	29	ILE	O-C-N	5.45	127.25	121.91
6	F	153	VAL	CA-C-O	5.45	126.14	120.36
17	T	51	TYR	CA-C-N	5.45	128.03	120.29
17	T	51	TYR	C-N-CA	5.45	128.03	120.29
28	H	106	ILE	CB-CA-C	-5.45	103.61	111.19
28	H	342	GLY	CA-C-O	-5.45	118.21	122.52
30	K	190	LEU	CA-C-O	-5.45	112.69	120.16
31	L	290	ARG	NE-CZ-NH2	5.45	124.11	119.20
32	M	109	ASP	CA-CB-CG	5.45	118.05	112.60
33	J	24	GLU	CA-C-N	5.45	128.13	120.28
33	J	24	GLU	C-N-CA	5.45	128.13	120.28
7	g	118	GLN	N-CA-CB	5.45	118.70	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	164	ILE	CA-C-O	-5.45	115.39	121.17
13	m	173	ASN	OD1-CG-ND2	5.45	128.05	122.60
21	N	902	VAL	CB-CA-C	5.45	118.24	111.15
5	e	114	GLN	CA-C-O	-5.45	113.70	119.97
5	E	41	ALA	N-CA-CB	5.45	117.98	109.97
28	H	292	ARG	N-CA-CB	-5.45	102.11	110.01
29	I	145	CYS	N-CA-CB	5.45	118.73	110.45
4	d	238	GLN	N-CA-C	5.45	117.30	111.36
7	g	225	ASN	OD1-CG-ND2	-5.45	117.15	122.60
14	n	155	ASN	CA-CB-CG	-5.45	107.15	112.60
2	B	44	VAL	N-CA-C	-5.45	100.63	108.53
2	B	108	LYS	CA-C-N	5.45	127.58	120.28
2	B	108	LYS	C-N-CA	5.45	127.58	120.28
7	G	99	PHE	CA-C-N	5.45	128.03	120.29
7	G	99	PHE	C-N-CA	5.45	128.03	120.29
24	Q	167	LYS	CB-CA-C	-5.45	100.21	110.67
25	R	245	SER	CA-C-N	5.45	129.82	120.72
25	R	245	SER	C-N-CA	5.45	129.82	120.72
28	H	344	ASP	CA-C-N	5.45	125.39	119.78
28	H	344	ASP	C-N-CA	5.45	125.39	119.78
33	J	298	ASP	N-CA-CB	5.45	118.13	110.12
4	D	60	THR	CA-C-O	-5.45	114.91	119.76
22	S	300	ALA	CA-C-O	-5.45	114.91	119.76
25	R	95	ASP	CA-CB-CG	-5.45	107.15	112.60
27	O	134	ALA	CB-CA-C	-5.45	101.75	110.79
29	I	252	LEU	N-CA-C	-5.45	106.68	113.38
1	a	247	ALA	CA-C-N	5.45	128.15	120.42
1	a	247	ALA	C-N-CA	5.45	128.15	120.42
10	j	157	ASN	CB-CG-OD1	-5.45	109.91	120.80
8	1	193	GLU	O-C-N	-5.45	116.94	123.31
10	3	189	ILE	CA-C-O	-5.45	114.70	120.53
24	Q	336	ASN	CA-C-O	-5.45	114.65	120.42
1	a	99	ALA	CA-C-N	5.44	128.02	120.29
1	a	99	ALA	C-N-CA	5.44	128.02	120.29
12	l	275	VAL	CA-C-N	5.44	127.52	120.44
12	l	275	VAL	C-N-CA	5.44	127.52	120.44
4	D	128	PRO	CA-C-N	5.44	128.60	120.87
4	D	128	PRO	C-N-CA	5.44	128.60	120.87
11	4	100	VAL	N-CA-CB	5.44	118.92	111.41
29	I	274	ASN	CA-CB-CG	5.44	118.04	112.60
6	f	211	LEU	N-CA-CB	5.44	117.97	109.97
9	2	211	LYS	CA-C-N	5.44	128.57	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	211	LYS	C-N-CA	5.44	128.57	120.90
12	5	244	ALA	CB-CA-C	-5.44	101.00	110.09
19	Y	60	TRP	O-C-N	5.44	129.18	123.03
22	S	480	ARG	N-CA-C	5.44	119.64	112.89
25	R	184	GLN	CA-C-N	5.44	128.02	120.29
25	R	184	GLN	C-N-CA	5.44	128.02	120.29
25	R	360	SER	CA-C-N	5.44	127.42	120.56
25	R	360	SER	C-N-CA	5.44	127.42	120.56
26	U	167	GLU	N-CA-CB	5.44	118.12	110.12
29	I	170	VAL	CA-C-O	5.44	126.94	121.17
33	J	308	GLY	O-C-N	5.44	129.21	122.41
9	i	158	SER	N-CA-C	-5.44	106.48	113.23
11	4	80	VAL	CA-C-N	5.44	128.01	120.29
11	4	80	VAL	C-N-CA	5.44	128.01	120.29
20	Z	254	PRO	CA-C-N	5.44	131.93	121.54
20	Z	254	PRO	C-N-CA	5.44	131.93	121.54
23	P	107	SER	N-CA-CB	5.44	118.21	110.16
23	P	137	ALA	CA-C-N	5.44	128.58	120.31
23	P	137	ALA	C-N-CA	5.44	128.58	120.31
30	K	278	ALA	CA-C-N	5.44	130.44	122.77
30	K	278	ALA	C-N-CA	5.44	130.44	122.77
32	M	330	VAL	O-C-N	-5.44	116.76	122.25
12	l	158	LEU	CA-C-O	-5.44	113.72	119.97
2	B	79	GLY	CA-C-N	5.44	125.09	119.05
2	B	79	GLY	C-N-CA	5.44	125.09	119.05
24	Q	192	ALA	N-CA-C	-5.44	105.27	111.14
32	M	306	LEU	CA-C-O	-5.44	114.66	120.42
33	J	402	LYS	N-CA-C	-5.44	105.43	111.36
4	d	60	THR	CA-C-N	5.44	126.64	119.84
4	d	60	THR	C-N-CA	5.44	126.64	119.84
11	4	63	ASN	N-CA-C	5.44	117.29	111.36
24	Q	144	LEU	N-CA-C	5.44	117.21	111.28
28	H	283	TYR	N-CA-C	-5.44	101.11	109.76
25	R	305	PHE	CA-C-O	-5.44	112.71	120.16
27	O	314	SER	CB-CA-C	-5.44	101.77	110.79
29	I	352	ASN	CA-C-N	5.44	125.44	119.90
29	I	352	ASN	C-N-CA	5.44	125.44	119.90
31	L	310	THR	CA-C-N	5.44	128.57	120.31
31	L	310	THR	C-N-CA	5.44	128.57	120.31
2	b	133	SER	O-C-N	5.43	129.77	123.30
9	i	115	HIS	CA-CB-CG	5.43	119.23	113.80
20	Z	625	THR	CA-C-O	-5.43	113.63	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	59	GLU	N-CA-C	5.43	117.20	111.28
25	R	380	VAL	CA-C-O	-5.43	116.25	121.63
29	I	221	LEU	N-CA-C	-5.43	100.38	109.24
29	I	278	ILE	CA-C-O	5.43	126.04	120.39
30	K	330	ARG	O-C-N	-5.43	115.70	121.30
22	S	429	ASP	N-CA-C	-5.43	106.65	113.28
28	H	210	ASP	N-CA-C	-5.43	105.46	113.61
30	K	200	GLN	N-CA-CB	5.43	118.20	110.16
31	L	64	LEU	CA-C-N	5.43	127.56	120.28
31	L	64	LEU	C-N-CA	5.43	127.56	120.28
4	D	116	VAL	N-CA-C	-5.43	105.23	110.72
21	N	317	SER	N-CA-C	-5.43	105.44	111.36
24	Q	99	THR	N-CA-C	5.43	117.20	111.28
32	M	189	GLN	OE1-CD-NE2	5.43	128.03	122.60
33	J	180	ALA	CA-C-N	5.43	127.94	120.39
33	J	180	ALA	C-N-CA	5.43	127.94	120.39
3	c	94	HIS	CG-CD2-NE2	5.43	112.63	107.20
21	N	696	LYS	N-CA-CB	5.43	118.19	110.16
25	R	214	TYR	N-CA-C	-5.43	105.52	111.82
26	U	241	THR	CA-C-N	5.43	125.52	119.87
26	U	241	THR	C-N-CA	5.43	125.52	119.87
28	H	112	SER	CA-C-N	5.43	131.34	122.65
28	H	112	SER	C-N-CA	5.43	131.34	122.65
2	b	79	GLY	CA-C-N	5.43	125.07	119.05
2	b	79	GLY	C-N-CA	5.43	125.07	119.05
12	l	163	TYR	CA-C-N	5.43	127.55	120.28
12	l	163	TYR	C-N-CA	5.43	127.55	120.28
5	E	203	ILE	CA-C-N	5.43	127.50	120.44
5	E	203	ILE	C-N-CA	5.43	127.50	120.44
7	G	72	ARG	NE-CZ-NH2	5.43	124.08	119.20
16	V	216	LEU	O-C-N	-5.43	115.81	122.05
22	S	391	GLY	O-C-N	-5.43	116.37	122.28
25	R	411	LEU	CA-C-N	5.43	127.82	120.44
25	R	411	LEU	C-N-CA	5.43	127.82	120.44
30	K	236	ARG	NE-CZ-NH1	5.43	126.93	121.50
33	J	240	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
10	3	35	GLY	CA-C-N	-5.42	117.66	122.97
10	3	35	GLY	C-N-CA	-5.42	117.66	122.97
14	7	92	ASP	CA-CB-CG	-5.42	107.17	112.60
16	V	218	LYS	CA-CB-CG	5.42	124.95	114.10
17	T	98	GLU	O-C-N	5.42	129.62	123.27
21	N	142	GLU	CA-C-N	5.42	127.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	142	GLU	C-N-CA	5.42	127.55	120.28
21	N	873	ARG	CA-C-N	5.42	130.59	123.11
21	N	873	ARG	C-N-CA	5.42	130.59	123.11
23	P	148	LYS	O-C-N	-5.42	116.37	122.12
24	Q	412	ALA	N-CA-C	5.42	117.95	111.71
27	O	183	ASN	N-CA-CB	5.42	119.66	110.49
5	e	40	ILE	O-C-N	-5.42	118.09	122.97
1	A	193	HIS	CA-C-N	5.42	130.54	123.06
1	A	193	HIS	C-N-CA	5.42	130.54	123.06
25	R	309	LEU	N-CA-CB	5.42	118.19	110.16
30	K	198	TYR	CA-C-N	5.42	128.09	120.28
30	K	198	TYR	C-N-CA	5.42	128.09	120.28
32	M	369	THR	N-CA-CB	5.42	118.31	109.69
33	J	371	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	a	135	ARG	CA-C-N	5.42	125.43	119.90
1	a	135	ARG	C-N-CA	5.42	125.43	119.90
8	h	73	GLU	CA-C-N	5.42	127.54	120.28
8	h	73	GLU	C-N-CA	5.42	127.54	120.28
1	A	22	GLU	CB-CA-C	-5.42	101.03	110.09
3	C	48	ALA	N-CA-C	5.42	117.43	109.24
5	E	16	SER	N-CA-C	-5.42	103.90	110.13
8	1	59	ALA	N-CA-C	5.42	117.19	111.28
9	2	54	ILE	CA-C-N	5.42	129.39	121.80
9	2	54	ILE	C-N-CA	5.42	129.39	121.80
21	N	261	LEU	N-CA-CB	5.42	117.93	110.07
30	K	100	LEU	CA-C-N	-5.42	113.99	122.56
30	K	100	LEU	C-N-CA	-5.42	113.99	122.56
33	J	380	GLU	CA-C-N	5.42	127.54	120.28
33	J	380	GLU	C-N-CA	5.42	127.54	120.28
2	b	215	GLY	CA-C-N	5.42	129.45	120.94
2	b	215	GLY	C-N-CA	5.42	129.45	120.94
3	c	191	GLU	CA-C-N	5.42	128.55	120.31
3	c	191	GLU	C-N-CA	5.42	128.55	120.31
6	f	233	TYR	CA-CB-CG	-5.42	104.14	113.90
9	i	144	ALA	N-CA-CB	5.42	117.93	110.07
30	K	326	PRO	N-CA-C	-5.42	106.95	114.27
10	j	160	PRO	N-CD-CG	5.42	111.33	103.20
17	T	222	LEU	O-C-N	5.42	127.94	122.09
23	P	210	ASN	CA-CB-CG	-5.42	107.18	112.60
24	Q	181	GLU	CA-C-N	5.42	127.54	120.28
24	Q	181	GLU	C-N-CA	5.42	127.54	120.28
1	a	65	ASP	N-CA-CB	5.42	118.03	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	272	PHE	O-C-N	5.42	127.86	122.12
22	S	220	ILE	O-C-N	5.42	127.53	121.90
24	Q	51	ARG	CA-C-N	5.42	127.80	120.38
24	Q	51	ARG	C-N-CA	5.42	127.80	120.38
33	J	229	MET	CA-C-N	5.42	128.11	120.42
33	J	229	MET	C-N-CA	5.42	128.11	120.42
7	g	105	THR	CA-C-N	5.42	125.71	119.92
7	g	105	THR	C-N-CA	5.42	125.71	119.92
9	2	174	ASP	N-CA-CB	5.42	119.64	110.49
13	6	91	LYS	N-CA-C	-5.42	102.86	110.50
15	W	43	SER	O-C-N	-5.42	115.98	122.15
24	Q	280	ASN	CA-C-N	5.42	127.88	120.46
24	Q	280	ASN	C-N-CA	5.42	127.88	120.46
26	U	146	ASP	N-CA-C	-5.42	107.23	112.97
8	h	35	ILE	N-CA-C	-5.41	100.62	108.36
10	j	113	ASN	CA-CB-CG	-5.41	107.19	112.60
11	k	41	HIS	CG-CD2-NE2	5.41	112.61	107.20
15	W	79	THR	N-CA-C	5.41	117.28	110.24
23	P	421	GLU	CA-C-N	5.41	127.98	120.29
23	P	421	GLU	C-N-CA	5.41	127.98	120.29
24	Q	130	ARG	CA-C-N	5.41	129.18	120.30
24	Q	130	ARG	C-N-CA	5.41	129.18	120.30
2	b	229	THR	N-CA-C	-5.41	106.05	113.30
3	c	38	ILE	N-CA-CB	5.41	119.18	111.82
10	3	164	PHE	N-CA-C	-5.41	105.46	111.36
25	R	27	SER	O-C-N	-5.41	116.39	122.12
27	O	138	LEU	CA-C-O	5.41	126.19	119.97
31	L	406	ASP	O-C-N	5.41	129.79	122.59
7	g	127	ASN	CA-C-N	5.41	127.80	120.44
7	g	127	ASN	C-N-CA	5.41	127.80	120.44
11	k	74	GLU	N-CA-CB	5.41	118.33	109.95
4	d	245	GLU	CA-C-N	5.41	127.53	120.28
4	d	245	GLU	C-N-CA	5.41	127.53	120.28
7	g	55	THR	N-CA-C	-5.41	106.69	113.72
18	X	21	SER	CA-C-N	5.41	129.81	122.19
18	X	21	SER	C-N-CA	5.41	129.81	122.19
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
12	l	199	GLY	CA-C-O	-5.41	116.55	121.47
9	2	101	ARG	NE-CZ-NH2	5.41	124.06	119.20
21	N	103	SER	CB-CA-C	-5.41	101.49	110.68
22	S	151	GLU	N-CA-C	-5.41	101.35	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	312	PRO	N-CA-C	-5.41	107.12	114.80
28	H	127	SER	CA-C-O	-5.41	115.67	121.45
28	H	227	LEU	CA-C-O	-5.41	112.75	120.16
4	d	167	ASN	N-CA-CB	5.40	119.92	111.71
1	A	12	TYR	N-CA-C	-5.40	105.35	113.89
33	J	342	ASN	O-C-N	5.40	129.34	122.04
7	g	68	GLN	CA-C-O	-5.40	114.79	121.06
11	k	166	GLN	CA-C-N	5.40	127.52	120.28
11	k	166	GLN	C-N-CA	5.40	127.52	120.28
1	A	198	SER	N-CA-C	-5.40	100.22	108.76
3	C	185	LYS	CA-C-N	5.40	128.09	120.42
3	C	185	LYS	C-N-CA	5.40	128.09	120.42
4	D	87	GLU	N-CA-C	5.40	117.17	111.28
9	2	146	GLY	N-CA-C	-5.40	107.58	115.63
2	b	149	GLN	CB-CG-CD	-5.40	103.42	112.60
3	C	239	LEU	O-C-N	5.40	128.91	122.27
6	F	138	ASP	N-CA-CB	5.40	115.60	108.96
21	N	817	THR	CA-C-N	5.40	128.06	120.28
21	N	817	THR	C-N-CA	5.40	128.06	120.28
22	S	485	LYS	N-CA-CB	5.40	117.84	110.01
24	Q	175	VAL	CA-C-N	5.40	127.52	120.28
24	Q	175	VAL	C-N-CA	5.40	127.52	120.28
24	Q	201	ALA	CA-C-N	5.40	127.96	120.29
24	Q	201	ALA	C-N-CA	5.40	127.96	120.29
27	O	130	ASP	CA-C-O	-5.40	114.83	120.55
1	a	36	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	166	TYR	CB-CA-C	-5.40	101.36	110.43
21	N	861	TYR	N-CA-C	-5.40	99.80	108.55
22	S	188	TYR	CA-C-N	5.40	127.96	120.29
22	S	188	TYR	C-N-CA	5.40	127.96	120.29
22	S	270	ALA	CA-C-N	5.40	127.52	120.28
22	S	270	ALA	C-N-CA	5.40	127.52	120.28
2	b	188	ALA	CB-CA-C	-5.40	101.83	110.79
24	Q	1	MET	CG-SD-CE	-5.40	89.03	100.90
24	Q	215	VAL	CB-CA-C	-5.40	104.77	112.22
28	H	309	ASP	N-CA-CB	5.40	118.21	110.06
30	K	193	VAL	CA-C-O	-5.40	114.47	120.46
32	M	45	ARG	CA-C-O	-5.40	113.29	119.60
13	6	44	ASN	N-CA-CB	5.40	118.24	110.20
28	H	249	TYR	N-CA-CB	5.40	120.83	111.39
4	d	181	ARG	NE-CZ-NH2	5.39	124.06	119.20
5	e	30	ALA	CA-C-N	5.39	127.85	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	30	ALA	C-N-CA	5.39	127.85	120.46
7	g	110	PRO	N-CA-CB	5.39	109.26	103.33
10	j	48	HIS	N-CA-C	-5.39	106.07	113.30
20	Z	224	LEU	CA-C-N	5.39	127.82	120.54
20	Z	224	LEU	C-N-CA	5.39	127.82	120.54
4	d	21	GLU	CA-C-O	-5.39	114.70	120.42
12	l	255	VAL	CB-CA-C	-5.39	103.09	110.96
13	m	110	PHE	CA-CB-CG	-5.39	108.41	113.80
9	2	95	HIS	N-CA-C	5.39	117.16	111.28
11	4	63	ASN	CA-C-O	-5.39	114.70	120.42
16	V	235	GLU	CA-C-N	5.39	127.95	120.29
16	V	235	GLU	C-N-CA	5.39	127.95	120.29
22	S	259	TYR	CA-C-N	5.39	125.15	119.76
22	S	259	TYR	C-N-CA	5.39	125.15	119.76
1	a	169	THR	CA-CB-OG1	5.39	117.69	109.60
4	d	85	LEU	CA-C-N	5.39	128.07	120.42
4	d	85	LEU	C-N-CA	5.39	128.07	120.42
12	5	157	ILE	O-C-N	-5.39	116.64	121.87
31	L	339	ARG	NE-CZ-NH2	-5.39	114.35	119.20
6	f	19	LEU	CB-CA-C	-5.39	100.39	109.72
8	h	131	LEU	N-CA-C	-5.39	100.14	108.55
4	D	165	GLY	CA-C-N	5.39	131.83	121.54
4	D	165	GLY	C-N-CA	5.39	131.83	121.54
8	1	76	THR	O-C-N	5.39	128.29	122.15
13	6	87	HIS	CA-CB-CG	-5.39	108.41	113.80
19	Y	16	LEU	N-CA-CB	5.39	119.15	110.85
21	N	201	LYS	N-CA-C	5.39	116.84	111.07
22	S	458	GLN	CG-CD-OE1	5.39	131.58	120.80
4	d	52	LEU	N-CA-C	-5.39	102.22	110.14
6	f	7	ASP	CA-CB-CG	-5.39	107.21	112.60
8	h	155	MET	CA-C-N	5.39	129.40	120.94
8	h	155	MET	C-N-CA	5.39	129.40	120.94
12	l	278	GLU	CA-C-N	5.39	127.94	120.29
12	l	278	GLU	C-N-CA	5.39	127.94	120.29
27	O	369	ARG	NE-CZ-NH1	-5.39	116.11	121.50
31	L	366	ALA	CA-C-N	5.39	127.44	120.44
31	L	366	ALA	C-N-CA	5.39	127.44	120.44
6	f	170	THR	N-CA-C	-5.39	105.49	111.36
7	g	93	ARG	CA-C-N	5.39	127.94	120.29
7	g	93	ARG	C-N-CA	5.39	127.94	120.29
3	C	162	ALA	CA-C-O	5.39	126.78	120.75
22	S	199	GLU	N-CA-C	-5.39	98.43	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	412	THR	CA-C-N	5.39	127.50	120.28
25	R	412	THR	C-N-CA	5.39	127.50	120.28
30	K	188	VAL	CB-CA-C	-5.39	107.13	111.71
32	M	27	THR	O-C-N	5.39	127.83	122.12
32	M	56	ASN	CA-C-N	5.39	127.84	120.46
32	M	56	ASN	C-N-CA	5.39	127.84	120.46
4	D	24	LEU	N-CA-CB	5.38	118.13	110.16
17	T	206	LYS	CG-CD-CE	5.38	123.69	111.30
18	X	99	PHE	CA-C-O	-5.38	114.81	121.11
21	N	551	GLY	O-C-N	5.38	127.46	122.13
25	R	249	ILE	CA-C-N	5.38	127.94	120.29
25	R	249	ILE	C-N-CA	5.38	127.94	120.29
28	H	442	ASP	CA-C-N	5.38	127.50	120.28
28	H	442	ASP	C-N-CA	5.38	127.50	120.28
29	I	360	LYS	CA-C-N	5.38	129.16	120.55
29	I	360	LYS	C-N-CA	5.38	129.16	120.55
1	A	68	THR	O-C-N	-5.38	115.73	122.24
2	B	175	LEU	CA-C-N	5.38	127.44	120.44
2	B	175	LEU	C-N-CA	5.38	127.44	120.44
10	3	194	GLU	O-C-N	5.38	129.29	123.10
20	Z	946	THR	N-CA-C	-5.38	99.75	108.52
21	N	458	ALA	CA-C-O	-5.38	114.11	120.57
2	B	110	LEU	CA-C-N	5.38	127.83	120.46
2	B	110	LEU	C-N-CA	5.38	127.83	120.46
21	N	535	LEU	CA-C-N	5.38	127.83	120.46
21	N	535	LEU	C-N-CA	5.38	127.83	120.46
31	L	96	LYS	CA-C-N	5.38	127.93	120.29
31	L	96	LYS	C-N-CA	5.38	127.93	120.29
14	n	153	GLN	CA-C-N	5.38	128.49	120.31
14	n	153	GLN	C-N-CA	5.38	128.49	120.31
8	h	127	SER	N-CA-C	-5.38	100.56	108.79
8	h	204	GLN	N-CA-CB	-5.38	102.21	110.12
21	N	761	ILE	CA-C-N	5.38	128.98	121.24
21	N	761	ILE	C-N-CA	5.38	128.98	121.24
23	P	268	LEU	CA-C-N	5.38	128.06	120.42
23	P	268	LEU	C-N-CA	5.38	128.06	120.42
25	R	113	LEU	CA-C-O	-5.38	114.72	120.42
32	M	105	ASN	N-CA-C	5.38	117.67	110.35
1	a	19	PHE	CA-C-O	5.38	127.65	121.47
1	a	23	GLY	CA-C-O	5.38	124.99	119.02
14	n	158	GLN	CG-CD-OE1	-5.38	110.05	120.80
12	5	281	SER	CA-C-N	5.38	130.00	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	281	SER	C-N-CA	5.38	130.00	122.36
21	N	776	TYR	N-CA-C	-5.38	100.53	109.46
22	S	65	ASN	OD1-CG-ND2	5.38	127.98	122.60
23	P	345	VAL	O-C-N	-5.38	116.29	121.83
14	n	190	LYS	CB-CA-C	-5.38	102.44	110.88
4	D	95	SER	CA-C-N	5.38	127.48	120.28
4	D	95	SER	C-N-CA	5.38	127.48	120.28
23	P	361	THR	CA-CB-OG1	5.38	117.66	109.60
3	c	31	HIS	CA-CB-CG	-5.37	108.43	113.80
14	n	206	ALA	O-C-N	5.37	127.61	122.07
6	F	206	LEU	N-CA-CB	5.37	117.87	109.97
22	S	450	ASN	CA-CB-CG	5.37	117.97	112.60
23	P	395	ARG	CA-C-N	5.37	125.04	119.56
23	P	395	ARG	C-N-CA	5.37	125.04	119.56
25	R	216	ILE	CA-C-O	5.37	126.51	119.85
27	O	203	THR	CA-C-O	5.37	126.33	120.58
9	i	38	ASN	N-CA-C	5.37	117.14	111.28
16	V	150	LYS	O-C-N	-5.37	116.91	123.30
21	N	335	ALA	CB-CA-C	-5.37	102.45	110.88
21	N	355	TRP	CA-C-N	5.37	127.42	120.44
21	N	355	TRP	C-N-CA	5.37	127.42	120.44
29	I	299	GLU	CA-C-N	5.37	127.42	120.44
29	I	299	GLU	C-N-CA	5.37	127.42	120.44
30	K	71	GLU	N-CA-C	-5.37	105.42	111.28
33	J	217	GLU	N-CA-CB	5.37	118.40	110.56
8	h	95	CYS	CB-CA-C	-5.37	101.88	110.79
12	l	83	PHE	CA-C-N	5.37	127.47	120.28
12	l	83	PHE	C-N-CA	5.37	127.47	120.28
10	3	103	TYR	N-CA-CB	5.37	118.23	109.69
2	B	80	PRO	CA-C-N	5.37	127.47	120.28
2	B	80	PRO	C-N-CA	5.37	127.47	120.28
11	4	147	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
16	V	214	MET	CA-C-N	5.37	128.97	121.24
16	V	214	MET	C-N-CA	5.37	128.97	121.24
17	T	179	ASP	CA-CB-CG	-5.37	107.23	112.60
21	N	138	GLU	CA-C-N	5.37	128.47	120.31
21	N	138	GLU	C-N-CA	5.37	128.47	120.31
21	N	731	VAL	CA-CB-CG2	-5.37	101.27	110.40
25	R	29	LYS	CA-C-N	5.37	128.01	120.28
25	R	29	LYS	C-N-CA	5.37	128.01	120.28
32	M	139	LYS	CB-CA-C	-5.37	101.13	110.09
32	M	185	GLY	CA-C-O	-5.37	115.74	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	145	HIS	N-CA-CB	5.37	118.10	110.16
1	a	27	GLN	CG-CD-NE2	-5.37	108.35	116.40
4	d	136	ALA	N-CA-C	-5.37	101.37	109.85
14	n	200	LYS	CA-C-O	-5.37	112.99	119.27
25	R	401	HIS	O-C-N	-5.37	116.43	122.12
28	H	99	VAL	N-CA-CB	5.37	116.38	110.53
10	j	19	ASP	CB-CA-C	-5.36	104.11	111.73
10	j	160	PRO	N-CA-CB	5.36	109.37	103.26
11	k	41	HIS	ND1-CE1-NE2	5.36	113.76	108.40
12	l	247	GLY	N-CA-C	-5.36	100.47	113.18
21	N	705	ILE	CA-C-N	5.36	127.47	120.28
21	N	705	ILE	C-N-CA	5.36	127.47	120.28
23	P	165	VAL	O-C-N	5.36	128.51	122.18
27	O	202	SER	N-CA-CB	5.36	117.79	109.48
33	J	399	SER	CA-CB-OG	5.36	121.83	111.10
9	i	212	ASP	N-CA-C	-5.36	103.45	110.53
5	E	185	ASN	CA-CB-CG	-5.36	107.24	112.60
23	P	182	GLU	CA-C-O	5.36	126.42	120.63
33	J	84	VAL	N-CA-C	-5.36	101.27	108.35
13	m	100	ASN	N-CA-C	-5.36	105.35	111.14
2	B	119	GLN	CG-CD-NE2	5.36	124.44	116.40
8	1	161	VAL	CA-C-N	5.36	127.46	120.28
8	1	161	VAL	C-N-CA	5.36	127.46	120.28
12	5	101	VAL	N-CA-CB	-5.36	104.89	111.00
21	N	613	HIS	CA-CB-CG	-5.36	108.44	113.80
24	Q	392	GLN	N-CA-C	-5.36	106.61	112.72
30	K	146	LEU	CA-C-O	5.36	126.66	120.60
7	g	52	LYS	N-CA-C	-5.36	98.51	107.99
9	i	193	TRP	O-C-N	-5.36	116.04	122.15
11	4	149	ARG	CA-C-N	5.36	124.97	119.56
11	4	149	ARG	C-N-CA	5.36	124.97	119.56
15	W	160	ALA	CB-CA-C	-5.36	101.90	110.79
24	Q	107	VAL	CA-CB-CG1	5.36	119.51	110.40
24	Q	261	VAL	CA-C-O	-5.36	115.17	120.85
24	Q	366	ILE	N-CA-C	5.36	117.79	111.09
33	J	331	HIS	CG-CD2-NE2	5.36	112.56	107.20
7	g	106	PRO	N-CA-CB	5.36	108.42	103.39
3	C	151	SER	CA-C-O	5.36	126.82	120.66
16	V	157	ARG	NE-CZ-NH2	-5.36	114.38	119.20
17	T	31	LYS	CA-C-N	5.36	127.31	120.56
17	T	31	LYS	C-N-CA	5.36	127.31	120.56
28	H	189	PRO	CA-C-N	5.36	131.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	189	PRO	C-N-CA	5.36	131.77	121.54
30	K	343	LEU	CA-C-N	5.36	133.49	121.76
30	K	343	LEU	C-N-CA	5.36	133.49	121.76
30	K	379	SER	CA-C-N	5.36	126.83	120.14
30	K	379	SER	C-N-CA	5.36	126.83	120.14
33	J	168	VAL	CB-CA-C	-5.36	104.96	111.87
21	N	97	PHE	CB-CA-C	-5.35	100.78	109.13
26	U	269	THR	CA-C-N	5.35	130.51	121.14
26	U	269	THR	C-N-CA	5.35	130.51	121.14
1	a	101	ALA	CA-C-N	5.35	127.45	120.28
1	a	101	ALA	C-N-CA	5.35	127.45	120.28
10	3	141	THR	CA-C-O	5.35	125.95	119.31
11	4	175	ASP	CA-C-O	-5.35	114.94	121.36
28	H	52	THR	O-C-N	-5.35	116.45	122.12
8	1	71	HIS	N-CA-CB	5.35	118.08	110.16
13	6	88	ASN	CB-CG-ND2	-5.35	108.37	116.40
29	I	311	ASN	N-CA-C	-5.35	105.53	111.36
30	K	182	GLN	OE1-CD-NE2	5.35	127.95	122.60
2	b	32	VAL	CA-C-O	5.35	126.82	120.72
4	d	250	LYS	CA-C-N	5.35	127.89	120.29
4	d	250	LYS	C-N-CA	5.35	127.89	120.29
7	g	183	HIS	ND1-CE1-NE2	5.35	113.75	108.40
12	5	271	LEU	CA-C-N	5.35	127.45	120.28
12	5	271	LEU	C-N-CA	5.35	127.45	120.28
16	V	23	THR	N-CA-C	-5.35	101.32	108.86
17	T	128	TYR	N-CA-C	-5.35	105.45	111.28
25	R	159	SER	CB-CA-C	-5.35	101.91	110.79
1	a	249	ALA	N-CA-CB	5.35	118.08	110.16
3	c	94	HIS	CB-CG-CD2	-5.35	124.25	131.20
3	C	194	LEU	O-C-N	5.35	127.79	122.12
7	G	171	SER	O-C-N	5.35	128.25	122.15
21	N	700	CYS	O-C-N	5.35	129.18	122.23
30	K	420	THR	CA-C-N	5.35	131.59	121.97
30	K	420	THR	C-N-CA	5.35	131.59	121.97
1	A	187	LYS	CA-C-O	5.35	126.21	120.70
25	R	339	ALA	N-CA-C	5.35	117.11	111.28
8	h	161	VAL	N-CA-CB	5.34	116.80	110.55
9	i	164	MET	CB-CA-C	-5.34	101.92	110.79
10	j	155	GLU	N-CA-C	-5.34	98.14	108.45
10	3	45	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
14	7	121	GLU	CA-C-O	5.34	125.42	120.50
25	R	388	VAL	N-CA-CB	5.34	118.19	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	373	ARG	N-CA-CB	5.34	118.99	110.65
29	I	294	SER	O-C-N	-5.34	115.84	122.25
12	5	238	ALA	CB-CA-C	-5.34	101.92	110.79
17	T	20	TYR	CA-C-N	5.34	128.43	120.31
17	T	20	TYR	C-N-CA	5.34	128.43	120.31
23	P	172	GLU	CA-C-N	5.34	127.39	120.44
23	P	172	GLU	C-N-CA	5.34	127.39	120.44
25	R	248	SER	N-CA-CB	5.34	118.07	110.16
9	i	211	LYS	CA-CB-CG	5.34	124.78	114.10
11	k	139	TYR	N-CA-C	-5.34	107.31	113.88
14	n	84	VAL	CB-CA-C	5.34	118.76	110.96
14	7	126	PHE	N-CA-CB	-5.34	102.26	110.01
22	S	26	ALA	CA-C-N	5.34	127.38	120.44
22	S	26	ALA	C-N-CA	5.34	127.38	120.44
24	Q	246	TYR	CA-CB-CG	-5.34	104.29	113.90
28	H	442	ASP	CA-CB-CG	5.34	117.94	112.60
3	c	219	GLY	CA-C-N	5.34	131.74	121.54
3	c	219	GLY	C-N-CA	5.34	131.74	121.54
11	4	133	HIS	N-CA-C	-5.34	101.60	109.18
14	7	54	ILE	N-CA-CB	5.34	119.08	111.82
29	I	351	GLU	CA-C-O	-5.34	115.56	121.33
30	K	101	GLU	CA-C-N	5.34	126.48	120.66
30	K	101	GLU	C-N-CA	5.34	126.48	120.66
31	L	209	ARG	O-C-N	5.34	127.78	122.12
33	J	81	ASP	CA-C-N	5.34	131.74	121.54
33	J	81	ASP	C-N-CA	5.34	131.74	121.54
9	i	207	MET	N-CA-C	-5.34	98.52	108.02
8	1	83	SER	CA-C-N	5.34	127.43	120.28
8	1	83	SER	C-N-CA	5.34	127.43	120.28
10	3	143	SER	CA-C-N	5.34	127.70	120.44
10	3	143	SER	C-N-CA	5.34	127.70	120.44
17	T	82	PHE	CB-CG-CD2	5.34	129.78	120.70
21	N	760	GLY	CA-C-O	5.34	126.55	121.64
27	O	354	GLN	OE1-CD-NE2	5.34	127.94	122.60
9	i	95	HIS	CG-CD2-NE2	5.34	112.54	107.20
12	l	158	LEU	CA-C-N	5.34	127.87	120.29
12	l	158	LEU	C-N-CA	5.34	127.87	120.29
1	A	172	GLY	CA-C-N	5.34	126.51	119.84
1	A	172	GLY	C-N-CA	5.34	126.51	119.84
11	4	127	GLU	N-CA-C	-5.34	100.60	109.46
21	N	114	SER	CA-C-N	5.34	127.43	120.28
21	N	114	SER	C-N-CA	5.34	127.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	417	GLN	CA-C-N	5.34	127.38	120.44
22	S	417	GLN	C-N-CA	5.34	127.38	120.44
31	L	105	ILE	N-CA-CB	5.34	117.39	110.99
31	L	191	ARG	CA-C-N	5.34	127.43	120.28
31	L	191	ARG	C-N-CA	5.34	127.43	120.28
32	M	80	ALA	O-C-N	-5.34	116.71	123.17
32	M	158	THR	N-CA-CB	5.34	119.39	110.85
1	a	198	SER	CA-C-N	5.33	129.63	120.72
1	a	198	SER	C-N-CA	5.33	129.63	120.72
13	m	224	PHE	CA-CB-CG	-5.33	108.47	113.80
23	P	402	PHE	CA-C-O	-5.33	114.65	120.36
27	O	72	LYS	N-CA-C	-5.33	105.42	112.94
12	l	141	HIS	CA-CB-CG	5.33	119.13	113.80
3	C	151	SER	N-CA-C	-5.33	100.34	109.24
8	1	128	VAL	CA-C-O	-5.33	115.19	120.90
11	4	59	TYR	CA-C-N	5.33	127.76	120.46
11	4	59	TYR	C-N-CA	5.33	127.76	120.46
12	5	207	GLY	N-CA-C	-5.33	106.77	115.46
27	O	133	ILE	CA-C-N	5.33	127.42	120.28
27	O	133	ILE	C-N-CA	5.33	127.42	120.28
30	K	260	LEU	CA-C-N	5.33	127.37	120.44
30	K	260	LEU	C-N-CA	5.33	127.37	120.44
11	k	157	GLY	CA-C-N	5.33	127.86	120.29
11	k	157	GLY	C-N-CA	5.33	127.86	120.29
7	G	12	ASN	OD1-CG-ND2	5.33	127.93	122.60
21	N	602	VAL	CA-C-O	-5.33	115.12	118.69
21	N	847	LYS	CA-C-O	5.33	125.09	118.43
22	S	30	GLN	CA-C-N	5.33	127.76	120.46
22	S	30	GLN	C-N-CA	5.33	127.76	120.46
23	P	253	ASP	CA-CB-CG	5.33	117.93	112.60
24	Q	394	ASN	CB-CA-C	-5.33	99.81	110.42
28	H	51	GLN	CA-C-O	-5.33	114.90	120.55
32	M	56	ASN	CA-CB-CG	-5.33	107.27	112.60
7	g	72	ARG	CA-C-O	5.33	124.98	119.97
22	S	344	PRO	CA-C-N	5.33	127.86	120.29
22	S	344	PRO	C-N-CA	5.33	127.86	120.29
22	S	435	LYS	O-C-N	-5.33	117.18	123.41
23	P	377	GLU	CA-C-O	-5.33	115.20	120.90
27	O	259	THR	N-CA-CB	5.33	117.74	110.01
30	K	316	MET	N-CA-CB	5.33	120.56	111.66
1	a	186	PHE	N-CA-C	-5.33	106.28	112.89
11	k	46	PHE	CA-CB-CG	-5.33	108.47	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	208	LYS	CA-C-O	-5.33	115.21	120.70
22	S	111	ARG	NE-CZ-NH2	-5.33	114.41	119.20
2	b	53	SER	CA-C-N	5.33	126.50	119.84
2	b	53	SER	C-N-CA	5.33	126.50	119.84
14	n	143	LEU	CB-CA-C	-5.33	101.56	110.19
17	T	196	SER	N-CA-C	5.33	117.08	111.28
22	S	109	GLU	N-CA-C	-5.33	106.17	113.30
22	S	127	THR	OG1-CB-CG2	5.33	119.95	109.30
26	U	26	GLN	CB-CA-C	5.33	119.45	111.89
5	e	184	LEU	N-CA-CB	5.32	118.53	110.28
12	l	93	SER	CB-CA-C	-5.32	102.88	111.18
13	m	20	ILE	CA-C-O	-5.32	116.24	121.67
9	2	68	PRO	CA-C-N	5.32	130.57	122.37
9	2	68	PRO	C-N-CA	5.32	130.57	122.37
14	7	129	LEU	CA-C-O	-5.32	114.78	120.42
22	S	180	ASN	CA-C-N	5.32	129.73	120.68
22	S	180	ASN	C-N-CA	5.32	129.73	120.68
23	P	101	MET	O-C-N	5.32	127.76	122.12
28	H	73	ASP	CA-C-N	5.32	130.07	122.72
28	H	73	ASP	C-N-CA	5.32	130.07	122.72
31	L	319	GLY	CA-C-N	5.32	128.37	120.17
31	L	319	GLY	C-N-CA	5.32	128.37	120.17
13	m	27	ASP	CA-CB-CG	-5.32	107.28	112.60
17	T	265	ASP	CA-C-N	5.32	127.41	120.28
17	T	265	ASP	C-N-CA	5.32	127.41	120.28
24	Q	183	LYS	N-CA-CB	5.32	117.94	110.12
25	R	207	ARG	NE-CZ-NH1	5.32	126.82	121.50
33	J	93	LYS	N-CA-C	-5.32	101.03	109.76
10	j	140	GLY	CA-C-O	-5.32	116.49	122.24
6	F	146	GLU	N-CA-C	-5.32	99.74	108.41
8	1	139	GLY	N-CA-C	-5.32	106.52	115.62
16	V	127	LYS	O-C-N	5.32	127.76	122.12
17	T	255	GLN	CB-CG-CD	-5.32	103.56	112.60
27	O	229	ASN	O-C-N	-5.32	115.33	122.19
6	F	27	GLU	N-CA-CB	5.32	118.03	110.16
21	N	276	GLU	CB-CG-CD	-5.32	103.56	112.60
29	I	116	ASP	CA-CB-CG	-5.32	107.28	112.60
9	i	115	HIS	ND1-CE1-NE2	5.32	113.72	108.40
10	j	3	ASP	O-C-N	-5.32	114.89	121.64
1	A	234	PHE	N-CA-CB	5.32	120.70	111.39
7	G	144	ASN	N-CA-CB	5.32	118.18	110.47
14	7	58	ASP	N-CA-C	5.32	117.19	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	35	PHE	CA-CB-CG	-5.32	108.48	113.80
25	R	81	HIS	O-C-N	-5.32	115.52	122.59
25	R	84	LYS	N-CA-C	-5.32	100.02	109.06
26	U	276	ILE	CA-C-N	5.32	127.67	120.38
26	U	276	ILE	C-N-CA	5.32	127.67	120.38
30	K	302	GLN	OE1-CD-NE2	-5.32	117.28	122.60
6	f	103	LEU	O-C-N	-5.32	116.74	123.01
2	B	237	LYS	N-CA-C	-5.32	100.58	109.24
3	C	115	LEU	CA-C-O	-5.32	113.86	119.97
9	2	60	CYS	N-CA-C	-5.32	99.48	110.80
10	3	166	THR	CB-CA-C	-5.32	102.50	110.90
14	7	94	GLN	OE1-CD-NE2	-5.32	117.28	122.60
15	W	15	TYR	CB-CA-C	-5.32	101.58	110.56
22	S	54	TRP	CG-CD2-CE3	-5.32	128.58	133.90
27	O	370	LEU	CA-C-O	-5.32	114.09	120.10
28	H	124	ASN	OD1-CG-ND2	5.32	127.92	122.60
30	K	100	LEU	N-CA-CB	5.32	118.43	110.19
31	L	193	LEU	CA-C-O	5.32	126.06	120.42
8	h	160	THR	O-C-N	5.31	128.21	122.15
17	T	221	ALA	O-C-N	-5.31	116.00	122.22
4	d	251	LYS	CB-CA-C	-5.31	101.82	110.85
3	C	35	ALA	N-CA-CB	5.31	119.53	110.71
21	N	714	THR	N-CA-C	-5.31	101.28	109.52
23	P	142	ASP	CA-CB-CG	-5.31	107.29	112.60
25	R	123	ASP	CA-CB-CG	-5.31	107.29	112.60
26	U	7	LYS	CB-CG-CD	5.31	123.52	111.30
30	K	371	LEU	CA-C-O	5.31	125.45	119.18
31	L	262	ILE	N-CA-CB	5.31	116.20	110.62
33	J	171	PRO	N-CA-C	-5.31	107.22	114.98
6	f	52	ASN	OD1-CG-ND2	5.31	127.91	122.60
13	6	58	ILE	N-CA-C	-5.31	99.91	107.77
27	O	368	ASP	CB-CA-C	-5.31	101.97	110.79
6	f	70	MET	CA-CB-CG	5.31	124.72	114.10
14	n	181	ALA	CA-C-O	5.31	126.05	120.42
2	B	159	TRP	CE3-CZ3-CH2	5.31	128.00	121.10
28	H	250	GLY	CA-C-N	5.31	125.85	120.38
28	H	250	GLY	C-N-CA	5.31	125.85	120.38
28	H	376	GLU	CA-C-N	5.31	129.47	122.30
28	H	376	GLU	C-N-CA	5.31	129.47	122.30
1	a	122	ALA	CA-C-N	5.31	127.39	120.28
1	a	122	ALA	C-N-CA	5.31	127.39	120.28
2	b	18	LEU	N-CA-C	-5.31	100.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	14	SER	N-CA-CB	5.31	119.82	110.37
24	Q	78	ILE	O-C-N	-5.31	115.05	121.10
25	R	372	ILE	CA-C-O	-5.31	114.34	118.85
26	U	196	SER	CA-CB-OG	-5.31	100.49	111.10
26	U	290	ASP	CA-C-O	-5.31	114.90	120.63
26	U	230	GLN	CB-CA-C	-5.31	101.83	110.85
29	I	284	ILE	CA-C-O	5.31	125.67	119.89
29	I	385	ASP	CB-CA-C	-5.31	100.78	109.80
30	K	330	ARG	CA-C-N	5.31	126.47	119.84
30	K	330	ARG	C-N-CA	5.31	126.47	119.84
9	i	183	LEU	CA-C-N	5.30	127.39	120.28
9	i	183	LEU	C-N-CA	5.30	127.39	120.28
12	l	241	HIS	ND1-CE1-NE2	5.30	113.70	108.40
2	B	219	PRO	N-CA-CB	5.30	108.24	103.20
5	E	92	ALA	CA-C-N	5.30	127.34	120.44
5	E	92	ALA	C-N-CA	5.30	127.34	120.44
6	F	54	ASP	N-CA-CB	5.30	119.63	111.46
9	2	197	GLY	N-CA-C	-5.30	107.38	115.66
12	5	223	LEU	O-C-N	-5.30	117.43	123.48
13	6	80	VAL	N-CA-C	5.30	116.03	110.62
21	N	379	LEU	CA-C-N	5.30	127.39	120.28
21	N	379	LEU	C-N-CA	5.30	127.39	120.28
23	P	184	MET	CA-C-N	5.30	127.82	120.29
23	P	184	MET	C-N-CA	5.30	127.82	120.29
24	Q	425	GLN	O-C-N	-5.30	116.10	122.15
1	a	220	LYS	CB-CG-CD	5.30	123.50	111.30
32	M	358	ALA	CA-C-O	5.30	126.57	120.90
1	a	158	ASP	O-C-N	-5.30	114.45	121.34
6	F	117	GLN	OE1-CD-NE2	5.30	127.90	122.60
12	5	215	LEU	O-C-N	5.30	128.59	122.17
15	W	3	LEU	N-CA-CB	5.30	119.97	111.91
18	X	62	ASP	CA-CB-CG	-5.30	107.30	112.60
21	N	308	ASN	CA-C-O	5.30	126.20	120.32
24	Q	213	GLN	O-C-N	5.30	127.53	122.07
28	H	183	ILE	N-CA-CB	5.30	116.83	110.31
29	I	181	TYR	CB-CG-CD1	5.30	128.75	120.80
5	e	124	GLY	O-C-N	-5.30	118.58	122.71
14	n	127	GLU	CA-C-N	5.30	127.33	120.44
14	n	127	GLU	C-N-CA	5.30	127.33	120.44
2	B	41	ASN	O-C-N	5.30	128.09	121.84
16	V	135	ARG	N-CA-C	-5.30	105.26	112.26
16	V	298	ALA	N-CA-CB	5.30	117.69	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	179	THR	CA-CB-OG1	5.30	117.55	109.60
24	Q	425	GLN	CG-CD-NE2	-5.30	108.45	116.40
27	O	286	PHE	CA-CB-CG	-5.30	108.50	113.80
12	l	191	ASP	CA-C-N	5.30	129.57	120.72
12	l	191	ASP	C-N-CA	5.30	129.57	120.72
19	Y	44	ALA	CA-C-N	5.30	131.31	121.62
19	Y	44	ALA	C-N-CA	5.30	131.31	121.62
14	n	138	SER	O-C-N	-5.30	115.15	122.46
29	I	371	LEU	CA-C-N	5.30	128.29	120.82
29	I	371	LEU	C-N-CA	5.30	128.29	120.82
33	J	288	ILE	N-CA-C	-5.30	99.33	106.85
5	e	99	HIS	CA-CB-CG	5.29	119.09	113.80
14	n	111	ASN	N-CA-C	-5.29	102.11	108.25
22	S	246	GLU	CA-C-N	5.29	128.98	120.30
22	S	246	GLU	C-N-CA	5.29	128.98	120.30
1	A	45	VAL	N-CA-CB	5.29	121.33	112.44
1	A	178	ILE	CA-C-N	5.29	127.37	120.28
1	A	178	ILE	C-N-CA	5.29	127.37	120.28
16	V	135	ARG	CA-C-N	5.29	128.36	120.95
16	V	135	ARG	C-N-CA	5.29	128.36	120.95
21	N	379	LEU	CA-C-O	-5.29	114.94	120.55
25	R	338	TYR	N-CA-CB	5.29	118.00	110.16
30	K	65	GLU	CA-C-O	5.29	126.16	120.55
31	L	72	ASP	N-CA-C	-5.29	106.78	113.18
32	M	241	ALA	CA-C-O	-5.29	115.77	121.38
1	a	140	ILE	N-CA-CB	5.29	117.34	110.99
7	g	213	GLU	CB-CG-CD	-5.29	103.60	112.60
12	l	113	ASN	OD1-CG-ND2	5.29	127.89	122.60
13	6	90	LYS	N-CA-C	-5.29	102.65	110.48
13	6	97	ALA	CA-C-O	-5.29	114.94	120.55
21	N	70	TYR	CB-CG-CD2	5.29	128.74	120.80
27	O	322	ASP	CA-CB-CG	-5.29	107.31	112.60
29	I	128	TYR	CA-C-N	5.29	130.20	122.85
29	I	128	TYR	C-N-CA	5.29	130.20	122.85
30	K	228	ASN	OD1-CG-ND2	5.29	127.89	122.60
13	m	35	THR	O-C-N	-5.29	115.84	122.35
13	m	109	ARG	NE-CZ-NH2	-5.29	114.44	119.20
7	G	14	VAL	O-C-N	5.29	128.98	122.95
7	G	22	PHE	CA-C-O	-5.29	115.45	121.00
8	1	144	TYR	N-CA-C	5.29	117.05	111.28
21	N	196	THR	N-CA-C	-5.29	107.48	114.04
10	3	10	GLY	N-CA-C	-5.29	104.79	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	227	MET	N-CA-CB	5.29	119.61	111.46
22	S	50	PRO	CA-C-N	5.29	127.62	120.38
22	S	50	PRO	C-N-CA	5.29	127.62	120.38
22	S	65	ASN	CA-CB-CG	-5.29	107.31	112.60
24	Q	80	HIS	N-CA-C	-5.29	106.51	113.17
29	I	420	LYS	N-CA-CB	-5.29	102.35	110.12
31	L	409	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
33	J	375	ILE	N-CA-CB	5.29	116.38	110.51
21	N	409	GLY	CA-C-N	5.29	127.36	120.28
21	N	409	GLY	C-N-CA	5.29	127.36	120.28
27	O	173	SER	N-CA-C	5.29	117.12	111.36
31	L	97	ALA	N-CA-C	-5.29	105.60	111.36
32	M	53	HIS	CA-C-N	5.29	127.36	120.28
32	M	53	HIS	C-N-CA	5.29	127.36	120.28
1	a	51	THR	OG1-CB-CG2	-5.28	98.73	109.30
3	c	214	ALA	N-CA-C	-5.28	101.04	109.23
17	T	59	LYS	O-C-N	5.28	128.17	122.15
25	R	156	LYS	N-CA-C	-5.28	105.69	111.82
25	R	285	ALA	O-C-N	5.28	128.17	122.15
25	R	363	PHE	O-C-N	5.28	127.72	122.12
27	O	128	LEU	O-C-N	5.28	127.72	122.12
27	O	361	ASP	CA-CB-CG	5.28	117.88	112.60
13	6	123	ASP	N-CA-CB	5.28	117.67	110.38
24	Q	238	TYR	CA-CB-CG	-5.28	104.39	113.90
32	M	324	LEU	CA-C-O	-5.28	115.02	121.36
4	d	156	TYR	N-CA-CB	5.28	120.56	111.00
3	C	31	HIS	N-CA-C	-5.28	104.27	111.56
3	C	70	ASN	N-CA-C	-5.28	101.27	108.24
21	N	762	ARG	CA-CB-CG	5.28	124.66	114.10
24	Q	343	LEU	O-C-N	5.28	127.79	122.09
28	H	251	PRO	CA-C-O	-5.28	112.90	120.56
2	b	240	SER	O-C-N	-5.28	116.52	122.12
7	G	147	HIS	CA-CB-CG	5.28	119.08	113.80
15	W	37	PHE	CA-C-N	5.28	127.79	120.29
15	W	37	PHE	C-N-CA	5.28	127.79	120.29
16	V	279	HIS	N-CA-C	-5.28	105.61	111.36
21	N	70	TYR	CB-CG-CD1	-5.28	112.88	120.80
10	j	29	LEU	N-CA-C	-5.28	100.58	109.07
3	C	216	ILE	CA-C-O	5.28	125.95	120.36
8	1	83	SER	N-CA-C	-5.28	102.65	110.46
12	5	210	PHE	CA-C-N	5.28	128.33	120.31
12	5	210	PHE	C-N-CA	5.28	128.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	257	GLU	N-CA-CB	-5.28	101.63	110.39
19	Y	78	LYS	N-CA-C	5.28	117.03	111.28
22	S	292	TYR	N-CA-C	5.28	117.78	111.71
23	P	214	GLU	CA-C-N	5.28	128.33	120.31
23	P	214	GLU	C-N-CA	5.28	128.33	120.31
25	R	74	ASN	CA-CB-CG	5.28	117.88	112.60
26	U	106	ILE	CA-C-N	5.28	127.88	120.28
26	U	106	ILE	C-N-CA	5.28	127.88	120.28
28	H	307	PHE	CA-C-O	-5.28	114.68	120.70
29	I	356	SER	CA-C-O	-5.28	114.83	120.42
29	I	415	ASP	CA-C-N	5.28	127.35	120.28
29	I	415	ASP	C-N-CA	5.28	127.35	120.28
29	I	432	LEU	CA-C-N	5.28	131.23	122.73
29	I	432	LEU	C-N-CA	5.28	131.23	122.73
30	K	202	GLY	CA-C-N	5.28	127.57	120.50
30	K	202	GLY	C-N-CA	5.28	127.57	120.50
5	e	74	ILE	N-CA-CB	5.28	118.11	111.46
12	l	227	ASP	N-CA-C	-5.28	106.35	112.89
11	4	146	HIS	CG-CD2-NE2	5.28	112.48	107.20
20	Z	237	VAL	CA-C-N	5.28	128.73	120.82
20	Z	237	VAL	C-N-CA	5.28	128.73	120.82
20	Z	728	LYS	CG-CD-CE	5.28	123.44	111.30
21	N	169	ALA	O-C-N	-5.28	116.39	122.09
25	R	371	PHE	N-CA-C	5.28	118.18	111.69
28	H	229	LEU	N-CA-CB	5.28	118.12	110.26
30	K	37	ASN	CA-CB-CG	5.28	117.88	112.60
4	d	167	ASN	CA-C-O	-5.27	116.15	122.27
2	B	164	ILE	N-CA-C	-5.27	100.27	108.44
16	V	38	LEU	CA-C-O	-5.27	115.28	120.82
27	O	285	SER	CA-C-O	5.27	126.36	120.82
32	M	16	ASP	N-CA-CB	5.27	118.44	110.42
2	b	248	GLU	N-CA-C	-5.27	105.61	111.36
10	3	71	THR	O-C-N	5.27	128.16	122.15
23	P	115	ARG	NE-CZ-NH1	5.27	126.77	121.50
23	P	273	TYR	N-CA-CB	5.27	119.40	110.49
25	R	200	LYS	N-CA-CB	5.27	117.96	110.16
28	H	342	GLY	CA-C-N	5.27	127.87	120.28
28	H	342	GLY	C-N-CA	5.27	127.87	120.28
14	n	147	ILE	CA-C-N	5.27	130.11	123.10
14	n	147	ILE	C-N-CA	5.27	130.11	123.10
4	D	111	ARG	N-CA-CB	5.27	117.87	110.12
5	E	16	SER	CA-C-N	5.27	125.35	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	16	SER	C-N-CA	5.27	125.35	119.87
28	H	71	GLU	N-CA-CB	5.27	119.40	110.49
33	J	336	ASN	N-CA-CB	5.27	120.67	111.13
3	c	108	VAL	O-C-N	-5.27	116.40	121.83
7	G	81	LEU	N-CA-CB	5.27	118.02	110.06
21	N	811	LYS	CB-CG-CD	5.27	123.42	111.30
25	R	49	PHE	CB-CA-C	-5.27	102.04	110.79
27	O	176	SER	N-CA-C	5.27	117.11	111.36
28	H	432	ARG	NE-CZ-NH1	-5.27	116.23	121.50
3	c	107	PRO	CA-C-O	-5.27	115.36	121.95
6	f	3	ARG	CA-C-N	5.27	131.18	121.70
6	f	3	ARG	C-N-CA	5.27	131.18	121.70
6	f	52	ASN	N-CA-C	-5.27	101.07	109.23
8	h	28	ARG	N-CA-CB	5.27	118.76	110.23
8	h	33	ALA	N-CA-C	-5.27	105.83	113.21
1	A	12	TYR	N-CA-CB	5.27	118.54	110.95
15	W	111	VAL	CA-C-O	5.27	125.92	120.39
17	T	149	ASP	N-CA-C	-5.27	105.54	111.28
18	X	111	LEU	O-C-N	5.27	129.68	122.41
20	Z	857	LEU	N-CA-C	-5.27	106.90	113.38
21	N	35	LEU	N-CA-C	-5.27	105.31	112.26
21	N	445	GLY	O-C-N	-5.27	116.28	122.34
33	J	222	TYR	CA-C-N	5.27	127.30	120.56
33	J	222	TYR	C-N-CA	5.27	127.30	120.56
6	f	178	THR	CA-C-O	-5.27	115.28	120.70
21	N	906	ARG	NE-CZ-NH2	-5.27	114.46	119.20
30	K	180	GLN	O-C-N	-5.27	115.19	122.46
11	k	111	LYS	N-CA-C	-5.26	107.88	114.56
4	D	17	ILE	CA-C-N	5.26	127.86	120.28
4	D	17	ILE	C-N-CA	5.26	127.86	120.28
16	V	51	GLY	CA-C-O	-5.26	116.50	121.87
18	X	55	LYS	CA-C-N	5.26	125.27	119.90
18	X	55	LYS	C-N-CA	5.26	125.27	119.90
21	N	469	VAL	N-CA-CB	5.26	117.70	110.54
28	H	366	LEU	CA-C-O	-5.26	114.84	120.42
2	b	182	GLU	CB-CG-CD	-5.26	103.65	112.60
6	f	113	CYS	N-CA-CB	5.26	117.95	110.16
8	h	65	ALA	CA-C-N	5.26	127.76	120.29
8	h	65	ALA	C-N-CA	5.26	127.76	120.29
7	G	226	GLY	CA-C-O	5.26	124.89	119.00
9	2	231	SER	N-CA-C	-5.26	101.12	109.96
13	6	186	GLU	N-CA-C	5.26	117.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	434	TYR	CB-CG-CD1	5.26	128.69	120.80
30	K	161	MET	CG-SD-CE	-5.26	89.32	100.90
32	M	33	ARG	O-C-N	-5.26	116.65	122.07
1	a	211	ILE	CA-C-O	-5.26	115.59	121.17
2	b	168	SER	N-CA-C	5.26	116.70	111.07
4	d	89	ALA	O-C-N	5.26	127.49	122.07
13	m	28	PHE	N-CA-C	-5.26	101.12	108.96
28	H	105	ILE	CB-CA-C	-5.26	105.61	111.35
32	M	310	ASN	CA-CB-CG	-5.26	107.34	112.60
5	e	213	ASP	CA-C-O	-5.26	115.79	121.36
7	g	92	GLY	O-C-N	5.26	127.27	122.17
11	k	38	LEU	O-C-N	5.26	129.07	122.23
9	2	106	VAL	N-CA-C	5.26	115.98	110.62
16	V	100	ARG	N-CA-C	-5.26	106.09	112.88
19	Y	55	THR	N-CA-CB	5.26	117.94	110.16
20	Z	361	HIS	CA-C-N	5.26	127.85	120.28
20	Z	361	HIS	C-N-CA	5.26	127.85	120.28
28	H	359	ASN	CA-CB-CG	-5.26	107.34	112.60
28	H	465	GLN	N-CA-C	-5.26	104.30	111.56
4	d	217	PRO	CA-C-N	5.26	130.41	122.68
4	d	217	PRO	C-N-CA	5.26	130.41	122.68
4	d	233	VAL	CA-CB-CG1	5.26	119.34	110.40
12	5	233	LYS	CA-C-O	-5.26	114.40	120.24
21	N	306	ASN	N-CA-C	-5.26	106.45	112.92
21	N	768	ILE	CA-C-O	-5.26	115.36	119.20
24	Q	40	ALA	N-CA-C	5.26	118.88	111.52
28	H	392	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
8	h	133	TYR	N-CA-C	-5.26	101.08	109.07
12	5	136	SER	CA-C-N	5.26	127.75	120.29
12	5	136	SER	C-N-CA	5.26	127.75	120.29
14	7	39	VAL	CA-C-O	-5.26	114.91	120.48
15	W	12	ASN	N-CA-CB	5.26	119.02	110.77
20	Z	196	SER	CA-C-N	5.26	127.32	120.28
20	Z	196	SER	C-N-CA	5.26	127.32	120.28
23	P	401	ASN	CA-CB-CG	5.26	117.86	112.60
25	R	47	ALA	N-CA-CB	5.26	117.85	110.12
26	U	130	VAL	CA-C-O	5.26	125.56	119.36
27	O	323	ASN	CA-C-N	5.26	127.88	120.42
27	O	323	ASN	C-N-CA	5.26	127.88	120.42
31	L	255	TYR	N-CA-C	5.26	116.88	110.41
4	d	215	VAL	N-CA-C	5.25	115.47	108.11
4	D	169	LYS	CA-C-O	5.25	126.12	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	52	ASN	N-CA-C	-5.25	101.42	109.41
13	6	50	LYS	N-CA-C	-5.25	106.87	113.28
21	N	614	ASN	O-C-N	-5.25	117.23	123.22
24	Q	219	ASP	N-CA-CB	-5.25	102.40	110.12
1	a	46	ARG	NE-CZ-NH2	5.25	123.93	119.20
7	g	153	PRO	CA-C-N	5.25	128.30	120.31
7	g	153	PRO	C-N-CA	5.25	128.30	120.31
14	n	74	ARG	N-CA-C	-5.25	106.55	113.12
14	7	127	GLU	CA-C-N	5.25	128.09	120.79
14	7	127	GLU	C-N-CA	5.25	128.09	120.79
17	T	241	GLU	CA-C-N	5.25	127.32	120.28
17	T	241	GLU	C-N-CA	5.25	127.32	120.28
18	X	16	GLU	N-CA-C	5.25	117.70	110.35
21	N	811	LYS	O-C-N	5.25	127.69	122.12
25	R	254	SER	CA-C-N	5.25	127.38	120.60
25	R	254	SER	C-N-CA	5.25	127.38	120.60
3	c	199	LYS	O-C-N	5.25	129.06	122.23
16	V	146	SER	O-C-N	5.25	128.64	122.34
21	N	584	ARG	CA-C-N	5.25	127.32	120.28
21	N	584	ARG	C-N-CA	5.25	127.32	120.28
24	Q	336	ASN	N-CA-CB	5.25	117.93	110.16
24	Q	430	ALA	CA-C-N	5.25	129.49	120.72
24	Q	430	ALA	C-N-CA	5.25	129.49	120.72
10	3	153	LEU	CA-C-O	-5.25	113.93	119.97
7	g	165	THR	O-C-N	-5.25	117.75	123.26
11	k	79	ALA	N-CA-C	-5.25	105.23	111.69
14	n	253	ASP	CA-CB-CG	5.25	117.85	112.60
4	D	162	GLN	CA-CB-CG	5.25	124.60	114.10
8	1	47	HIS	CA-CB-CG	5.25	119.05	113.80
14	7	68	ARG	N-CA-C	5.25	116.69	111.07
21	N	895	LYS	CA-C-O	-5.25	115.40	121.49
26	U	60	GLU	N-CA-C	-5.25	107.25	113.97
28	H	242	PRO	N-CA-C	-5.25	104.30	110.70
30	K	50	LYS	CB-CA-C	-5.25	102.61	110.90
1	a	176	GLN	CA-C-N	5.25	127.31	120.28
1	a	176	GLN	C-N-CA	5.25	127.31	120.28
2	b	188	ALA	O-C-N	5.25	127.68	122.12
3	c	75	VAL	CA-C-N	5.25	130.47	122.65
3	c	75	VAL	C-N-CA	5.25	130.47	122.65
12	l	185	PRO	N-CA-CB	5.25	107.98	103.31
23	P	17	LEU	CA-C-N	5.25	131.00	121.92
23	P	17	LEU	C-N-CA	5.25	131.00	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	406	LYS	CA-C-N	5.25	129.74	120.87
23	P	406	LYS	C-N-CA	5.25	129.74	120.87
24	Q	178	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
26	U	132	LEU	CA-C-O	-5.25	115.10	120.87
2	b	182	GLU	N-CA-CB	5.25	119.96	110.83
10	3	14	ALA	O-C-N	-5.25	116.87	123.27
17	T	168	SER	N-CA-C	-5.25	106.11	112.88
18	X	19	GLU	CA-C-N	5.25	128.28	120.31
18	X	19	GLU	C-N-CA	5.25	128.28	120.31
29	I	280	PHE	CA-CB-CG	-5.25	108.56	113.80
33	J	221	LYS	CB-CA-C	-5.25	101.33	110.09
4	d	210	ILE	N-CA-C	-5.24	100.77	108.11
13	m	24	ALA	CA-C-N	5.24	128.02	121.83
13	m	24	ALA	C-N-CA	5.24	128.02	121.83
13	m	103	HIS	ND1-CE1-NE2	5.24	113.64	108.40
21	N	395	ALA	CA-C-N	5.24	127.31	120.28
21	N	395	ALA	C-N-CA	5.24	127.31	120.28
21	N	914	VAL	O-C-N	-5.24	117.52	123.03
22	S	47	THR	CA-CB-CG2	5.24	119.42	110.50
23	P	16	ILE	O-C-N	-5.24	116.78	121.87
23	P	263	HIS	CA-C-O	-5.24	114.86	120.42
33	J	212	ARG	CD-NE-CZ	-5.24	117.06	124.40
8	1	180	GLY	N-CA-C	-5.24	100.76	113.18
14	7	38	ILE	CB-CG1-CD1	5.24	124.81	113.80
14	7	55	ILE	N-CA-C	-5.24	100.93	108.53
27	O	318	HIS	CG-CD2-NE2	5.24	112.44	107.20
30	K	80	LYS	CA-C-O	-5.24	114.99	120.55
6	f	165	SER	N-CA-C	-5.24	106.66	113.16
7	g	141	VAL	N-CA-C	-5.24	100.65	108.46
17	T	247	ASP	CB-CA-C	-5.24	101.94	110.85
21	N	87	ASP	CA-CB-CG	-5.24	107.36	112.60
21	N	177	ASP	CA-CB-CG	5.24	117.84	112.60
33	J	160	ILE	CA-C-O	-5.24	113.24	119.58
7	g	122	ALA	N-CA-C	-5.24	105.74	111.82
8	h	58	ALA	CA-C-N	5.24	127.25	120.44
8	h	58	ALA	C-N-CA	5.24	127.25	120.44
6	F	216	VAL	N-CA-C	-5.24	100.93	108.42
13	6	185	VAL	CA-C-N	5.24	127.30	120.28
13	6	185	VAL	C-N-CA	5.24	127.30	120.28
13	6	213	LEU	N-CA-CB	5.24	119.12	110.69
16	V	42	ARG	NE-CZ-NH2	5.24	123.92	119.20
17	T	169	GLN	N-CA-C	-5.24	106.04	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	274	GLU	CA-C-O	-5.24	114.94	120.55
15	W	87	MET	CG-SD-CE	-5.24	89.38	100.90
16	V	240	ALA	O-C-N	5.24	127.46	122.07
6	f	148	GLN	CA-C-O	5.24	125.82	120.64
6	f	189	LEU	CA-C-N	5.24	127.26	120.56
6	f	189	LEU	C-N-CA	5.24	127.26	120.56
5	E	95	ALA	CB-CA-C	-5.24	102.10	110.79
9	2	64	HIS	ND1-CE1-NE2	5.24	113.64	108.40
21	N	747	HIS	CG-CD2-NE2	5.24	112.44	107.20
22	S	283	GLN	CA-C-N	5.24	129.99	122.35
22	S	283	GLN	C-N-CA	5.24	129.99	122.35
33	J	274	GLU	O-C-N	5.24	128.50	122.17
4	d	139	ASP	CA-C-O	-5.23	115.47	120.97
21	N	745	LEU	CA-C-O	-5.23	116.22	122.13
2	b	24	ALA	O-C-N	5.23	128.71	122.27
11	k	138	PHE	CA-C-O	-5.23	113.95	119.97
9	2	187	ALA	N-CA-C	5.23	117.06	111.36
10	3	86	THR	O-C-N	5.23	128.71	122.27
17	T	130	ASP	CA-CB-CG	5.23	117.83	112.60
19	Y	48	THR	N-CA-CB	5.23	119.13	111.54
20	Z	29	ASP	CA-C-N	5.23	127.24	120.44
20	Z	29	ASP	C-N-CA	5.23	127.24	120.44
23	P	110	LEU	N-CA-CB	5.23	117.73	110.04
24	Q	156	ALA	CA-C-O	-5.23	115.00	120.55
28	H	218	ILE	O-C-N	-5.23	115.89	121.80
1	a	240	ASN	CA-CB-CG	-5.23	107.37	112.60
2	b	117	ILE	N-CA-C	-5.23	105.61	110.53
10	3	103	TYR	CA-C-N	-5.23	115.40	123.14
10	3	103	TYR	C-N-CA	-5.23	115.40	123.14
24	Q	70	ALA	CB-CA-C	-5.23	101.74	109.90
26	U	252	HIS	CB-CG-CD2	-5.23	124.40	131.20
29	I	354	ASP	CA-CB-CG	5.23	117.83	112.60
9	i	133	ASP	N-CA-C	-5.23	103.42	108.07
4	D	112	TYR	N-CA-CB	5.23	117.65	110.07
11	4	170	LYS	CG-CD-CE	5.23	123.33	111.30
28	H	137	ASP	CA-C-N	5.23	131.53	121.54
28	H	137	ASP	C-N-CA	5.23	131.53	121.54
33	J	276	LEU	CA-C-N	5.23	127.81	120.28
33	J	276	LEU	C-N-CA	5.23	127.81	120.28
1	A	41	ASN	N-CA-CB	5.23	119.92	110.83
11	4	168	LEU	CA-C-N	5.23	127.60	120.54
11	4	168	LEU	C-N-CA	5.23	127.60	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	172	SER	CA-C-O	-5.23	114.69	119.76
15	W	56	GLY	CA-C-O	-5.23	118.82	122.22
21	N	301	THR	N-CA-C	-5.23	105.58	111.28
13	m	78	ASN	OD1-CG-ND2	5.23	127.83	122.60
11	4	40	PRO	CA-C-O	-5.23	111.00	118.89
32	M	196	ALA	CA-C-N	-5.23	117.80	123.08
32	M	196	ALA	C-N-CA	-5.23	117.80	123.08
3	c	204	SER	CB-CA-C	-5.22	102.65	110.90
8	1	170	GLN	N-CA-C	-5.22	105.76	111.82
22	S	246	GLU	CB-CA-C	-5.22	104.51	111.88
22	S	278	LYS	CB-CA-C	-5.22	102.68	110.88
30	K	188	VAL	O-C-N	5.22	125.82	121.85
13	m	116	HIS	CB-CG-CD2	-5.22	124.41	131.20
20	Z	727	GLU	CA-C-O	-5.22	115.45	121.19
23	P	118	VAL	CA-C-N	5.22	127.62	120.46
23	P	118	VAL	C-N-CA	5.22	127.62	120.46
24	Q	252	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
28	H	264	ALA	N-CA-CB	5.22	118.38	110.28
26	U	33	CYS	N-CA-C	-5.22	99.15	108.13
29	I	95	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	b	204	PHE	CA-CB-CG	-5.22	108.58	113.80
3	c	129	ARG	N-CA-CB	-5.22	102.49	110.11
5	E	97	VAL	CA-CB-CG2	-5.22	101.53	110.40
18	X	55	LYS	CA-C-O	5.22	124.13	119.59
24	Q	47	ASP	N-CA-CB	5.22	119.31	110.49
28	H	391	ILE	N-CA-C	-5.22	104.99	112.35
31	L	162	GLU	CA-C-N	5.22	130.78	122.74
31	L	162	GLU	C-N-CA	5.22	130.78	122.74
33	J	112	ARG	CB-CA-C	5.22	118.35	109.84
9	2	78	ALA	CA-C-N	5.22	127.22	120.44
9	2	78	ALA	C-N-CA	5.22	127.22	120.44
11	4	93	ARG	N-CA-C	-5.22	105.58	112.94
11	4	129	PRO	N-CA-C	-5.22	107.22	114.27
15	W	30	ILE	CB-CA-C	-5.22	105.29	111.97
20	Z	247	GLN	CA-C-N	5.22	127.27	120.28
20	Z	247	GLN	C-N-CA	5.22	127.27	120.28
20	Z	524	ALA	CA-C-N	5.22	129.03	120.63
20	Z	524	ALA	C-N-CA	5.22	129.03	120.63
23	P	266	TYR	CB-CG-CD2	-5.22	112.97	120.80
29	I	216	PRO	CB-CA-C	-5.22	104.73	111.46
5	e	189	SER	N-CA-C	-5.22	106.50	112.92
4	D	18	PHE	CA-CB-CG	-5.22	108.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	37	SER	O-C-N	-5.22	117.21	123.31
20	Z	252	CYS	CA-C-N	5.22	124.50	120.33
20	Z	252	CYS	C-N-CA	5.22	124.50	120.33
28	H	404	TRP	CA-C-N	5.22	128.24	120.31
28	H	404	TRP	C-N-CA	5.22	128.24	120.31
32	M	344	ASP	N-CA-C	-5.22	106.98	113.55
1	a	144	VAL	N-CA-CB	5.21	119.13	111.52
5	e	71	ASP	N-CA-C	-5.21	100.99	108.60
6	f	223	THR	N-CA-CB	5.21	120.57	111.13
4	D	135	ILE	O-C-N	5.21	128.73	123.20
5	E	26	TYR	CB-CG-CD2	5.21	128.62	120.80
6	F	45	VAL	N-CA-CB	5.21	120.00	111.45
8	1	65	ALA	O-C-N	-5.21	116.70	122.07
10	3	177	ARG	CD-NE-CZ	-5.21	117.10	124.40
12	5	112	ILE	N-CA-C	-5.21	105.52	110.42
29	I	142	GLU	CA-C-O	-5.21	113.90	119.22
11	k	98	TYR	N-CA-C	-5.21	99.92	108.41
1	A	62	LYS	CA-C-O	5.21	125.45	119.35
4	D	220	ASP	CA-CB-CG	5.21	117.81	112.60
12	5	181	ARG	CA-CB-CG	5.21	124.52	114.10
17	T	94	HIS	ND1-CE1-NE2	5.21	113.61	108.40
26	U	20	ASP	CA-C-N	5.21	129.54	120.68
26	U	20	ASP	C-N-CA	5.21	129.54	120.68
11	4	33	ASP	N-CA-C	-5.21	103.81	110.53
22	S	200	GLU	N-CA-C	-5.21	100.54	109.24
25	R	93	LYS	CA-C-O	5.21	127.96	120.51
5	e	111	SER	CA-C-N	5.21	127.26	120.28
5	e	111	SER	C-N-CA	5.21	127.26	120.28
12	l	228	ALA	N-CA-CB	5.21	117.87	110.16
9	2	49	SER	N-CA-C	-5.21	99.47	108.69
16	V	220	GLN	OE1-CD-NE2	-5.21	117.39	122.60
23	P	91	LEU	CB-CA-C	-5.21	102.04	110.79
29	I	310	LEU	N-CA-CB	5.21	117.87	110.16
31	L	299	ARG	CD-NE-CZ	-5.21	117.11	124.40
2	b	58	SER	N-CA-C	-5.21	105.80	113.61
1	A	203	VAL	N-CA-CB	5.21	117.62	110.54
4	D	121	THR	CA-C-O	-5.21	114.90	120.42
26	U	271	ASP	CA-C-N	5.21	129.53	120.68
26	U	271	ASP	C-N-CA	5.21	129.53	120.68
28	H	188	PRO	CA-C-N	5.21	125.21	119.90
28	H	188	PRO	C-N-CA	5.21	125.21	119.90
30	K	223	VAL	O-C-N	5.21	128.71	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	369	ALA	CA-C-N	5.21	129.48	120.58
33	J	369	ALA	C-N-CA	5.21	129.48	120.58
9	i	235	PRO	CA-C-N	5.21	128.16	120.82
9	i	235	PRO	C-N-CA	5.21	128.16	120.82
10	3	48	HIS	CA-CB-CG	5.21	119.00	113.80
24	Q	424	ASP	CA-C-N	5.21	127.68	120.29
24	Q	424	ASP	C-N-CA	5.21	127.68	120.29
3	c	56	LEU	O-C-N	5.20	128.99	122.22
4	d	5	ASP	CA-CB-CG	-5.20	107.40	112.60
5	e	21	LEU	N-CA-C	-5.20	99.28	108.23
6	f	113	CYS	CA-C-O	-5.20	114.91	120.42
9	i	250	CYS	CA-C-N	5.20	128.10	120.71
9	i	250	CYS	C-N-CA	5.20	128.10	120.71
23	P	432	LEU	CA-C-N	5.20	127.81	120.42
23	P	432	LEU	C-N-CA	5.20	127.81	120.42
24	Q	158	ILE	CA-C-N	5.20	127.25	120.28
24	Q	158	ILE	C-N-CA	5.20	127.25	120.28
31	L	361	PHE	CA-C-N	5.20	127.77	120.28
31	L	361	PHE	C-N-CA	5.20	127.77	120.28
32	M	359	GLN	CA-C-N	5.20	127.59	120.46
32	M	359	GLN	C-N-CA	5.20	127.59	120.46
12	5	207	GLY	CA-C-N	5.20	127.77	120.28
12	5	207	GLY	C-N-CA	5.20	127.77	120.28
20	Z	729	GLU	CB-CA-C	-5.20	100.07	110.42
23	P	31	ASP	CA-C-N	5.20	127.68	120.29
23	P	31	ASP	C-N-CA	5.20	127.68	120.29
14	n	215	ARG	NE-CZ-NH2	5.20	123.88	119.20
16	V	287	THR	CA-C-N	5.20	127.51	120.44
16	V	287	THR	C-N-CA	5.20	127.51	120.44
17	T	138	ASP	N-CA-C	5.20	121.88	110.80
19	Y	57	THR	N-CA-C	-5.20	100.12	108.55
20	Z	257	PRO	CA-C-N	5.20	125.74	120.38
20	Z	257	PRO	C-N-CA	5.20	125.74	120.38
21	N	264	SER	CA-C-O	5.20	126.06	120.70
23	P	400	VAL	CB-CA-C	5.20	118.33	110.63
27	O	20	PRO	N-CA-C	-5.20	107.63	114.03
27	O	71	ASP	CA-CB-CG	5.20	117.80	112.60
27	O	255	LEU	CA-C-N	5.20	127.67	120.29
27	O	255	LEU	C-N-CA	5.20	127.67	120.29
4	d	180	ASP	N-CA-C	-5.20	99.49	108.69
6	F	38	LEU	N-CA-CB	5.20	119.47	111.46
14	7	135	GLN	N-CA-C	-5.20	105.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	222	ALA	N-CA-CB	5.20	117.52	109.98
21	N	686	ILE	CA-C-O	-5.20	115.34	120.85
22	S	237	ILE	CA-C-N	5.20	127.25	120.28
22	S	237	ILE	C-N-CA	5.20	127.25	120.28
33	J	310	ILE	CA-C-N	5.20	131.47	121.54
33	J	310	ILE	C-N-CA	5.20	131.47	121.54
7	g	20	ARG	CA-C-O	-5.20	115.09	120.70
28	H	263	VAL	O-C-N	-5.20	115.24	122.05
2	b	64	VAL	N-CA-C	-5.20	99.68	107.37
7	g	91	ARG	NE-CZ-NH2	5.20	123.88	119.20
12	l	262	TYR	O-C-N	5.20	129.23	122.89
20	Z	793	PHE	CA-CB-CG	-5.20	108.61	113.80
21	N	444	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
28	H	59	ILE	CA-C-N	5.20	127.67	120.29
28	H	59	ILE	C-N-CA	5.20	127.67	120.29
30	K	119	VAL	N-CA-CB	5.20	117.22	110.99
31	L	293	GLU	N-CA-C	-5.20	105.28	113.02
32	M	35	LYS	O-C-N	-5.20	115.88	122.27
13	m	35	THR	N-CA-CB	5.19	118.44	110.70
10	j	90	LEU	CB-CA-C	-5.19	102.73	110.88
11	k	188	GLY	O-C-N	5.19	127.78	122.85
12	l	137	GLN	O-C-N	-5.19	116.23	122.15
14	n	116	ALA	O-C-N	-5.19	115.68	122.59
4	D	172	ARG	CA-CB-CG	-5.19	103.72	114.10
6	F	48	ALA	CA-C-O	5.19	126.83	120.60
8	1	18	LYS	O-C-N	-5.19	116.62	122.12
21	N	672	ASN	N-CA-C	-5.19	98.33	109.81
23	P	203	ILE	N-CA-CB	5.19	117.73	110.56
25	R	141	TYR	CA-C-N	5.19	127.24	120.28
25	R	141	TYR	C-N-CA	5.19	127.24	120.28
27	O	284	GLU	CA-C-N	5.19	127.19	120.44
27	O	284	GLU	C-N-CA	5.19	127.19	120.44
27	O	349	THR	CA-CB-OG1	5.19	117.39	109.60
6	f	81	ALA	CA-C-N	5.19	127.23	120.28
6	f	81	ALA	C-N-CA	5.19	127.23	120.28
13	m	15	ASP	CA-CB-CG	5.19	117.79	112.60
8	1	143	ILE	O-C-N	-5.19	116.08	122.57
13	6	169	GLU	CA-C-N	5.19	126.33	119.84
13	6	169	GLU	C-N-CA	5.19	126.33	119.84
21	N	740	TRP	CA-C-O	5.19	125.36	119.18
24	Q	150	GLN	N-CA-C	-5.19	100.06	108.52
32	M	189	GLN	CA-C-O	-5.19	114.92	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	201	LEU	N-CA-C	5.19	116.94	111.28
32	M	231	LEU	N-CA-C	5.19	116.62	111.07
2	b	69	PRO	CA-C-N	5.19	130.38	122.23
2	b	69	PRO	C-N-CA	5.19	130.38	122.23
5	e	200	VAL	CA-C-N	5.19	127.23	120.28
5	e	200	VAL	C-N-CA	5.19	127.23	120.28
8	h	127	SER	CB-CA-C	-5.19	100.97	110.62
9	i	151	GLY	O-C-N	5.19	129.44	122.70
6	F	11	VAL	N-CA-C	-5.19	108.07	113.10
16	V	126	GLN	CA-CB-CG	5.19	124.47	114.10
18	X	26	PRO	N-CA-CB	5.19	107.86	103.19
21	N	92	ASP	CA-CB-CG	-5.19	107.41	112.60
21	N	752	SER	O-C-N	5.19	128.06	122.15
22	S	329	GLU	CB-CG-CD	-5.19	103.78	112.60
22	S	358	LYS	N-CA-C	5.19	116.94	111.28
27	O	103	LYS	CA-C-N	5.19	127.23	120.28
27	O	103	LYS	C-N-CA	5.19	127.23	120.28
28	H	80	HIS	CB-CG-CD2	-5.19	124.46	131.20
33	J	390	MET	CA-C-O	-5.19	114.92	120.42
13	m	185	VAL	CB-CA-C	5.19	119.14	112.14
1	A	33	LYS	CA-C-O	-5.19	113.36	119.48
13	6	42	SER	CA-C-N	5.19	129.72	122.93
13	6	42	SER	C-N-CA	5.19	129.72	122.93
13	6	221	ARG	NE-CZ-NH1	5.19	126.69	121.50
31	L	111	GLU	N-CA-CB	5.19	117.62	109.69
12	l	128	GLN	N-CA-CB	5.18	117.74	110.12
4	D	175	LEU	N-CA-C	5.18	116.62	111.07
13	6	218	ASP	CA-C-O	-5.18	113.28	119.35
14	7	74	ARG	NE-CZ-NH2	-5.18	114.53	119.20
15	W	127	ARG	N-CA-CB	5.18	117.53	110.01
21	N	428	VAL	CA-CB-CG1	-5.18	101.59	110.40
25	R	258	LEU	N-CA-C	5.18	117.33	111.11
29	I	63	GLU	CA-C-N	5.18	127.49	120.44
29	I	63	GLU	C-N-CA	5.18	127.49	120.44
30	K	241	GLU	O-C-N	5.18	128.28	122.27
32	M	391	LEU	N-CA-C	-5.18	106.46	112.89
2	b	67	LEU	CA-C-O	5.18	126.10	120.55
4	d	16	HIS	N-CA-CB	5.18	118.48	110.60
5	e	18	GLU	CA-C-O	5.18	125.70	119.59
11	k	193	ASP	N-CA-CB	5.18	118.17	110.29
6	F	82	ARG	O-C-N	-5.18	116.63	122.12
12	5	199	GLY	N-CA-C	-5.18	103.67	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	385	PHE	CA-C-N	5.18	128.66	120.47
20	Z	385	PHE	C-N-CA	5.18	128.66	120.47
21	N	559	TYR	N-CA-C	-5.18	106.54	112.92
22	S	214	MET	CA-C-N	5.18	129.49	120.68
22	S	214	MET	C-N-CA	5.18	129.49	120.68
24	Q	186	HIS	CG-CD2-NE2	5.18	112.38	107.20
27	O	302	VAL	CA-CB-CG2	5.18	119.21	110.40
29	I	157	VAL	CA-C-O	-5.18	112.95	119.48
33	J	157	ILE	CA-C-O	-5.18	115.36	120.85
2	b	222	LEU	O-C-N	-5.18	115.50	122.23
23	P	41	VAL	CA-C-O	-5.18	115.56	120.95
27	O	157	LEU	CB-CA-C	-5.18	102.75	110.88
28	H	198	MET	CA-C-N	5.18	128.19	120.31
28	H	198	MET	C-N-CA	5.18	128.19	120.31
1	a	168	ALA	N-CA-C	-5.18	100.86	108.99
5	e	109	VAL	CB-CA-C	-5.18	105.23	112.02
11	k	194	ASP	CA-CB-CG	5.18	117.78	112.60
13	m	193	ARG	O-C-N	5.18	127.61	122.12
21	N	910	PRO	N-CA-C	-5.18	107.44	114.80
22	S	187	ILE	CA-C-N	5.18	127.17	120.44
22	S	187	ILE	C-N-CA	5.18	127.17	120.44
28	H	94	GLU	N-CA-C	-5.18	106.64	113.17
2	b	159	TRP	CD2-CE2-CZ2	-5.18	117.22	122.40
2	b	242	GLU	O-C-N	5.18	128.05	122.15
5	E	224	LYS	CA-C-N	5.18	127.47	120.38
5	E	224	LYS	C-N-CA	5.18	127.47	120.38
11	4	135	TYR	CA-CB-CG	-5.18	104.58	113.90
13	6	217	LYS	CA-CB-CG	5.18	124.45	114.10
21	N	666	GLN	CA-CB-CG	5.18	124.45	114.10
21	N	715	ILE	O-C-N	5.18	128.78	123.03
21	N	869	ASP	CA-C-N	5.18	128.82	121.42
21	N	869	ASP	C-N-CA	5.18	128.82	121.42
23	P	93	ILE	CA-CB-CG1	5.18	119.20	110.40
30	K	156	SER	N-CA-CB	5.18	117.76	110.36
7	g	109	ILE	CB-CA-C	-5.17	108.86	114.35
6	F	186	PRO	CA-C-N	5.17	127.21	120.28
6	F	186	PRO	C-N-CA	5.17	127.21	120.28
21	N	571	LEU	CA-C-N	5.17	127.48	120.44
21	N	571	LEU	C-N-CA	5.17	127.48	120.44
22	S	251	SER	N-CA-C	-5.17	105.72	111.36
33	J	157	ILE	N-CA-C	-5.17	105.49	110.72
33	J	177	LEU	O-C-N	5.17	128.05	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	165	GLU	CA-C-N	5.17	127.48	120.44
10	3	165	GLU	C-N-CA	5.17	127.48	120.44
23	P	69	ARG	NE-CZ-NH2	5.17	123.86	119.20
23	P	148	LYS	CA-C-O	5.17	126.03	120.55
1	a	204	GLU	O-C-N	5.17	127.60	122.12
5	E	112	LEU	N-CA-CB	-5.17	102.52	110.12
21	N	518	ALA	CB-CA-C	-5.17	102.06	110.85
22	S	463	GLU	CA-C-N	5.17	127.21	120.28
22	S	463	GLU	C-N-CA	5.17	127.21	120.28
27	O	297	ILE	CA-C-O	5.17	126.33	120.85
28	H	84	ILE	CA-CB-CG1	5.17	119.19	110.40
29	I	244	PHE	N-CA-C	-5.17	99.36	108.20
11	k	63	ASN	CA-C-O	-5.17	115.38	120.70
32	M	228	LYS	N-CA-C	5.17	116.60	111.07
13	m	202	ARG	NE-CZ-NH1	-5.17	116.33	121.50
17	T	235	PHE	CA-C-N	5.17	127.63	120.29
17	T	235	PHE	C-N-CA	5.17	127.63	120.29
21	N	283	ASP	N-CA-CB	5.17	118.09	109.98
21	N	406	TYR	CA-C-O	-5.17	115.07	120.55
21	N	713	VAL	CA-C-O	5.17	126.46	120.67
24	Q	175	VAL	N-CA-C	-5.17	105.35	110.62
25	R	108	SER	N-CA-C	5.17	117.33	111.02
25	R	119	LYS	CB-CA-C	-5.17	101.07	110.63
27	O	135	ARG	N-CA-CB	5.17	117.72	110.12
31	L	67	HIS	ND1-CE1-NE2	5.17	113.57	108.40
31	L	105	ILE	CB-CA-C	-5.17	103.81	110.84
5	e	13	SER	CA-C-N	5.17	128.89	121.50
5	e	13	SER	C-N-CA	5.17	128.89	121.50
9	i	244	GLU	N-CA-C	-5.17	101.56	109.41
3	C	223	GLY	N-CA-C	-5.17	108.49	115.21
4	D	43	VAL	CB-CA-C	-5.17	102.92	110.62
9	2	165	ALA	O-C-N	5.17	127.60	122.12
10	3	119	PRO	N-CD-CG	5.17	110.95	103.20
19	Y	1	MET	CB-CA-C	5.17	119.92	110.10
22	S	95	PHE	CB-CA-C	-5.17	102.07	110.85
23	P	354	SER	CA-C-N	5.17	127.63	120.29
23	P	354	SER	C-N-CA	5.17	127.63	120.29
28	H	381	ASP	CA-C-N	5.17	127.46	120.38
28	H	381	ASP	C-N-CA	5.17	127.46	120.38
33	J	18	GLY	CA-C-O	-5.17	114.62	120.30
33	J	402	LYS	CA-C-N	5.17	127.20	120.28
33	J	402	LYS	C-N-CA	5.17	127.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	254	PRO	O-C-N	5.17	129.61	122.64
23	P	60	ALA	CA-C-O	-5.17	115.08	120.55
29	I	247	ILE	O-C-N	-5.17	117.11	123.00
4	d	25	GLU	CA-C-N	5.16	127.72	120.28
4	d	25	GLU	C-N-CA	5.16	127.72	120.28
6	f	215	ILE	CA-C-N	5.16	129.67	122.23
6	f	215	ILE	C-N-CA	5.16	129.67	122.23
31	L	375	ASP	CA-CB-CG	-5.16	107.44	112.60
32	M	407	GLN	CA-C-O	-5.16	115.88	121.87
9	i	203	ASP	N-CA-CB	-5.16	102.38	110.69
6	F	168	ALA	N-CA-C	-5.16	105.28	112.45
24	Q	34	ASP	CB-CA-C	-5.16	102.07	110.85
24	Q	192	ALA	CB-CA-C	-5.16	102.74	110.90
31	L	138	SER	N-CA-C	-5.16	106.09	114.09
32	M	339	ARG	N-CA-C	-5.16	99.80	110.80
32	M	423	GLN	CB-CA-C	-5.16	100.15	110.42
1	a	145	SER	CB-CA-C	-5.16	101.05	111.17
2	b	149	GLN	N-CA-C	-5.16	100.04	108.76
3	c	103	ASN	N-CA-CB	5.16	119.92	112.13
10	j	98	ARG	N-CA-C	-5.16	100.75	108.96
9	2	170	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
11	4	190	ARG	NE-CZ-NH1	-5.16	116.34	121.50
20	Z	748	LEU	N-CA-C	-5.16	105.83	111.82
22	S	19	HIS	ND1-CE1-NE2	5.16	113.56	108.40
24	Q	313	ASP	CA-CB-CG	-5.16	107.44	112.60
28	H	206	VAL	CB-CA-C	5.16	117.86	111.15
31	L	422	VAL	N-CA-CB	5.16	117.56	110.54
7	g	191	GLU	N-CA-CB	5.16	118.95	110.39
14	n	103	LEU	CA-C-N	5.16	127.75	120.42
14	n	103	LEU	C-N-CA	5.16	127.75	120.42
15	W	30	ILE	CA-C-N	5.16	127.19	120.28
15	W	30	ILE	C-N-CA	5.16	127.19	120.28
17	T	20	TYR	N-CA-C	-5.16	107.66	114.31
17	T	161	TRP	CA-C-N	5.16	127.61	120.29
17	T	161	TRP	C-N-CA	5.16	127.61	120.29
22	S	173	LEU	N-CA-C	-5.16	103.88	110.53
24	Q	273	ASN	N-CA-CB	5.16	120.50	112.25
24	Q	306	TYR	N-CA-CB	5.16	117.55	110.07
24	Q	396	TRP	CE2-CD2-CE3	5.16	123.96	118.80
32	M	254	MET	CG-SD-CE	-5.16	89.55	100.90
7	g	8	TYR	O-C-N	5.16	127.40	121.88
13	m	111	PHE	CA-CB-CG	5.16	118.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	70	LYS	N-CA-C	5.16	116.98	111.36
29	I	268	PHE	N-CA-CB	-5.16	102.86	110.49
4	d	102	ASP	CA-CB-CG	5.16	117.76	112.60
5	e	201	LEU	O-C-N	-5.16	116.66	122.12
8	h	90	VAL	CA-C-N	5.16	127.14	120.44
8	h	90	VAL	C-N-CA	5.16	127.14	120.44
7	G	209	GLU	CA-C-O	-5.16	115.09	120.55
16	V	39	LYS	CA-C-O	5.16	126.23	120.82
17	T	88	TYR	N-CA-CB	5.16	117.70	110.12
21	N	682	PHE	CA-CB-CG	5.16	118.96	113.80
24	Q	183	LYS	CB-CA-C	-5.16	102.23	110.79
26	U	62	ASN	O-C-N	-5.16	117.28	123.31
2	B	95	THR	O-C-N	-5.15	116.76	122.07
3	C	50	ARG	NH1-CZ-NH2	5.15	126.00	119.30
6	F	152	ASN	CA-C-N	5.15	130.15	122.99
6	F	152	ASN	C-N-CA	5.15	130.15	122.99
28	H	176	VAL	CA-CB-CG2	5.15	119.16	110.40
33	J	394	GLN	CB-CG-CD	-5.15	103.84	112.60
12	l	199	GLY	CA-C-N	5.15	131.54	122.42
12	l	199	GLY	C-N-CA	5.15	131.54	122.42
15	W	169	SER	CB-CA-C	5.15	118.21	109.50
17	T	186	ARG	N-CA-C	5.15	116.58	111.07
21	N	461	GLU	CB-CA-C	-5.15	102.24	110.79
21	N	476	THR	CA-C-O	5.15	124.48	118.97
27	O	94	GLU	N-CA-C	-5.15	105.74	111.36
32	M	61	LYS	N-CA-C	-5.15	106.84	113.23
33	J	234	PHE	CB-CA-C	-5.15	102.79	110.88
1	a	166	TYR	CA-C-N	5.15	132.42	122.53
1	a	166	TYR	C-N-CA	5.15	132.42	122.53
2	b	244	ASN	CA-CB-CG	5.15	117.75	112.60
3	c	136	ILE	N-CA-C	-5.15	101.00	108.36
1	A	128	TYR	CB-CG-CD2	-5.15	113.07	120.80
1	A	175	GLN	CA-C-N	5.15	127.18	120.28
1	A	175	GLN	C-N-CA	5.15	127.18	120.28
5	E	247	GLU	N-CA-C	5.15	117.80	111.82
8	1	13	MET	O-C-N	-5.15	117.85	123.26
9	2	45	ALA	O-C-N	-5.15	117.71	123.48
16	V	248	ALA	CA-C-O	-5.15	114.05	119.97
17	T	229	VAL	N-CA-C	-5.15	100.15	107.77
21	N	241	LEU	CA-C-O	5.15	125.88	120.42
17	T	44	LEU	N-CA-CB	5.15	119.19	110.49
31	L	309	LEU	CB-CA-C	-5.15	102.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	4	ASN	CB-CG-ND2	5.15	124.12	116.40
6	f	225	TYR	CB-CG-CD1	5.15	128.52	120.80
7	g	30	ALA	CA-C-N	5.15	128.74	120.30
7	g	30	ALA	C-N-CA	5.15	128.74	120.30
12	l	102	ALA	CA-C-N	5.15	131.51	121.63
12	l	102	ALA	C-N-CA	5.15	131.51	121.63
12	5	228	ALA	N-CA-C	-5.15	105.36	111.69
13	6	27	ASP	CA-CB-CG	5.15	117.75	112.60
21	N	438	ASP	CA-C-N	5.15	127.73	120.42
21	N	438	ASP	C-N-CA	5.15	127.73	120.42
22	S	229	THR	N-CA-CB	5.15	117.78	110.16
22	S	235	ASN	N-CA-C	5.15	116.89	111.28
22	S	244	ASN	OD1-CG-ND2	-5.15	117.45	122.60
24	Q	192	ALA	CA-C-N	5.15	130.44	122.26
24	Q	192	ALA	C-N-CA	5.15	130.44	122.26
29	I	280	PHE	CB-CA-C	5.15	118.53	110.19
30	K	296	LEU	CA-C-N	5.15	127.51	120.46
30	K	296	LEU	C-N-CA	5.15	127.51	120.46
31	L	169	ASN	N-CA-C	-5.15	105.36	111.69
21	N	354	PRO	CA-C-N	5.15	127.60	120.29
21	N	354	PRO	C-N-CA	5.15	127.60	120.29
22	S	233	LEU	CA-C-N	5.15	127.51	120.46
22	S	233	LEU	C-N-CA	5.15	127.51	120.46
23	P	420	ASP	CA-CB-CG	-5.15	107.45	112.60
24	Q	178	HIS	CA-C-O	5.15	126.00	120.55
7	g	107	ILE	CA-C-N	5.14	125.05	119.85
7	g	107	ILE	C-N-CA	5.14	125.05	119.85
8	h	154	ASN	OD1-CG-ND2	-5.14	117.46	122.60
10	3	31	SER	CB-CA-C	-5.14	104.96	111.70
16	V	190	HIS	CG-CD2-NE2	5.14	112.34	107.20
24	Q	139	ILE	N-CA-C	-5.14	105.37	110.62
25	R	397	ASN	CA-CB-CG	5.14	117.74	112.60
29	I	106	ILE	N-CA-CB	5.14	116.33	110.72
32	M	393	ALA	N-CA-CB	5.14	117.93	110.47
6	f	193	GLY	N-CA-C	5.14	120.11	113.27
3	C	8	SER	CA-C-O	5.14	120.92	117.94
3	C	194	LEU	CA-C-N	5.14	127.12	120.44
3	C	194	LEU	C-N-CA	5.14	127.12	120.44
7	G	156	SER	N-CA-C	-5.14	101.02	109.40
8	1	67	ILE	N-CA-C	5.14	117.52	111.09
9	2	143	HIS	O-C-N	-5.14	115.59	122.94
10	3	114	SER	N-CA-C	-5.14	106.32	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	155	ASN	N-CA-C	-5.14	105.90	113.61
24	Q	424	ASP	CA-CB-CG	-5.14	107.46	112.60
26	U	297	GLN	CA-C-N	5.14	127.12	120.44
26	U	297	GLN	C-N-CA	5.14	127.12	120.44
30	K	203	ILE	CA-CB-CG2	5.14	119.24	110.50
3	c	182	ASP	CA-C-O	5.14	125.44	119.32
8	h	37	ASN	N-CA-C	-5.14	100.22	108.55
9	i	107	SER	N-CA-CB	5.14	117.77	110.16
14	n	109	TYR	CB-CG-CD1	5.14	128.51	120.80
25	R	30	ALA	CA-C-N	5.14	127.68	120.28
25	R	30	ALA	C-N-CA	5.14	127.68	120.28
29	I	226	GLY	N-CA-C	5.14	122.20	115.36
14	n	110	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	24	ARG	N-CA-C	-5.14	101.73	109.85
8	1	133	TYR	N-CA-C	-5.14	100.92	108.99
9	2	132	VAL	N-CA-C	-5.14	100.80	108.46
24	Q	68	MET	N-CA-CB	5.14	119.24	110.50
25	R	325	HIS	CA-C-O	-5.14	113.53	119.59
28	H	60	GLU	N-CA-C	-5.14	105.76	111.36
31	L	55	LYS	O-C-N	5.14	128.01	122.15
32	M	84	GLU	CA-C-N	5.14	129.66	122.93
32	M	84	GLU	C-N-CA	5.14	129.66	122.93
6	f	225	TYR	CB-CG-CD2	-5.14	113.09	120.80
13	6	111	PHE	CA-C-O	-5.14	113.12	120.16
2	b	60	THR	CA-C-N	5.14	130.65	122.94
2	b	60	THR	C-N-CA	5.14	130.65	122.94
11	k	7	ILE	O-C-N	-5.14	117.13	123.09
2	B	200	VAL	CA-C-N	5.14	130.94	121.85
2	B	200	VAL	C-N-CA	5.14	130.94	121.85
13	6	52	PHE	CB-CA-C	-5.14	100.31	109.71
21	N	48	ALA	CA-C-N	5.14	127.58	120.29
21	N	48	ALA	C-N-CA	5.14	127.58	120.29
23	P	194	SER	CA-C-N	5.14	127.16	120.28
23	P	194	SER	C-N-CA	5.14	127.16	120.28
23	P	375	GLN	O-C-N	5.14	128.00	122.15
24	Q	304	GLU	CB-CG-CD	-5.14	103.87	112.60
31	L	67	HIS	CA-CB-CG	-5.14	108.66	113.80
31	L	332	THR	N-CA-C	-5.14	106.42	113.30
1	a	213	ALA	CA-C-O	-5.13	115.11	120.55
8	h	101	ASN	N-CA-CB	5.13	118.77	110.40
1	A	226	GLY	O-C-N	-5.13	118.65	123.48
2	B	171	ALA	N-CA-C	5.13	117.78	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	136	GLY	N-CA-C	-5.13	101.02	110.83
12	5	181	ARG	NE-CZ-NH2	-5.13	114.58	119.20
16	V	95	LEU	CA-C-O	-5.13	112.94	119.31
29	I	152	LYS	N-CA-CB	5.13	118.21	110.30
7	g	220	SER	CA-C-N	5.13	127.16	120.28
7	g	220	SER	C-N-CA	5.13	127.16	120.28
2	B	89	SER	N-CA-CB	5.13	117.67	110.12
6	F	148	GLN	O-C-N	-5.13	118.42	121.71
9	2	203	ASP	CA-CB-CG	5.13	117.73	112.60
11	4	159	ASP	CA-C-N	5.13	127.58	120.29
11	4	159	ASP	C-N-CA	5.13	127.58	120.29
16	V	235	GLU	N-CA-C	5.13	116.88	111.28
21	N	193	ALA	CA-C-N	5.13	127.13	120.56
21	N	193	ALA	C-N-CA	5.13	127.13	120.56
25	R	357	PHE	N-CA-CB	5.13	117.76	110.16
33	J	22	TYR	N-CA-C	-5.13	105.38	111.69
33	J	383	GLU	CA-C-N	5.13	127.58	120.29
33	J	383	GLU	C-N-CA	5.13	127.58	120.29
5	e	204	LEU	CA-C-O	-5.13	115.43	120.82
13	m	229	ARG	CD-NE-CZ	5.13	131.59	124.40
14	n	213	ALA	O-C-N	5.13	128.58	122.27
4	D	199	LEU	N-CA-C	-5.13	106.28	112.54
6	F	194	VAL	CA-CB-CG2	-5.13	101.67	110.40
7	G	224	THR	CA-CB-OG1	5.13	117.30	109.60
29	I	254	GLN	CA-C-O	5.13	126.91	121.11
30	K	286	THR	CA-CB-OG1	5.13	117.30	109.60
9	2	241	VAL	N-CA-C	-5.13	100.95	108.85
11	4	27	VAL	N-CA-C	-5.13	99.87	107.51
15	W	181	LEU	O-C-N	5.13	127.36	122.03
21	N	215	MET	CA-C-N	5.13	129.40	120.68
21	N	215	MET	C-N-CA	5.13	129.40	120.68
5	e	188	HIS	ND1-CE1-NE2	5.13	113.53	108.40
14	n	98	ARG	O-C-N	5.13	128.90	122.23
15	W	17	ARG	N-CA-C	-5.13	106.61	112.92
21	N	292	GLY	CA-C-N	5.13	126.50	120.09
21	N	292	GLY	C-N-CA	5.13	126.50	120.09
25	R	25	GLU	CA-C-N	5.13	127.02	120.56
25	R	25	GLU	C-N-CA	5.13	127.02	120.56
31	L	344	ASP	CA-CB-CG	-5.13	107.47	112.60
2	B	55	LEU	N-CA-C	-5.13	106.98	113.18
3	C	213	PHE	CA-CB-CG	-5.13	108.67	113.80
6	F	206	LEU	CA-C-N	5.13	131.42	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	206	LEU	C-N-CA	5.13	131.42	122.81
10	3	42	LYS	N-CA-CB	5.13	118.02	110.33
11	4	73	TYR	N-CA-C	-5.13	100.73	108.52
12	5	228	ALA	CA-C-N	5.13	128.10	120.31
12	5	228	ALA	C-N-CA	5.13	128.10	120.31
17	T	78	PHE	CA-C-N	5.13	127.15	120.28
17	T	78	PHE	C-N-CA	5.13	127.15	120.28
21	N	33	ASP	N-CA-CB	5.13	119.01	110.91
21	N	140	MET	N-CA-CB	5.13	117.75	110.16
30	K	163	GLU	N-CA-C	-5.13	105.09	113.19
2	b	63	LYS	CA-C-N	5.12	130.08	123.11
2	b	63	LYS	C-N-CA	5.12	130.08	123.11
14	n	102	ASP	CA-CB-CG	5.12	117.72	112.60
9	2	95	HIS	CA-CB-CG	5.12	118.92	113.80
20	Z	747	ALA	CB-CA-C	-5.12	102.83	110.88
14	n	54	ILE	N-CA-C	-5.12	100.94	108.11
9	2	46	ASP	CA-C-N	5.12	130.68	121.66
9	2	46	ASP	C-N-CA	5.12	130.68	121.66
11	4	35	THR	CB-CA-C	5.12	120.93	109.56
15	W	150	ASN	N-CA-C	-5.12	99.89	110.80
16	V	195	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
21	N	77	SER	N-CA-C	5.12	118.79	112.54
2	b	119	GLN	CA-C-O	-5.12	114.99	120.42
6	f	35	THR	N-CA-CB	5.12	120.40	111.13
5	E	80	GLY	N-CA-C	-5.12	101.04	113.18
28	H	186	PRO	CA-C-O	-5.12	115.52	122.08
30	K	217	THR	N-CA-C	5.12	119.40	113.20
33	J	95	ILE	CA-C-N	-5.12	115.10	121.96
33	J	95	ILE	C-N-CA	-5.12	115.10	121.96
1	a	221	ASN	N-CA-C	-5.12	106.28	112.88
4	d	70	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	209	HIS	N-CA-C	-5.12	105.78	111.36
16	V	234	GLU	CA-C-N	5.12	127.14	120.28
16	V	234	GLU	C-N-CA	5.12	127.14	120.28
23	P	374	SER	CA-C-O	5.12	126.20	120.82
26	U	20	ASP	CA-CB-CG	5.12	117.72	112.60
28	H	331	ARG	CA-C-O	5.12	125.98	120.55
1	a	124	LEU	CA-C-O	5.12	125.97	120.70
6	f	146	GLU	CB-CG-CD	-5.12	103.90	112.60
9	i	142	ILE	CA-CB-CG2	5.12	119.20	110.50
2	B	120	GLU	N-CA-CB	5.12	118.89	110.39
4	D	209	ASN	OD1-CG-ND2	5.12	127.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	239	ALA	CB-CA-C	-5.12	101.16	110.63
21	N	491	GLY	O-C-N	-5.12	116.86	122.65
21	N	565	ASN	CA-C-N	5.12	127.45	120.54
21	N	565	ASN	C-N-CA	5.12	127.45	120.54
21	N	624	ALA	CA-C-O	-5.12	115.12	120.55
25	R	395	ASN	CA-CB-CG	5.12	117.72	112.60
33	J	367	MET	CA-C-N	5.12	127.56	120.29
33	J	367	MET	C-N-CA	5.12	127.56	120.29
4	D	120	TYR	N-CA-CB	5.12	117.73	110.16
28	H	288	ALA	CA-C-O	-5.12	115.00	120.42
11	4	147	HIS	CA-C-O	5.12	124.98	119.15
16	V	159	ILE	CA-C-N	5.12	128.47	120.75
16	V	159	ILE	C-N-CA	5.12	128.47	120.75
19	Y	83	ARG	N-CA-C	5.12	116.86	111.28
21	N	737	SER	N-CA-C	-5.12	106.82	113.16
26	U	102	SER	CA-C-N	5.12	129.26	120.72
26	U	102	SER	C-N-CA	5.12	129.26	120.72
27	O	87	LYS	CA-CB-CG	-5.12	103.87	114.10
28	H	111	GLU	CA-C-N	5.12	129.88	122.36
28	H	111	GLU	C-N-CA	5.12	129.88	122.36
33	J	368	TYR	CB-CA-C	-5.12	102.15	110.85
6	f	204	GLU	CA-C-O	-5.11	115.98	121.45
8	h	161	VAL	O-C-N	5.11	126.92	121.91
4	D	116	VAL	CA-C-N	5.11	127.09	120.44
4	D	116	VAL	C-N-CA	5.11	127.09	120.44
9	2	157	GLY	O-C-N	5.11	130.47	122.70
21	N	149	GLU	CA-C-N	5.11	131.57	122.06
21	N	149	GLU	C-N-CA	5.11	131.57	122.06
21	N	259	PHE	N-CA-CB	5.11	117.73	110.16
22	S	86	SER	O-C-N	5.11	127.54	122.12
25	R	85	SER	CA-C-N	5.11	130.98	122.54
25	R	85	SER	C-N-CA	5.11	130.98	122.54
26	U	251	ASN	CA-CB-CG	-5.11	107.49	112.60
27	O	99	LEU	N-CA-C	5.11	116.54	111.07
3	c	31	HIS	CG-CD2-NE2	5.11	112.31	107.20
21	N	152	LEU	CA-C-N	5.11	127.13	120.28
21	N	152	LEU	C-N-CA	5.11	127.13	120.28
21	N	319	SER	CA-C-O	-5.11	115.00	120.42
23	P	345	VAL	CA-C-O	5.11	126.27	120.85
24	Q	428	GLU	CA-C-N	5.11	127.13	120.28
24	Q	428	GLU	C-N-CA	5.11	127.13	120.28
25	R	112	GLU	CA-C-N	5.11	127.55	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	112	GLU	C-N-CA	5.11	127.55	120.29
6	f	125	GLY	CA-C-O	-5.11	116.07	122.61
6	F	143	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
15	W	166	GLU	O-C-N	5.11	129.42	122.37
19	Y	59	ILE	O-C-N	5.11	128.96	122.57
21	N	719	ASN	CB-CG-ND2	-5.11	108.73	116.40
23	P	282	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
24	Q	51	ARG	N-CA-C	5.11	115.56	108.00
26	U	286	ILE	CA-C-N	5.11	127.13	120.28
26	U	286	ILE	C-N-CA	5.11	127.13	120.28
1	a	209	HIS	CA-CB-CG	-5.11	108.69	113.80
4	D	132	SER	N-CA-C	-5.11	101.36	109.59
27	O	267	ASP	CA-C-O	5.11	125.97	120.55
28	H	358	PRO	N-CA-C	-5.11	108.14	114.68
31	L	140	LEU	N-CA-C	-5.11	100.18	108.41
1	a	32	PHE	O-C-N	5.11	129.51	122.46
6	f	67	ASP	CA-C-N	5.11	131.13	122.65
6	f	67	ASP	C-N-CA	5.11	131.13	122.65
10	3	118	LYS	CA-C-N	5.11	124.87	119.76
10	3	118	LYS	C-N-CA	5.11	124.87	119.76
16	V	119	SER	N-CA-C	-5.11	103.66	110.55
20	Z	727	GLU	N-CA-C	5.11	117.64	110.23
22	S	480	ARG	CD-NE-CZ	-5.11	117.25	124.40
26	U	289	ASP	CA-C-N	5.11	127.38	120.38
26	U	289	ASP	C-N-CA	5.11	127.38	120.38
27	O	252	PHE	CA-CB-CG	5.11	118.91	113.80
30	K	286	THR	CA-C-N	5.11	126.71	120.22
30	K	286	THR	C-N-CA	5.11	126.71	120.22
31	L	397	GLU	CA-C-O	5.11	125.64	119.31
3	c	227	GLN	N-CA-CB	5.11	118.59	110.16
12	l	196	ARG	CG-CD-NE	-5.11	100.77	112.00
3	C	152	ASN	N-CA-CB	5.11	116.19	109.55
7	G	207	ASN	OD1-CG-ND2	-5.11	117.49	122.60
21	N	677	ASP	N-CA-C	5.11	116.65	111.14
22	S	302	HIS	CB-CG-ND1	5.11	130.36	122.70
30	K	344	ARG	CD-NE-CZ	-5.11	117.25	124.40
23	P	20	GLU	CA-C-N	5.10	126.47	120.09
23	P	20	GLU	C-N-CA	5.10	126.47	120.09
26	U	11	ALA	N-CA-CB	5.10	116.21	110.03
30	K	233	ALA	O-C-N	-5.10	116.66	122.89
2	b	188	ALA	CA-C-O	-5.10	115.14	120.55
12	l	114	PRO	CA-C-O	-5.10	111.19	118.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	248	GLY	O-C-N	5.10	129.33	122.70
1	A	184	ASN	N-CA-CB	5.10	118.19	110.28
12	5	266	HIS	ND1-CE1-NE2	5.10	113.50	108.40
27	O	349	THR	CA-C-N	5.10	130.66	122.50
27	O	349	THR	C-N-CA	5.10	130.66	122.50
28	H	218	ILE	CB-CA-C	-5.10	104.00	112.26
30	K	43	VAL	N-CA-C	-5.10	105.57	110.72
32	M	415	PHE	CA-C-O	-5.10	115.14	120.55
14	n	249	ASN	CA-CB-CG	-5.10	107.50	112.60
32	M	353	SER	CA-CB-OG	5.10	121.30	111.10
2	b	194	LEU	CA-C-N	5.10	127.07	120.44
2	b	194	LEU	C-N-CA	5.10	127.07	120.44
12	l	251	ASN	N-CA-C	-5.10	99.10	108.02
4	D	184	PRO	CA-C-N	5.10	125.01	119.76
4	D	184	PRO	C-N-CA	5.10	125.01	119.76
8	1	54	ARG	CA-C-O	-5.10	114.80	120.66
5	E	195	GLU	CA-C-N	5.10	127.11	120.28
5	E	195	GLU	C-N-CA	5.10	127.11	120.28
24	Q	138	SER	O-C-N	5.10	127.96	122.15
25	R	166	ALA	CA-C-N	5.10	127.11	120.28
25	R	166	ALA	C-N-CA	5.10	127.11	120.28
2	b	178	ARG	N-CA-C	5.10	119.55	113.23
3	C	175	LEU	CA-C-N	5.10	127.11	120.28
3	C	175	LEU	C-N-CA	5.10	127.11	120.28
28	H	182	ASN	N-CA-C	-5.10	99.94	110.80
5	e	242	GLU	N-CA-CB	5.09	117.61	110.12
14	7	223	ARG	O-C-N	-5.09	115.89	122.77
15	W	106	GLN	CA-C-O	-5.09	115.58	121.19
16	V	96	LYS	CA-C-O	5.09	125.82	120.42
26	U	5	HIS	N-CA-CB	5.09	120.35	111.13
26	U	123	VAL	N-CA-C	-5.09	99.92	107.51
28	H	284	VAL	O-C-N	-5.09	116.92	122.83
8	h	86	THR	CB-CA-C	-5.09	102.19	110.85
1	A	216	THR	CA-C-O	5.09	126.11	120.71
10	3	44	PHE	CA-CB-CG	5.09	118.89	113.80
11	4	31	SER	CA-C-N	5.09	130.69	122.29
11	4	31	SER	C-N-CA	5.09	130.69	122.29
15	W	105	VAL	CA-C-N	5.09	127.94	120.71
15	W	105	VAL	C-N-CA	5.09	127.94	120.71
20	Z	351	PRO	CA-C-N	5.09	127.52	120.29
20	Z	351	PRO	C-N-CA	5.09	127.52	120.29
22	S	293	ILE	CB-CG1-CD1	5.09	124.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	93	ASP	N-CA-CB	5.09	118.00	110.56
32	M	193	LEU	CA-C-N	5.09	127.44	120.46
32	M	193	LEU	C-N-CA	5.09	127.44	120.46
7	g	150	MET	CA-C-N	5.09	130.17	122.99
7	g	150	MET	C-N-CA	5.09	130.17	122.99
10	j	68	ARG	NE-CZ-NH2	-5.09	114.62	119.20
11	4	172	MET	CA-C-N	5.09	124.75	119.56
11	4	172	MET	C-N-CA	5.09	124.75	119.56
14	7	80	ASP	O-C-N	-5.09	116.68	122.23
16	V	186	GLN	N-CA-CB	5.09	119.09	110.49
17	T	86	LYS	N-CA-C	5.09	120.49	113.77
17	T	122	PHE	CA-C-O	5.09	125.95	120.55
22	S	113	SER	N-CA-CB	5.09	119.23	110.68
23	P	189	LEU	N-CA-C	-5.09	105.81	111.36
23	P	300	VAL	CA-C-N	5.09	127.61	120.28
23	P	300	VAL	C-N-CA	5.09	127.61	120.28
28	H	56	LEU	O-C-N	5.09	127.52	122.12
30	K	114	THR	N-CA-C	-5.09	107.12	113.38
31	L	178	ILE	N-CA-C	5.09	119.93	109.34
22	S	238	LEU	N-CA-C	5.09	116.83	111.28
24	Q	322	GLU	CA-C-N	5.09	129.22	120.72
24	Q	322	GLU	C-N-CA	5.09	129.22	120.72
28	H	118	ASP	CA-CB-CG	-5.09	107.51	112.60
29	I	266	GLN	CB-CA-C	-5.09	102.34	110.79
29	I	391	ASP	N-CA-C	-5.09	105.92	111.82
14	n	73	GLU	N-CA-CB	5.09	117.55	109.51
27	O	49	PHE	CA-C-N	5.09	127.52	120.29
27	O	49	PHE	C-N-CA	5.09	127.52	120.29
3	c	11	THR	CA-C-N	5.09	128.92	121.80
3	c	11	THR	C-N-CA	5.09	128.92	121.80
3	c	88	ILE	CA-C-N	5.09	127.36	120.44
3	c	88	ILE	C-N-CA	5.09	127.36	120.44
13	m	149	ALA	N-CA-C	5.09	116.83	111.28
2	B	99	ARG	CD-NE-CZ	-5.09	117.28	124.40
25	R	121	GLU	CA-C-N	5.09	127.05	120.44
25	R	121	GLU	C-N-CA	5.09	127.05	120.44
26	U	252	HIS	CG-CD2-NE2	5.09	112.29	107.20
29	I	208	TYR	CA-CB-CG	-5.09	104.74	113.90
30	K	394	ALA	CA-C-O	-5.09	114.12	119.97
32	M	226	THR	N-CA-C	-5.09	105.77	112.94
10	3	106	GLY	N-CA-C	-5.08	101.97	112.34
11	4	68	SER	N-CA-CB	5.08	117.69	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	106	GLU	N-CA-CB	5.08	117.44	110.07
24	Q	69	GLY	N-CA-C	-5.08	101.13	113.18
25	R	392	ARG	CA-C-N	5.08	124.99	119.85
25	R	392	ARG	C-N-CA	5.08	124.99	119.85
5	e	33	LEU	O-C-N	5.08	127.31	122.07
5	e	90	GLU	CA-C-N	5.08	127.05	120.44
5	e	90	GLU	C-N-CA	5.08	127.05	120.44
5	e	196	ALA	CA-C-O	-5.08	115.03	120.42
5	e	215	ASN	CA-CB-CG	-5.08	107.52	112.60
14	n	37	PRO	N-CA-C	5.08	119.29	111.21
18	X	9	LYS	O-C-N	5.08	129.84	123.23
20	Z	247	GLN	CA-C-O	-5.08	114.36	120.10
22	S	215	MET	CA-C-N	5.08	127.51	120.29
22	S	215	MET	C-N-CA	5.08	127.51	120.29
23	P	272	PRO	O-C-N	5.08	128.86	123.01
29	I	391	ASP	N-CA-CB	5.08	118.16	110.28
32	M	282	GLU	N-CA-CB	5.08	119.08	110.49
32	M	328	ASN	OD1-CG-ND2	5.08	127.68	122.60
3	c	152	ASN	O-C-N	-5.08	115.84	121.53
10	j	108	VAL	N-CA-CB	5.08	118.94	111.52
11	k	175	ASP	CA-CB-CG	5.08	117.68	112.60
4	D	149	GLN	CA-CB-CG	5.08	124.26	114.10
5	E	182	GLU	CA-C-O	-5.08	115.16	120.55
6	F	224	ILE	CA-C-N	5.08	130.30	122.93
6	F	224	ILE	C-N-CA	5.08	130.30	122.93
18	X	30	GLN	CA-C-O	-5.08	115.69	121.58
20	Z	735	GLU	N-CA-C	5.08	117.55	111.71
24	Q	315	ASN	CA-C-N	5.08	127.51	120.29
24	Q	315	ASN	C-N-CA	5.08	127.51	120.29
26	U	97	PRO	N-CD-CG	5.08	109.90	103.80
30	K	58	TYR	N-CA-C	-5.08	106.77	113.17
8	1	53	CYS	CA-C-N	-5.08	114.50	122.73
8	1	53	CYS	C-N-CA	-5.08	114.50	122.73
22	S	428	ARG	NE-CZ-NH2	5.08	123.77	119.20
33	J	246	PHE	O-C-N	5.08	128.83	122.63
5	e	132	ARG	N-CA-CB	5.08	117.53	109.71
6	f	199	GLN	OE1-CD-NE2	5.08	127.68	122.60
3	C	131	PHE	N-CA-C	-5.08	101.99	110.17
7	G	66	LYS	CB-CA-C	-5.08	101.61	110.09
7	G	183	HIS	CA-C-O	-5.08	115.26	121.00
12	5	172	MET	CA-C-N	5.08	131.37	121.41
12	5	172	MET	C-N-CA	5.08	131.37	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	134	ASP	CA-C-N	5.08	125.76	120.12
13	6	134	ASP	C-N-CA	5.08	125.76	120.12
20	Z	752	ILE	CA-C-N	5.08	126.49	120.14
20	Z	752	ILE	C-N-CA	5.08	126.49	120.14
21	N	699	ALA	CB-CA-C	-5.08	102.36	110.79
22	S	400	LYS	CB-CG-CD	5.08	122.98	111.30
23	P	216	LEU	CA-C-N	5.08	127.09	120.28
23	P	216	LEU	C-N-CA	5.08	127.09	120.28
26	U	53	ALA	N-CA-CB	5.08	117.48	110.17
1	a	16	ILE	CB-CA-C	-5.08	105.29	112.14
13	6	149	ALA	N-CA-C	5.08	116.81	111.28
17	T	28	PRO	CA-C-O	-5.08	113.20	120.56
19	Y	17	THR	CA-C-N	5.08	127.04	120.44
19	Y	17	THR	C-N-CA	5.08	127.04	120.44
21	N	357	GLY	N-CA-C	5.08	120.30	114.16
22	S	227	ASN	CA-CB-CG	-5.08	107.52	112.60
22	S	391	GLY	CA-C-O	5.08	125.89	120.30
3	c	176	LEU	CA-C-N	5.08	130.02	121.14
3	c	176	LEU	C-N-CA	5.08	130.02	121.14
3	c	217	ARG	O-C-N	5.08	129.31	123.17
1	A	72	ILE	N-CA-CB	5.08	116.25	110.72
2	B	150	VAL	CA-C-O	5.08	125.40	120.27
21	N	55	PHE	N-CA-CB	5.08	119.76	111.08
22	S	302	HIS	CG-CD2-NE2	5.08	112.28	107.20
25	R	47	ALA	CB-CA-C	-5.08	102.37	110.79
25	R	331	ARG	O-C-N	5.08	127.30	122.07
28	H	119	ASN	N-CA-CB	5.08	117.82	109.95
1	a	181	ASN	CA-C-N	5.07	127.49	120.29
1	a	181	ASN	C-N-CA	5.07	127.49	120.29
9	i	166	VAL	N-CA-C	-5.07	105.59	110.72
3	C	225	VAL	N-CA-CB	5.07	118.41	111.41
8	1	121	THR	CB-CA-C	5.07	117.90	109.53
10	3	183	TRP	N-CA-CB	5.07	118.70	110.43
14	7	39	VAL	O-C-N	5.07	128.51	123.18
22	S	22	GLU	CA-C-O	5.07	125.80	120.42
32	M	211	GLY	O-C-N	5.07	128.61	122.32
33	J	133	LEU	CA-C-N	5.07	127.41	120.46
33	J	133	LEU	C-N-CA	5.07	127.41	120.46
33	J	259	GLU	N-CA-C	-5.07	105.75	111.28
2	b	22	ASP	N-CA-CB	5.07	117.58	110.12
3	c	131	PHE	CA-CB-CG	-5.07	108.73	113.80
31	L	305	LEU	CA-C-N	5.07	127.49	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	305	LEU	C-N-CA	5.07	127.49	120.29
4	d	203	VAL	CA-C-N	5.07	131.22	121.54
4	d	203	VAL	C-N-CA	5.07	131.22	121.54
6	f	23	GLU	CA-C-N	5.07	129.19	120.72
6	f	23	GLU	C-N-CA	5.07	129.19	120.72
8	h	100	ASP	N-CA-C	-5.07	100.00	110.80
1	A	82	VAL	N-CA-C	-5.07	101.18	108.48
5	E	72	ARG	NE-CZ-NH2	5.07	123.76	119.20
13	6	10	PHE	CA-CB-CG	5.07	118.87	113.80
26	U	178	VAL	O-C-N	5.07	127.27	122.20
30	K	328	LEU	O-C-N	-5.07	115.52	122.46
32	M	232	ALA	N-CA-C	5.07	116.49	111.07
33	J	388	LYS	CA-C-N	5.07	127.62	120.42
33	J	388	LYS	C-N-CA	5.07	127.62	120.42
7	g	234	ASP	CA-C-N	5.07	127.07	120.28
7	g	234	ASP	C-N-CA	5.07	127.07	120.28
5	E	202	LYS	CB-CA-C	-5.07	102.38	110.79
23	P	297	GLU	CB-CA-C	-5.07	102.89	110.90
23	P	359	ARG	NE-CZ-NH1	5.07	126.57	121.50
24	Q	195	LYS	N-CA-CB	5.07	117.66	110.16
7	g	16	SER	O-C-N	-5.07	115.49	121.32
9	i	99	THR	CA-C-N	5.07	129.75	122.40
9	i	99	THR	C-N-CA	5.07	129.75	122.40
13	m	43	ILE	CA-C-N	5.07	127.33	120.44
13	m	43	ILE	C-N-CA	5.07	127.33	120.44
4	D	127	ARG	CD-NE-CZ	-5.07	117.31	124.40
5	E	169	ALA	CB-CA-C	-5.07	101.56	109.72
8	1	29	THR	N-CA-C	-5.07	100.03	108.34
10	3	176	ASP	N-CA-CB	5.07	118.14	110.28
11	4	41	HIS	CA-C-O	-5.07	115.21	119.97
15	W	66	THR	N-CA-C	-5.07	101.37	109.07
21	N	462	VAL	N-CA-C	-5.07	104.65	111.44
21	N	901	GLY	CA-C-N	5.07	128.65	121.66
21	N	901	GLY	C-N-CA	5.07	128.65	121.66
22	S	185	PHE	CA-CB-CG	-5.07	108.73	113.80
22	S	230	LYS	O-C-N	5.07	127.29	122.07
28	H	52	THR	N-CA-CB	5.07	117.57	110.12
31	L	383	SER	N-CA-CB	5.07	118.44	110.23
4	D	201	GLU	CB-CA-C	-5.07	102.38	110.79
7	G	111	ALA	N-CA-C	5.07	116.49	111.07
10	3	175	ALA	N-CA-C	5.07	116.88	111.36
11	4	145	ASP	O-C-N	-5.07	116.85	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	476	ASP	CA-C-N	5.07	127.48	120.29
20	Z	476	ASP	C-N-CA	5.07	127.48	120.29
21	N	517	LEU	CA-C-N	5.07	127.48	120.29
21	N	517	LEU	C-N-CA	5.07	127.48	120.29
25	R	178	GLY	O-C-N	-5.07	116.11	122.70
29	I	64	ARG	N-CA-CB	5.07	117.41	110.07
33	J	106	ASP	N-CA-C	-5.07	107.27	113.50
8	h	45	ARG	CB-CA-C	-5.06	101.98	110.29
10	3	31	SER	CA-C-N	5.06	131.21	121.54
10	3	31	SER	C-N-CA	5.06	131.21	121.54
21	N	492	THR	N-CA-C	5.06	116.49	111.07
21	N	754	THR	CA-C-O	-5.06	115.11	119.72
23	P	210	ASN	OD1-CG-ND2	5.06	127.66	122.60
5	e	166	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
8	h	10	THR	CA-CB-OG1	5.06	117.19	109.60
10	3	71	THR	CA-CB-OG1	5.06	117.19	109.60
17	T	31	LYS	CB-CG-CD	5.06	122.94	111.30
22	S	416	GLU	CA-C-N	5.06	127.06	120.28
22	S	416	GLU	C-N-CA	5.06	127.06	120.28
29	I	168	VAL	CA-C-N	5.06	127.06	120.28
29	I	168	VAL	C-N-CA	5.06	127.06	120.28
2	b	163	ALA	O-C-N	-5.06	117.48	123.25
3	C	244	ILE	O-C-N	5.06	127.33	122.07
21	N	710	GLY	N-CA-C	-5.06	107.29	115.08
1	a	53	VAL	N-CA-C	-5.06	100.78	108.17
6	f	210	ASN	CA-C-O	-5.06	115.49	120.70
10	j	41	GLU	O-C-N	-5.06	117.08	122.85
12	l	266	HIS	N-CA-C	-5.06	100.04	108.34
1	A	63	LEU	N-CA-C	-5.06	106.61	112.89
1	A	229	THR	CA-CB-CG2	-5.06	101.90	110.50
6	F	201	LEU	N-CA-C	5.06	117.23	110.35
10	3	131	ASP	O-C-N	5.06	130.65	122.96
13	6	195	SER	N-CA-CB	5.06	117.56	110.12
14	7	208	GLU	CA-C-O	-5.06	114.15	119.97
16	V	124	ASN	OD1-CG-ND2	-5.06	117.54	122.60
20	Z	298	PHE	CA-C-N	5.06	127.06	120.28
20	Z	298	PHE	C-N-CA	5.06	127.06	120.28
22	S	99	ASN	N-CA-C	-5.06	100.35	108.55
27	O	131	SER	CA-C-N	5.06	128.00	120.31
27	O	131	SER	C-N-CA	5.06	128.00	120.31
30	K	327	ALA	N-CA-C	-5.06	105.42	112.45
12	l	245	TYR	N-CA-C	-5.06	105.83	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	169	THR	CA-C-O	5.06	127.11	121.40
3	C	67	TYR	N-CA-C	-5.06	100.79	109.24
15	W	65	PHE	CA-CB-CG	-5.06	108.74	113.80
22	S	291	GLU	CA-C-N	5.06	127.56	120.28
22	S	291	GLU	C-N-CA	5.06	127.56	120.28
26	U	288	PHE	O-C-N	5.06	127.28	122.07
2	B	87	ASP	CA-C-O	5.06	125.91	120.55
7	G	95	GLU	O-C-N	-5.06	116.39	122.15
16	V	71	MET	CA-C-N	5.06	124.97	119.76
16	V	71	MET	C-N-CA	5.06	124.97	119.76
21	N	854	GLU	CA-C-N	5.05	132.68	123.13
21	N	854	GLU	C-N-CA	5.05	132.68	123.13
22	S	434	ALA	N-CA-C	5.05	116.36	109.18
23	P	191	GLY	CA-C-O	5.05	124.62	118.86
26	U	258	SER	N-CA-C	-5.05	105.77	111.28
31	L	278	ILE	N-CA-CB	5.05	117.83	111.46
32	M	334	ASP	CA-C-O	-5.05	115.22	120.88
2	b	139	HIS	CA-C-N	-5.05	114.08	122.11
2	b	139	HIS	C-N-CA	-5.05	114.08	122.11
3	c	48	ALA	N-CA-C	-5.05	101.61	109.24
25	R	268	SER	CB-CA-C	-5.05	100.97	110.67
6	f	218	LYS	CA-C-O	5.05	125.78	120.42
6	F	224	ILE	CA-CB-CG1	-5.05	101.81	110.40
10	3	26	ASP	N-CA-C	-5.05	103.04	110.52
12	5	253	TYR	CB-CG-CD2	-5.05	113.22	120.80
22	S	183	LEU	CA-C-N	5.05	127.99	120.31
22	S	183	LEU	C-N-CA	5.05	127.99	120.31
22	S	298	ARG	CA-C-N	5.05	127.46	120.29
22	S	298	ARG	C-N-CA	5.05	127.46	120.29
26	U	191	THR	CA-C-N	5.05	127.99	120.31
26	U	191	THR	C-N-CA	5.05	127.99	120.31
29	I	184	ILE	CA-C-N	5.05	124.77	119.92
29	I	184	ILE	C-N-CA	5.05	124.77	119.92
5	e	144	ILE	O-C-N	5.05	129.01	123.10
9	i	114	GLN	CB-CG-CD	-5.05	104.02	112.60
1	A	93	ALA	CA-C-O	5.05	125.90	120.55
17	T	100	ASP	CA-C-O	5.05	125.90	120.55
17	T	170	ASN	CA-CB-CG	-5.05	107.55	112.60
26	U	54	LEU	CA-C-N	5.05	125.20	119.90
26	U	54	LEU	C-N-CA	5.05	125.20	119.90
30	K	66	ASP	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	200	GLN	OE1-CD-NE2	5.05	127.65	122.60
9	i	198	SER	CA-C-N	5.05	130.30	121.97
9	i	198	SER	C-N-CA	5.05	130.30	121.97
14	n	101	LYS	N-CA-C	-5.05	105.86	111.36
8	h	31	THR	N-CA-C	-5.05	100.19	108.41
6	F	4	ASN	O-C-N	-5.05	114.92	123.00
9	2	200	SER	N-CA-C	5.05	115.98	108.31
15	W	92	GLN	OE1-CD-NE2	5.05	127.65	122.60
20	Z	809	MET	CA-C-N	5.05	127.46	120.29
20	Z	809	MET	C-N-CA	5.05	127.46	120.29
21	N	143	LYS	CA-C-N	5.05	127.04	120.28
21	N	143	LYS	C-N-CA	5.05	127.04	120.28
23	P	239	GLN	CB-CA-C	-5.05	102.41	110.79
5	E	105	GLU	CA-C-N	5.04	128.37	120.75
5	E	105	GLU	C-N-CA	5.04	128.37	120.75
23	P	75	LEU	N-CA-C	5.04	116.78	111.28
1	a	92	ASN	CA-C-N	5.04	127.04	120.28
1	a	92	ASN	C-N-CA	5.04	127.04	120.28
9	i	153	TYR	CB-CG-CD2	-5.04	113.24	120.80
10	j	137	ILE	CB-CA-C	-5.04	102.73	110.50
12	l	164	GLN	CA-C-N	5.04	130.85	122.73
12	l	164	GLN	C-N-CA	5.04	130.85	122.73
3	C	183	ASP	N-CA-C	-5.04	105.49	111.69
8	1	129	HIS	CG-CD2-NE2	5.04	112.24	107.20
14	7	258	ILE	O-C-N	5.04	129.08	122.47
17	T	101	LYS	N-CA-CB	5.04	117.53	110.12
28	H	50	LYS	CA-C-N	5.04	127.04	120.28
28	H	50	LYS	C-N-CA	5.04	127.04	120.28
29	I	302	ILE	CA-C-N	5.04	127.30	120.44
29	I	302	ILE	C-N-CA	5.04	127.30	120.44
25	R	147	LYS	CA-C-N	5.04	127.03	120.28
25	R	147	LYS	C-N-CA	5.04	127.03	120.28
28	H	213	GLY	O-C-N	-5.04	117.29	122.68
32	M	228	LYS	CA-C-N	5.04	127.04	120.28
32	M	228	LYS	C-N-CA	5.04	127.04	120.28
32	M	415	PHE	CB-CA-C	-5.04	102.42	110.79
11	k	140	THR	O-C-N	-5.04	116.15	122.35
13	m	172	THR	N-CA-C	-5.04	108.16	114.56
3	C	231	LYS	CG-CD-CE	5.04	122.89	111.30
21	N	190	LEU	N-CA-CB	5.04	117.62	110.16
25	R	371	PHE	CA-CB-CG	-5.04	108.76	113.80
12	l	132	THR	CA-C-N	5.04	127.97	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	132	THR	C-N-CA	5.04	127.97	120.31
14	n	35	GLN	O-C-N	5.04	129.74	123.19
7	G	44	ASP	N-CA-C	-5.04	104.88	112.99
14	7	241	PHE	CA-C-N	5.04	130.01	122.86
14	7	241	PHE	C-N-CA	5.04	130.01	122.86
16	V	192	LEU	CA-C-N	5.04	126.99	120.44
16	V	192	LEU	C-N-CA	5.04	126.99	120.44
17	T	85	LEU	CB-CA-C	-5.04	102.97	110.88
21	N	457	SER	CB-CA-C	-5.04	102.97	110.88
24	Q	138	SER	CA-C-O	-5.04	115.08	120.42
24	Q	210	CYS	CB-CA-C	5.04	115.51	109.31
25	R	132	GLN	CA-C-N	5.04	127.53	120.28
25	R	132	GLN	C-N-CA	5.04	127.53	120.28
26	U	33	CYS	CA-C-O	-5.04	113.21	120.11
31	L	118	ILE	O-C-N	5.04	128.62	123.03
32	M	71	ASN	CA-C-N	5.04	127.44	120.29
32	M	71	ASN	C-N-CA	5.04	127.44	120.29
1	a	161	GLY	CA-C-O	5.04	124.40	118.96
9	i	98	TYR	N-CA-C	-5.04	105.87	111.36
23	P	311	TRP	CE2-CD2-CE3	5.04	123.84	118.80
28	H	99	VAL	CA-CB-CG1	-5.04	101.84	110.40
1	a	147	ASP	O-C-N	-5.04	117.42	123.06
2	b	43	VAL	CB-CA-C	-5.04	101.79	110.65
11	k	133	HIS	CB-CG-ND1	5.04	130.25	122.70
8	1	197	PHE	CA-CB-CG	-5.04	108.76	113.80
20	Z	244	ARG	CA-C-N	5.04	126.91	120.56
20	Z	244	ARG	C-N-CA	5.04	126.91	120.56
21	N	636	SER	N-CA-C	5.04	116.77	111.28
31	L	349	ILE	CA-C-N	5.04	126.13	119.84
31	L	349	ILE	C-N-CA	5.04	126.13	119.84
12	5	147	GLU	CA-C-N	5.03	130.80	121.94
12	5	147	GLU	C-N-CA	5.03	130.80	121.94
16	V	112	PRO	CA-C-O	-5.03	111.44	120.60
16	V	166	ASN	OD1-CG-ND2	5.03	127.63	122.60
17	T	14	ALA	N-CA-CB	5.03	117.61	110.16
21	N	516	GLY	N-CA-C	-5.03	106.33	112.77
21	N	604	ARG	CA-C-N	5.03	127.57	120.42
21	N	604	ARG	C-N-CA	5.03	127.57	120.42
30	K	257	VAL	N-CA-CB	-5.03	104.13	110.57
7	g	64	ASN	N-CA-C	-5.03	99.91	108.26
10	j	109	VAL	CA-CB-CG2	-5.03	101.85	110.40
14	n	55	ILE	CB-CA-C	5.03	118.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	231	ASN	CB-CA-C	-5.03	102.95	110.90
28	H	201	GLU	CA-C-O	5.03	126.90	121.06
32	M	63	LYS	O-C-N	5.03	127.89	122.15
13	m	137	GLY	CA-C-N	5.03	131.15	121.54
13	m	137	GLY	C-N-CA	5.03	131.15	121.54
14	n	109	TYR	N-CA-C	5.03	117.33	110.24
9	2	160	SER	N-CA-C	5.03	117.66	111.82
21	N	66	SER	CA-C-N	5.03	126.98	120.44
21	N	66	SER	C-N-CA	5.03	126.98	120.44
26	U	41	ALA	N-CA-C	-5.03	101.60	108.24
29	I	420	LYS	CA-C-O	5.03	125.88	120.55
33	J	297	LEU	N-CA-CB	5.03	118.14	110.44
2	b	213	ILE	CA-CB-CG2	-5.03	101.95	110.50
14	7	260	GLY	N-CA-C	-5.03	103.53	112.58
16	V	36	LYS	N-CA-C	-5.03	105.88	111.36
21	N	880	ARG	N-CA-C	-5.03	107.14	113.28
1	a	108	TYR	CA-C-N	5.03	129.55	121.00
1	a	108	TYR	C-N-CA	5.03	129.55	121.00
2	b	198	GLU	N-CA-CB	5.03	117.60	110.16
10	j	19	ASP	N-CA-CB	5.03	119.72	112.13
10	3	60	VAL	CA-CB-CG1	5.03	118.95	110.40
15	W	82	GLU	N-CA-C	5.03	119.12	112.89
18	X	120	GLU	CA-CB-CG	-5.03	104.04	114.10
20	Z	741	LEU	N-CA-C	5.03	117.65	111.82
21	N	127	ASP	CA-CB-CG	-5.03	107.57	112.60
21	N	697	PHE	N-CA-CB	5.03	117.30	110.01
25	R	34	THR	CA-CB-CG2	-5.03	101.95	110.50
25	R	412	THR	CA-C-O	-5.03	115.52	120.70
26	U	298	ASN	CA-C-N	5.03	127.43	120.29
26	U	298	ASN	C-N-CA	5.03	127.43	120.29
28	H	119	ASN	OD1-CG-ND2	-5.03	117.57	122.60
30	K	392	LEU	N-CA-C	-5.03	106.31	112.90
7	g	243	ALA	CA-C-N	5.03	126.97	120.44
7	g	243	ALA	C-N-CA	5.03	126.97	120.44
2	B	217	GLU	N-CA-C	5.03	117.63	110.24
6	F	71	GLY	CA-C-O	-5.03	116.67	121.49
16	V	242	LYS	CA-C-O	-5.03	115.22	120.55
20	Z	352	LYS	CA-C-N	5.03	123.41	120.24
20	Z	352	LYS	C-N-CA	5.03	123.41	120.24
27	O	202	SER	CB-CA-C	-5.03	102.30	109.84
29	I	372	SER	CA-C-N	5.03	129.22	120.68
29	I	372	SER	C-N-CA	5.03	129.22	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	364	HIS	N-CA-C	-5.03	107.00	113.23
14	n	128	TYR	O-C-N	5.02	127.25	122.07
1	A	103	GLU	CA-C-O	-5.02	115.53	120.70
3	C	148	LEU	N-CA-C	-5.02	101.21	109.40
5	E	238	GLU	CA-C-N	5.02	129.22	120.68
5	E	238	GLU	C-N-CA	5.02	129.22	120.68
8	1	33	ALA	CA-C-N	5.02	129.27	122.19
8	1	33	ALA	C-N-CA	5.02	129.27	122.19
10	3	172	LEU	CA-C-O	-5.02	115.10	120.42
20	Z	623	ARG	CA-C-N	5.02	127.01	120.28
20	Z	623	ARG	C-N-CA	5.02	127.01	120.28
25	R	61	PRO	CA-C-N	5.02	129.93	121.14
25	R	61	PRO	C-N-CA	5.02	129.93	121.14
27	O	121	ASP	N-CA-C	-5.02	101.68	109.72
30	K	50	LYS	N-CA-C	-5.02	105.72	111.14
6	f	45	VAL	CA-C-N	5.02	130.07	122.99
6	f	45	VAL	C-N-CA	5.02	130.07	122.99
7	G	143	LYS	O-C-N	5.02	127.87	122.15
7	G	199	ILE	N-CA-CB	5.02	117.37	110.54
12	5	273	TRP	O-C-N	-5.02	116.43	122.15
22	S	25	TYR	CB-CG-CD2	-5.02	113.27	120.80
3	c	68	LYS	N-CA-CB	5.02	117.73	109.95
4	d	134	LEU	CA-C-O	5.02	126.12	120.70
9	2	253	GLN	OE1-CD-NE2	5.02	127.62	122.60
21	N	127	ASP	CA-C-N	5.02	126.98	120.56
21	N	127	ASP	C-N-CA	5.02	126.98	120.56
21	N	635	GLN	OE1-CD-NE2	-5.02	117.58	122.60
21	N	920	VAL	O-C-N	-5.02	117.27	122.14
22	S	421	TYR	N-CA-C	5.02	117.64	111.82
23	P	403	GLU	N-CA-C	-5.02	100.11	110.80
26	U	207	VAL	O-C-N	5.02	127.00	121.83
31	L	312	MET	N-CA-C	5.02	117.53	111.40
14	n	242	LYS	N-CA-C	-5.02	101.53	109.76
7	G	11	SER	N-CA-C	-5.02	101.44	109.07
9	2	251	ASP	CA-CB-CG	-5.02	107.58	112.60
16	V	258	GLU	N-CA-CB	5.02	120.28	112.25
21	N	106	ILE	N-CA-CB	5.02	116.99	110.57
21	N	869	ASP	CA-CB-CG	-5.02	107.58	112.60
23	P	271	SER	CA-C-N	5.02	125.25	119.83
23	P	271	SER	C-N-CA	5.02	125.25	119.83
24	Q	269	LYS	CA-C-N	5.02	126.98	120.56
24	Q	269	LYS	C-N-CA	5.02	126.98	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	386	PHE	N-CA-CB	5.02	118.97	110.49
31	L	241	ALA	CA-C-O	-5.02	116.31	121.98
5	e	15	PHE	CA-CB-CG	5.02	118.82	113.80
5	e	150	ASP	CA-CB-CG	-5.02	107.58	112.60
7	g	8	TYR	CB-CG-CD2	-5.02	113.28	120.80
14	n	96	ILE	O-C-N	-5.02	116.66	121.83
6	F	108	ALA	CA-C-N	5.02	126.59	120.22
6	F	108	ALA	C-N-CA	5.02	126.59	120.22
20	Z	290	GLU	CA-C-N	5.02	127.00	120.28
20	Z	290	GLU	C-N-CA	5.02	127.00	120.28
22	S	261	HIS	CB-CG-ND1	5.02	130.22	122.70
23	P	80	THR	N-CA-CB	5.02	117.41	109.94
27	O	149	LEU	O-C-N	5.02	128.44	122.27
6	f	23	GLU	CA-C-O	5.01	125.86	120.55
13	m	101	ILE	CA-C-N	5.01	127.00	120.28
13	m	101	ILE	C-N-CA	5.01	127.00	120.28
6	F	152	ASN	N-CA-CB	5.01	117.36	109.69
14	7	113	LEU	N-CA-CB	5.01	118.47	110.65
17	T	165	GLN	CG-CD-NE2	5.01	123.92	116.40
27	O	204	SER	N-CA-C	-5.01	105.27	113.19
29	I	223	GLY	CA-C-O	5.01	124.37	120.91
10	j	109	VAL	N-CA-C	-5.01	101.26	108.53
2	B	157	PHE	CA-C-N	5.01	125.45	120.14
2	B	157	PHE	C-N-CA	5.01	125.45	120.14
22	S	86	SER	CA-C-N	5.01	127.41	120.29
22	S	86	SER	C-N-CA	5.01	127.41	120.29
30	K	165	GLU	N-CA-CB	5.01	117.91	110.29
3	C	163	ILE	CA-C-O	5.01	125.17	120.96
3	C	164	SER	CA-C-O	5.01	126.61	120.60
6	F	6	TYR	CB-CG-CD2	-5.01	113.28	120.80
17	T	39	LEU	CA-C-N	5.01	127.41	120.29
17	T	39	LEU	C-N-CA	5.01	127.41	120.29
18	X	103	GLU	CA-C-N	5.01	130.81	122.54
18	X	103	GLU	C-N-CA	5.01	130.81	122.54
23	P	431	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
32	M	45	ARG	N-CA-CB	5.01	117.85	110.33
3	c	159	GLY	O-C-N	-5.01	116.05	123.11
5	E	232	ASP	CA-C-O	5.01	127.75	121.89
9	2	100	SER	CA-C-N	5.01	130.37	121.80
9	2	100	SER	C-N-CA	5.01	130.37	121.80
15	W	86	HIS	CG-CD2-NE2	5.01	112.21	107.20
17	T	105	LEU	CA-C-N	5.01	127.53	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	105	LEU	C-N-CA	5.01	127.53	120.42
22	S	459	GLN	N-CA-CB	5.01	117.48	110.12
23	P	396	PRO	N-CA-CB	-5.01	98.47	103.48
26	U	301	ILE	CA-C-O	-5.01	115.54	120.85
28	H	130	ASN	CA-CB-CG	-5.01	107.59	112.60
11	k	75	LEU	CA-C-O	-5.01	115.71	121.47
32	M	224	PRO	N-CD-CG	5.01	110.71	103.20
33	J	389	VAL	N-CA-CB	5.01	118.09	110.58
2	b	166	LYS	N-CA-CB	5.01	117.93	110.22
5	e	141	ALA	CA-C-O	-5.01	115.50	121.56
7	g	185	GLU	N-CA-C	-5.01	107.22	113.38
7	g	218	TRP	CA-CB-CG	5.01	123.11	113.60
13	m	180	LEU	N-CA-CB	5.01	117.38	110.17
2	B	197	LYS	CA-C-N	5.01	127.40	120.29
2	B	197	LYS	C-N-CA	5.01	127.40	120.29
3	C	79	GLY	CA-C-N	5.01	127.88	120.82
3	C	79	GLY	C-N-CA	5.01	127.88	120.82
8	1	91	PHE	O-C-N	5.01	127.43	122.12
8	1	173	LYS	N-CA-CB	5.01	117.48	110.12
16	V	191	GLY	CA-C-O	5.01	125.81	120.40
21	N	188	TYR	CA-C-N	5.01	127.40	120.29
21	N	188	TYR	C-N-CA	5.01	127.40	120.29
23	P	76	ASN	CA-C-N	5.01	126.99	120.28
23	P	76	ASN	C-N-CA	5.01	126.99	120.28
25	R	72	VAL	CB-CA-C	5.01	119.50	111.29
25	R	338	TYR	CB-CG-CD1	5.01	128.31	120.80
30	K	179	MET	CG-SD-CE	-5.01	89.89	100.90
32	M	381	ARG	NE-CZ-NH2	-5.01	114.69	119.20
2	b	103	GLU	N-CA-CB	5.00	119.47	111.56
5	e	162	GLY	CA-C-N	5.00	129.64	122.23
5	e	162	GLY	C-N-CA	5.00	129.64	122.23
5	E	166	ARG	NH1-CZ-NH2	-5.00	112.79	119.30
21	N	270	LEU	N-CA-CB	5.00	117.57	110.16
21	N	488	CYS	N-CA-CB	5.00	117.48	110.12
26	U	171	VAL	N-CA-C	-5.00	105.61	110.42
31	L	170	MET	CB-CA-C	-5.00	102.34	110.85
32	M	353	SER	CA-C-N	5.00	126.99	120.28
32	M	353	SER	C-N-CA	5.00	126.99	120.28
6	F	194	VAL	N-CA-CB	5.00	118.09	110.58
7	G	55	THR	CA-CB-OG1	5.00	117.10	109.60
7	G	172	ALA	CA-C-O	5.00	125.72	120.42
19	Y	55	THR	CA-CB-CG2	5.00	119.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	59	ILE	CA-CB-CG1	5.00	118.91	110.40
21	N	228	VAL	CA-C-N	5.00	126.86	120.56
21	N	228	VAL	C-N-CA	5.00	126.86	120.56
21	N	695	ALA	CA-C-N	5.00	127.39	120.29
21	N	695	ALA	C-N-CA	5.00	127.39	120.29
23	P	360	ILE	CA-C-O	-5.00	116.68	121.63
12	l	182	LYS	CA-C-O	5.00	124.68	118.43
2	B	169	VAL	N-CA-C	-5.00	105.67	110.72
5	E	248	ALA	CA-C-N	5.00	127.39	120.29
5	E	248	ALA	C-N-CA	5.00	127.39	120.29
25	R	293	THR	N-CA-CB	5.00	117.26	110.01
32	M	33	ARG	CA-C-N	5.00	127.39	120.29
32	M	33	ARG	C-N-CA	5.00	127.39	120.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	Z	748	LEU	CA

All (355) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	120	TYR	Sidechain
8	1	133	TYR	Sidechain
8	1	146	TYR	Sidechain
8	1	198	TYR	Sidechain
8	1	202	TYR	Sidechain
8	1	75	TYR	Sidechain
9	2	126	TYR	Sidechain
9	2	215	TYR	Sidechain
9	2	219	TYR	Sidechain
9	2	232	TYR	Sidechain
9	2	48	ARG	Sidechain
9	2	98	TYR	Sidechain
10	3	124	PHE	Sidechain
10	3	188	TYR	Sidechain
10	3	46	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	135	TYR	Sidechain
11	4	190	ARG	Sidechain
11	4	36	ARG	Sidechain
11	4	59	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	4	70	ARG	Sidechain
11	4	8	ARG	Sidechain
12	5	148	ARG	Sidechain
12	5	165	TYR	Sidechain
12	5	212	TYR	Sidechain
12	5	242	ARG	Sidechain
12	5	245	TYR	Sidechain
12	5	253	TYR	Sidechain
12	5	83	PHE	Sidechain
13	6	106	TYR	Sidechain
13	6	113	TYR	Sidechain
13	6	164	PHE	Sidechain
13	6	182	TYR	Sidechain
13	6	229	ARG	Sidechain
13	6	41	TYR	Sidechain
14	7	109	TYR	Sidechain
14	7	126	PHE	Sidechain
14	7	161	ARG	Sidechain
14	7	189	ARG	Sidechain
14	7	218	TYR	Sidechain
14	7	219	TYR	Sidechain,Peptide
14	7	226	ARG	Sidechain
14	7	74	ARG	Sidechain
14	7	98	ARG	Sidechain
1	A	106	TYR	Sidechain
1	A	108	TYR	Sidechain
1	A	11	GLY	Mainchain,Peptide
1	A	110	TYR	Sidechain
1	A	12	TYR	Peptide
1	A	120	ARG	Sidechain
1	A	14	ARG	Sidechain
1	A	166	TYR	Sidechain
1	A	234	PHE	Sidechain
1	A	24	ARG	Sidechain
1	A	244	ARG	Sidechain
2	B	157	PHE	Sidechain
2	B	178	ARG	Sidechain
2	B	236	ARG	Sidechain
2	B	5	TYR	Sidechain
2	B	6	SER	Mainchain,Peptide
2	B	7	PHE	Peptide
2	B	83	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	90	ARG	Sidechain
2	B	97	TYR	Sidechain
2	B	99	ARG	Sidechain
3	C	122	TYR	Sidechain
3	C	129	ARG	Sidechain
3	C	13	PHE	Peptide
3	C	208	TYR	Sidechain
3	C	24	TYR	Sidechain
4	D	108	TYR	Sidechain
4	D	11	PHE	Sidechain,Peptide
4	D	120	TYR	Sidechain
4	D	90	ARG	Sidechain
5	E	103	TYR	Sidechain
5	E	166	ARG	Sidechain
5	E	231	TYR	Sidechain
5	E	72	ARG	Sidechain
5	E	8	TYR	Sidechain
6	F	143	HIS	Sidechain
6	F	164	ARG	Sidechain
6	F	225	TYR	Sidechain
6	F	4	ASN	Peptide
6	F	6	TYR	Peptide
7	G	103	TYR	Sidechain
7	G	126	TYR	Sidechain
7	G	15	PHE	Sidechain
7	G	20	ARG	Sidechain
7	G	201	TYR	Sidechain
7	G	22	PHE	Sidechain
7	G	8	TYR	Peptide
7	G	93	ARG	Sidechain
28	H	145	TYR	Sidechain
28	H	173	ARG	Sidechain
28	H	272	ILE	Mainchain
28	H	273	ARG	Mainchain,Peptide
28	H	299	ARG	Sidechain
28	H	357	ARG	Sidechain
28	H	367	ARG	Peptide
28	H	373	ARG	Sidechain
28	H	385	ARG	Sidechain
28	H	403	ARG	Sidechain
28	H	409	ARG	Sidechain
28	H	435	ARG	Sidechain

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Mol	Chain	Res	Type	Group
28	H	462	ARG	Sidechain
28	H	70	LYS	Peptide
29	I	182	SER	Peptide
29	I	246	ARG	Sidechain
29	I	256	TYR	Sidechain
29	I	304	ARG	Sidechain
29	I	339	ILE	Peptide
29	I	61	ARG	Sidechain
29	I	87	LYS	Peptide
33	J	112	ARG	Sidechain
33	J	212	ARG	Sidechain
33	J	22	TYR	Sidechain
33	J	238	ARG	Sidechain
33	J	257	ARG	Sidechain
33	J	270	ARG	Sidechain
33	J	286	LYS	Peptide
33	J	296	ARG	Sidechain
33	J	339	ARG	Sidechain
33	J	374	ARG	Sidechain
33	J	376	HIS	Sidechain
33	J	404	PHE	Sidechain
33	J	43	ARG	Sidechain
30	K	171	TYR	Sidechain
30	K	207	ARG	Sidechain
30	K	212	TYR	Sidechain
30	K	235	ILE	Mainchain,Peptide
30	K	236	ARG	Sidechain
30	K	281	ARG	Sidechain
30	K	344	ARG	Sidechain
30	K	77	ARG	Sidechain
30	K	88	ARG	Sidechain
31	L	117	TYR	Sidechain
31	L	126	ARG	Sidechain
31	L	173	PHE	Sidechain
31	L	194	ARG	Sidechain
31	L	209	ARG	Sidechain
31	L	290	ARG	Sidechain
31	L	315	PHE	Peptide
31	L	342	ARG	Peptide
31	L	404	ARG	Sidechain
31	L	82	ARG	Sidechain
32	M	153	TYR	Sidechain

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Mol	Chain	Res	Type	Group
32	M	166	ARG	Sidechain
32	M	180	TYR	Sidechain
32	M	314	GLY	Peptide
32	M	315	PHE	Peptide
32	M	320	ARG	Sidechain
32	M	342	ARG	Sidechain
32	M	345	ARG	Sidechain
32	M	42	ARG	Sidechain
32	M	428	LYS	Mainchain,Peptide
32	M	44	PHE	Sidechain
32	M	50	ARG	Sidechain
21	N	117	TYR	Sidechain
21	N	282	TYR	Sidechain
21	N	389	TYR	Sidechain
21	N	398	ARG	Sidechain
21	N	422	TYR	Sidechain
21	N	50	TYR	Sidechain
21	N	559	TYR	Sidechain
21	N	58	ARG	Sidechain
21	N	653	ARG	Sidechain
21	N	697	PHE	Sidechain
21	N	739	PHE	Sidechain
21	N	741	TYR	Sidechain
21	N	785	PRO	Peptide
21	N	81	TYR	Sidechain
21	N	866	TYR	Sidechain
21	N	873	ARG	Sidechain
21	N	880	ARG	Sidechain
21	N	921	ARG	Sidechain
27	O	15	ARG	Sidechain
27	O	215	TYR	Sidechain
27	O	248	TYR	Sidechain
27	O	310	PHE	Sidechain
27	O	65	PHE	Sidechain
27	O	70	TYR	Sidechain
23	P	13	TYR	Sidechain
23	P	213	TYR	Sidechain
23	P	232	ARG	Sidechain
23	P	3	ARG	Sidechain
23	P	318	TYR	Sidechain
23	P	344	ARG	Sidechain
23	P	351	ARG	Sidechain

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Mol	Chain	Res	Type	Group
23	P	395	ARG	Sidechain
23	P	402	PHE	Sidechain
23	P	95	TYR	Sidechain
24	Q	130	ARG	Sidechain
24	Q	163	ARG	Sidechain
24	Q	165	PHE	Sidechain
24	Q	185	TYR	Sidechain
24	Q	209	TYR	Sidechain
24	Q	238	TYR	Sidechain
24	Q	255	TYR	Sidechain
24	Q	264	TYR	Sidechain
24	Q	291	TYR	Sidechain
24	Q	309	ARG	Sidechain
24	Q	65	TYR	Sidechain
24	Q	75	ARG	Sidechain
24	Q	84	TYR	Sidechain
24	Q	88	PHE	Sidechain
25	R	141	TYR	Sidechain
25	R	181	TYR	Sidechain
25	R	207	ARG	Sidechain
25	R	210	TYR	Sidechain
25	R	214	TYR	Sidechain
25	R	24	TYR	Sidechain
25	R	321	TYR	Sidechain
25	R	392	ARG	Sidechain
25	R	400	TYR	Sidechain
25	R	43	ARG	Sidechain
25	R	63	TYR	Sidechain
25	R	70	TYR	Peptide
22	S	160	ARG	Sidechain
22	S	171	TYR	Sidechain
22	S	174	ARG	Sidechain
22	S	196	ARG	Sidechain
22	S	239	ARG	Sidechain
22	S	241	PHE	Sidechain
22	S	292	TYR	Sidechain
22	S	345	TYR	Sidechain
22	S	384	ARG	Sidechain
22	S	399	TYR	Sidechain
22	S	413	LEU	Peptide
22	S	421	TYR	Sidechain
22	S	428	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	S	464	ARG	Sidechain
22	S	467	PHE	Sidechain
22	S	480	ARG	Sidechain
22	S	52	TYR	Sidechain
22	S	55	ARG	Sidechain
17	T	157	TYR	Sidechain
17	T	197	TYR	Sidechain
17	T	211	PHE	Sidechain
17	T	245	TYR	Sidechain
17	T	251	HIS	Peptide
17	T	60	ARG	Sidechain
17	T	91	SER	Peptide
26	U	210	TYR	Sidechain
26	U	72	TYR	Sidechain
26	U	93	TYR	Sidechain
16	V	100	ARG	Sidechain
16	V	230	TYR	Sidechain
16	V	269	ARG	Sidechain
16	V	270	TYR	Sidechain
16	V	28	TYR	Sidechain
16	V	57	PHE	Sidechain
15	W	179	ARG	Sidechain
18	X	11	ARG	Sidechain
18	X	22	ARG	Sidechain
18	X	97	TYR	Sidechain
18	X	98	PHE	Sidechain
19	Y	83	ARG	Sidechain
19	Y	84	TYR	Sidechain
20	Z	165	TYR	Sidechain
20	Z	248	TYR	Sidechain
20	Z	269	TYR	Sidechain
20	Z	738	TYR	Sidechain
20	Z	747	ALA	Mainchain,Peptide
20	Z	970	TYR	Sidechain
1	a	105	ARG	Sidechain
1	a	106	TYR	Sidechain
1	a	11	GLY	Peptide
1	a	12	TYR	Peptide
1	a	120	ARG	Sidechain
1	a	133	TYR	Sidechain
1	a	143	PHE	Sidechain
2	b	101	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	b	104	TYR	Sidechain
2	b	178	ARG	Sidechain
2	b	23	TYR	Sidechain
2	b	6	SER	Peptide
2	b	82	TYR	Sidechain
3	c	13	PHE	Peptide
3	c	157	TYR	Sidechain
3	c	18	ARG	Sidechain
3	c	217	ARG	Sidechain
3	c	230	PHE	Sidechain
3	c	50	ARG	Sidechain
3	c	98	TYR	Sidechain
4	d	11	PHE	Peptide
4	d	119	ARG	Sidechain
4	d	141	ARG	Sidechain
4	d	29	ARG	Sidechain
5	e	103	TYR	Sidechain
5	e	164	PHE	Sidechain
5	e	20	ARG	Sidechain
5	e	231	TYR	Sidechain
6	f	123	TYR	Sidechain
6	f	126	ARG	Peptide
6	f	128	TYR	Sidechain
6	f	147	PHE	Sidechain
6	f	164	ARG	Sidechain
6	f	18	ARG	Sidechain
6	f	4	ASN	Peptide
6	f	6	TYR	Sidechain,Peptide
6	f	89	ARG	Sidechain
7	g	119	TYR	Sidechain
7	g	160	TYR	Sidechain
7	g	22	PHE	Sidechain
7	g	26	TYR	Sidechain
7	g	8	TYR	Sidechain,Peptide
8	h	133	TYR	Sidechain
8	h	142	PHE	Sidechain
8	h	146	TYR	Sidechain
8	h	152	ARG	Sidechain
8	h	38	ARG	Sidechain
8	h	75	TYR	Sidechain
8	h	96	TYR	Sidechain
9	i	153	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	i	65	ARG	Sidechain
10	j	188	TYR	Sidechain
10	j	199	TYR	Sidechain
10	j	40	PHE	Sidechain
10	j	46	TYR	Sidechain
10	j	67	PHE	Sidechain
10	j	74	TYR	Sidechain
11	k	107	TYR	Sidechain
11	k	135	TYR	Sidechain
11	k	139	TYR	Sidechain
11	k	36	ARG	Sidechain
11	k	67	TYR	Sidechain
11	k	83	PHE	Sidechain
11	k	96	ARG	Sidechain
12	l	165	TYR	Sidechain
12	l	181	ARG	Sidechain
12	l	188	TYR	Sidechain
12	l	212	TYR	Sidechain
12	l	242	ARG	Sidechain
12	l	262	TYR	Sidechain
12	l	94	ARG	Sidechain
13	m	131	TYR	Sidechain
13	m	182	TYR	Sidechain
13	m	221	ARG	Sidechain
13	m	225	TYR	Sidechain
13	m	47	TYR	Sidechain
13	m	85	PHE	Sidechain
14	n	124	TYR	Sidechain
14	n	170	TYR	Sidechain
14	n	218	TYR	Sidechain
14	n	78	VAL	Peptide

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	1913	0	1906	6	0
1	a	1913	0	1906	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1881	0	1893	10	0
2	b	1881	0	1893	6	0
3	C	1884	0	1880	6	0
3	c	1884	0	1880	6	0
4	D	1863	0	1878	5	0
4	d	1986	0	1996	5	0
5	E	1883	0	1851	3	0
5	e	1883	0	1851	6	0
6	F	1784	0	1788	6	0
6	f	1784	0	1788	4	0
7	G	1897	0	1886	7	0
7	g	1897	0	1886	4	0
8	1	1512	0	1478	5	0
8	h	1512	0	1478	2	0
9	2	1720	0	1716	7	0
9	i	1720	0	1716	7	0
10	3	1581	0	1571	3	0
10	j	1581	0	1571	1	0
11	4	1562	0	1569	2	0
11	k	1562	0	1569	6	0
12	5	1644	0	1592	5	0
12	l	1644	0	1592	3	0
13	6	1757	0	1708	5	0
13	m	1757	0	1708	2	0
14	7	1790	0	1790	0	0
14	n	1816	0	1818	6	0
15	W	1535	0	1542	6	0
16	V	2274	0	2273	6	0
17	T	2193	0	2161	2	0
18	X	1033	0	1017	3	0
19	Y	731	0	675	2	0
20	Z	7006	0	6932	218	0
21	N	7158	0	7226	68	0
22	S	3895	0	3938	8	0
23	P	3609	0	3694	6	0
24	Q	3499	0	3524	7	0
25	R	3259	0	3263	1	0
26	U	2427	0	2462	7	0
27	O	3186	0	3213	12	0
28	H	3313	0	3320	24	0
29	I	3022	0	3091	159	0
30	K	3113	0	3168	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	L	3083	0	3156	6	0
32	M	3285	0	3322	9	0
33	J	3171	0	3312	14	0
34	H	31	0	12	0	0
34	I	31	0	12	0	0
34	K	31	0	12	0	0
34	L	31	0	11	0	0
34	M	31	0	12	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
36	J	27	0	12	0	0
All	All	110471	0	110518	461	0

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

All (461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:748:LEU:CA	20:Z:748:LEU:CB	1.83	1.56
20:Z:728:LYS:CB	20:Z:728:LYS:CG	2.02	1.38
20:Z:728:LYS:HG3	29:I:61:ARG:CB	1.51	1.37
20:Z:255:LEU:HD22	21:N:816:LYS:CG	1.67	1.22
20:Z:728:LYS:CG	29:I:62:MET:HE3	1.70	1.20
20:Z:728:LYS:HG2	29:I:62:MET:HG2	1.20	1.18
20:Z:255:LEU:CG	29:I:61:ARG:HH22	1.57	1.17
20:Z:255:LEU:HD11	21:N:812:ALA:O	1.50	1.11
20:Z:728:LYS:CG	29:I:61:ARG:HB3	1.80	1.11
20:Z:728:LYS:HG2	29:I:62:MET:N	1.64	1.10
20:Z:255:LEU:HG	29:I:61:ARG:HH12	1.14	1.10
20:Z:748:LEU:CA	29:I:85:PHE:H	1.63	1.10
20:Z:748:LEU:CA	20:Z:748:LEU:N	2.15	1.09
20:Z:748:LEU:CA	29:I:84:PRO:CD	2.33	1.06
20:Z:728:LYS:CG	29:I:62:MET:CE	2.32	1.06
20:Z:728:LYS:CG	29:I:62:MET:N	2.18	1.06
2:B:17:LYS:HB3	33:J:405:LYS:HE3	1.35	1.04
20:Z:255:LEU:CG	29:I:61:ARG:HH12	1.71	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:255:LEU:HD22	21:N:816:LYS:CB	1.88	1.02
20:Z:748:LEU:C	29:I:84:PRO:CD	2.31	1.02
20:Z:738:TYR:CZ	29:I:69:LEU:HB3	1.95	1.01
20:Z:728:LYS:CG	29:I:62:MET:HG2	1.91	1.01
20:Z:748:LEU:C	29:I:84:PRO:HD3	1.85	1.00
20:Z:728:LYS:HG2	29:I:62:MET:CG	1.91	1.00
20:Z:728:LYS:CD	29:I:61:ARG:HG3	1.92	1.00
20:Z:748:LEU:HA	29:I:85:PHE:H	1.25	1.00
20:Z:255:LEU:CD1	21:N:816:LYS:HE3	1.91	1.00
20:Z:748:LEU:CB	20:Z:748:LEU:N	2.26	0.99
20:Z:728:LYS:CG	29:I:61:ARG:CB	2.39	0.98
20:Z:255:LEU:CB	29:I:61:ARG:NH2	2.28	0.97
20:Z:748:LEU:CA	29:I:84:PRO:HG2	1.94	0.97
20:Z:255:LEU:HG	29:I:61:ARG:NH1	1.80	0.96
20:Z:255:LEU:CG	29:I:61:ARG:NH2	2.27	0.96
20:Z:255:LEU:CB	21:N:816:LYS:HD2	1.94	0.96
20:Z:738:TYR:CZ	20:Z:738:TYR:OH	2.17	0.96
20:Z:748:LEU:C	29:I:84:PRO:N	2.23	0.96
20:Z:748:LEU:CA	29:I:84:PRO:HD2	1.95	0.95
20:Z:728:LYS:HB2	29:I:58:LYS:O	1.67	0.95
20:Z:738:TYR:CZ	29:I:66:LYS:O	2.21	0.93
20:Z:255:LEU:HD22	21:N:816:LYS:HB2	1.50	0.92
20:Z:748:LEU:CA	29:I:84:PRO:CG	2.46	0.92
20:Z:255:LEU:CD1	29:I:61:ARG:NH1	2.32	0.91
20:Z:728:LYS:CD	29:I:62:MET:HE2	2.00	0.91
20:Z:255:LEU:CG	20:Z:255:LEU:CD1	2.48	0.91
20:Z:748:LEU:N	29:I:84:PRO:HG2	1.85	0.90
20:Z:728:LYS:HG2	29:I:62:MET:H	1.35	0.90
20:Z:255:LEU:HD22	21:N:816:LYS:HG3	1.52	0.90
20:Z:255:LEU:CG	21:N:816:LYS:HD2	2.02	0.90
20:Z:748:LEU:CA	29:I:81:ILE:O	2.19	0.90
20:Z:255:LEU:HG	21:N:813:ARG:HA	1.55	0.89
20:Z:738:TYR:CZ	29:I:70:LEU:N	2.40	0.89
20:Z:255:LEU:CB	21:N:816:LYS:CD	2.52	0.88
20:Z:255:LEU:CG	21:N:816:LYS:HE3	2.03	0.88
20:Z:255:LEU:CD2	21:N:813:ARG:HA	2.04	0.88
20:Z:255:LEU:HD22	21:N:816:LYS:CD	2.04	0.87
20:Z:738:TYR:OH	29:I:66:LYS:O	1.92	0.87
20:Z:738:TYR:OH	29:I:69:LEU:HB3	1.75	0.86
20:Z:728:LYS:CG	29:I:61:ARG:CG	2.53	0.86
2:B:17:LYS:CB	33:J:405:LYS:HE3	2.00	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:255:LEU:HA	21:N:813:ARG:NH1	1.92	0.85
20:Z:728:LYS:HG3	29:I:61:ARG:HB3	0.85	0.85
20:Z:255:LEU:CG	21:N:816:LYS:CD	2.55	0.84
20:Z:255:LEU:CG	29:I:61:ARG:NH1	2.37	0.83
20:Z:748:LEU:C	29:I:84:PRO:CA	2.51	0.83
20:Z:748:LEU:HB3	29:I:85:PHE:HB2	1.59	0.83
20:Z:255:LEU:HB3	21:N:816:LYS:CD	2.07	0.83
20:Z:255:LEU:HD12	29:I:61:ARG:NH1	1.94	0.83
20:Z:255:LEU:CD1	21:N:812:ALA:O	2.25	0.82
2:B:17:LYS:HB3	33:J:405:LYS:CE	2.09	0.82
28:H:201:GLU:HB2	28:H:273:ARG:HH21	1.44	0.82
20:Z:748:LEU:CA	29:I:85:PHE:N	2.43	0.81
20:Z:748:LEU:CB	29:I:81:ILE:O	2.29	0.81
20:Z:255:LEU:CD1	29:I:61:ARG:HH12	1.91	0.80
20:Z:739:ALA:HB2	20:Z:764:LEU:HD13	1.63	0.80
20:Z:748:LEU:HB2	29:I:81:ILE:O	1.82	0.80
20:Z:255:LEU:HD13	21:N:816:LYS:HE3	1.62	0.79
20:Z:728:LYS:CD	29:I:61:ARG:O	2.30	0.79
20:Z:255:LEU:HD21	21:N:813:ARG:O	1.81	0.78
20:Z:728:LYS:HD3	29:I:61:ARG:O	1.84	0.78
20:Z:255:LEU:CG	21:N:816:LYS:CE	2.61	0.78
20:Z:255:LEU:CD2	21:N:816:LYS:HD2	2.14	0.78
20:Z:728:LYS:CB	29:I:62:MET:HE3	2.13	0.78
20:Z:255:LEU:HD21	21:N:813:ARG:HA	1.65	0.77
20:Z:738:TYR:OH	29:I:69:LEU:N	2.18	0.77
20:Z:748:LEU:N	29:I:81:ILE:O	2.18	0.76
20:Z:748:LEU:C	29:I:84:PRO:CB	2.58	0.76
20:Z:729:GLU:H	29:I:62:MET:HG3	1.50	0.76
20:Z:728:LYS:CG	29:I:61:ARG:HG3	2.15	0.76
20:Z:738:TYR:OH	29:I:70:LEU:N	2.19	0.76
20:Z:255:LEU:CD2	21:N:816:LYS:HB2	2.17	0.75
20:Z:728:LYS:HG3	29:I:61:ARG:CG	2.15	0.75
20:Z:255:LEU:HD21	21:N:813:ARG:C	2.12	0.74
20:Z:255:LEU:CD2	21:N:816:LYS:CG	2.59	0.74
6:F:155:GLU:H	7:G:64:ASN:HD21	1.36	0.73
20:Z:255:LEU:CG	21:N:813:ARG:HA	2.18	0.73
20:Z:255:LEU:CD2	21:N:816:LYS:CD	2.67	0.73
20:Z:248:TYR:HB3	20:Z:249:MET:HE2	1.71	0.72
20:Z:748:LEU:CB	29:I:85:PHE:HB2	2.20	0.72
20:Z:255:LEU:CG	29:I:61:ARG:CZ	2.69	0.71
20:Z:738:TYR:CE2	29:I:66:LYS:O	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:728:LYS:HD2	29:I:62:MET:HA	1.71	0.71
20:Z:255:LEU:HD21	21:N:813:ARG:CA	2.22	0.70
20:Z:748:LEU:C	29:I:84:PRO:HB3	2.16	0.70
20:Z:738:TYR:OH	29:I:69:LEU:CB	2.39	0.69
28:H:272:ILE:HG22	28:H:273:ARG:H	1.58	0.69
20:Z:741:LEU:HD23	20:Z:744:ALA:HB3	1.75	0.69
28:H:272:ILE:HG22	28:H:273:ARG:N	2.08	0.69
20:Z:738:TYR:CE1	29:I:70:LEU:N	2.61	0.69
20:Z:748:LEU:N	20:Z:748:LEU:HG	2.08	0.69
20:Z:728:LYS:HG2	29:I:62:MET:CA	2.22	0.68
20:Z:255:LEU:CD2	21:N:813:ARG:O	2.41	0.68
26:U:89:LEU:HD22	26:U:89:LEU:H	1.59	0.67
20:Z:748:LEU:HD12	29:I:81:ILE:HG23	1.76	0.67
20:Z:748:LEU:N	20:Z:748:LEU:CG	2.58	0.67
21:N:498:ILE:HD11	21:N:525:ASN:HD21	1.60	0.66
20:Z:728:LYS:CG	29:I:62:MET:CG	2.64	0.66
20:Z:255:LEU:HB3	21:N:816:LYS:HD3	1.76	0.66
20:Z:255:LEU:HD11	21:N:812:ALA:C	2.21	0.66
22:S:155:LEU:H	22:S:155:LEU:HD12	1.61	0.66
20:Z:748:LEU:HB3	29:I:85:PHE:O	1.96	0.66
20:Z:748:LEU:CA	29:I:84:PRO:N	2.59	0.65
20:Z:255:LEU:HG	29:I:61:ARG:HH22	1.60	0.65
20:Z:738:TYR:HH	29:I:66:LYS:C	2.06	0.64
20:Z:728:LYS:CG	29:I:61:ARG:C	2.70	0.64
20:Z:748:LEU:HA	29:I:85:PHE:N	2.07	0.64
20:Z:738:TYR:OH	29:I:69:LEU:CA	2.47	0.63
20:Z:255:LEU:CB	21:N:816:LYS:NZ	2.62	0.63
20:Z:255:LEU:CD2	21:N:816:LYS:HG3	2.26	0.62
20:Z:255:LEU:HG	29:I:61:ARG:NH2	2.12	0.62
20:Z:728:LYS:CD	29:I:61:ARG:C	2.72	0.62
20:Z:728:LYS:CB	29:I:62:MET:HG2	2.29	0.62
5:e:157:HIS:CE1	5:e:172:ILE:HG21	2.35	0.62
20:Z:728:LYS:CD	29:I:62:MET:HA	2.29	0.62
20:Z:748:LEU:N	29:I:84:PRO:CG	2.62	0.61
1:A:41:ASN:HD21	1:A:174:LYS:H	1.48	0.61
20:Z:738:TYR:CZ	29:I:69:LEU:CB	2.80	0.61
21:N:256:GLN:HB2	21:N:904:VAL:HG12	1.81	0.61
2:b:11:THR:HA	3:c:21:GLN:HE22	1.64	0.61
12:l:119:THR:HG21	12:l:175:MET:HE3	1.82	0.60
20:Z:738:TYR:HA	29:I:70:LEU:HD13	1.84	0.60
20:Z:209:PRO:HB3	29:I:54:ARG:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:CZ	1:A:209:HIS:CE1	2.91	0.59
3:C:133:VAL:HG11	3:C:135:PHE:CZ	2.38	0.59
28:H:273:ARG:CZ	29:I:316:PHE:CG	2.85	0.59
20:Z:809:MET:SD	29:I:205:PRO:HD2	2.42	0.59
29:I:258:GLY:HA2	29:I:304:ARG:HH12	1.66	0.58
28:H:273:ARG:HA	28:H:307:PHE:O	2.03	0.58
20:Z:741:LEU:HD11	29:I:74:GLU:HB2	1.85	0.58
32:M:253:GLN:HE21	32:M:253:GLN:HA	1.67	0.58
20:Z:255:LEU:HG	29:I:61:ARG:CZ	2.30	0.58
20:Z:248:TYR:HA	29:I:54:ARG:NH2	2.19	0.57
20:Z:738:TYR:OH	29:I:66:LYS:C	2.47	0.57
20:Z:255:LEU:CB	29:I:61:ARG:HH21	2.17	0.57
2:B:17:LYS:CB	33:J:405:LYS:CE	2.77	0.57
20:Z:748:LEU:HA	29:I:84:PRO:N	2.20	0.56
12:l:106:VAL:HG22	12:l:107:LYS:H	1.70	0.56
2:B:177:LYS:HE2	24:Q:168:LEU:HD13	1.87	0.56
16:V:66:VAL:HG21	16:V:102:GLN:HE22	1.69	0.56
20:Z:747:ALA:O	29:I:85:PHE:CD2	2.58	0.56
9:2:38:ASN:HD21	9:2:174:ASP:HB3	1.71	0.56
28:H:272:ILE:CG2	28:H:273:ARG:N	2.69	0.56
20:Z:748:LEU:C	29:I:83:LYS:C	2.73	0.56
27:O:242:ILE:HG22	27:O:248:TYR:CD1	2.40	0.56
20:Z:255:LEU:HB2	29:I:61:ARG:NH2	2.20	0.55
20:Z:746:ILE:C	29:I:84:PRO:HG3	2.31	0.55
20:Z:254:PRO:HB2	29:I:61:ARG:HE	1.71	0.55
28:H:272:ILE:CG2	28:H:273:ARG:H	2.20	0.55
20:Z:727:GLU:HB3	29:I:62:MET:HE1	1.89	0.55
18:X:68:LEU:HD22	18:X:128:VAL:HG11	1.87	0.55
21:N:59:GLU:H	21:N:59:GLU:CD	2.14	0.55
28:H:271:PHE:CE1	28:H:273:ARG:NH1	2.75	0.55
20:Z:728:LYS:HG3	29:I:61:ARG:CA	2.31	0.55
20:Z:154:ILE:HG21	28:H:43:ALA:HB3	1.89	0.54
20:Z:255:LEU:HD22	21:N:816:LYS:HD2	1.76	0.54
20:Z:728:LYS:HG2	29:I:62:MET:CB	2.36	0.54
28:H:273:ARG:NH1	29:I:316:PHE:CG	2.75	0.54
20:Z:154:ILE:HG21	28:H:43:ALA:CB	2.38	0.54
20:Z:741:LEU:HD12	29:I:70:LEU:CD1	2.37	0.54
29:I:326:MET:HE1	29:I:338:LEU:HD11	1.89	0.54
20:Z:729:GLU:N	29:I:62:MET:HG3	2.19	0.54
21:N:735:MET:HE2	21:N:735:MET:HA	1.89	0.54
6:f:132:LEU:H	6:f:147:PHE:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:224:LEU:HD21	20:Z:248:TYR:CZ	2.43	0.54
7:g:112:PHE:CZ	7:g:116:LEU:HD11	2.43	0.54
31:L:135:VAL:HG11	31:L:157:ARG:HA	1.90	0.53
21:N:672:ASN:HD22	21:N:675:VAL:HG23	1.73	0.53
3:c:13:PHE:HB2	4:d:19:GLN:HE22	1.73	0.53
14:n:215:ARG:HH11	9:2:169:SER:HA	1.73	0.53
21:N:498:ILE:CD1	21:N:525:ASN:HD21	2.22	0.53
20:Z:249:MET:O	20:Z:253:VAL:HG23	2.09	0.53
21:N:588:VAL:HG13	21:N:609:LEU:HD13	1.91	0.53
32:M:146:VAL:HG12	32:M:158:THR:HG22	1.91	0.53
11:k:141:PHE:HB3	12:5:242:ARG:HE	1.74	0.52
3:C:106:ILE:HD13	3:C:111:LEU:HD13	1.92	0.52
1:A:92:ASN:HA	7:G:118:GLN:HE22	1.74	0.52
20:Z:738:TYR:CE1	29:I:70:LEU:CA	2.93	0.52
27:O:320:PRO:O	27:O:324:VAL:HG23	2.09	0.52
20:Z:741:LEU:HB3	29:I:73:GLU:OE2	2.10	0.52
14:n:84:VAL:HG22	14:n:149:VAL:HG13	1.91	0.52
26:U:244:ASP:HA	26:U:247:ILE:HD12	1.90	0.52
11:4:101:ASN:HB2	11:4:133:HIS:CD2	2.44	0.52
20:Z:738:TYR:CE1	29:I:69:LEU:HD23	2.44	0.52
20:Z:728:LYS:CG	29:I:62:MET:H	2.04	0.51
7:g:49:ALA:HB2	7:g:196:ALA:HB1	1.92	0.51
13:6:35:THR:HB	13:6:48:GLU:H	1.74	0.51
24:Q:356:CYS:HG	24:Q:396:TRP:CG	2.29	0.51
20:Z:248:TYR:HA	29:I:54:ARG:HH22	1.75	0.51
20:Z:809:MET:HE1	29:I:205:PRO:HB2	1.92	0.51
20:Z:728:LYS:CD	29:I:62:MET:CE	2.83	0.51
6:F:19:LEU:HD11	7:G:130:ARG:HH11	1.75	0.51
20:Z:741:LEU:HD21	29:I:74:GLU:OE1	2.11	0.51
33:J:88:VAL:HG22	33:J:115:LEU:HD21	1.92	0.51
24:Q:419:LEU:HD22	26:U:267:VAL:HG21	1.91	0.50
12:l:233:LYS:HG2	12:l:252:LEU:HD11	1.93	0.50
20:Z:738:TYR:CE1	29:I:70:LEU:HA	2.46	0.50
20:Z:747:ALA:O	29:I:85:PHE:CE2	2.65	0.50
20:Z:255:LEU:HA	21:N:813:ARG:HH12	1.72	0.50
20:Z:255:LEU:HB3	21:N:816:LYS:HZ3	1.76	0.50
28:H:273:ARG:HD2	29:I:316:PHE:HB3	1.94	0.50
20:Z:728:LYS:CG	29:I:62:MET:HE2	2.34	0.50
9:i:139:LEU:HG	9:i:154:LEU:HD12	1.94	0.50
20:Z:255:LEU:CB	29:I:61:ARG:HH22	2.19	0.50
21:N:256:GLN:HB2	21:N:904:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:249:ILE:HD13	10:3:195:VAL:HG23	1.94	0.49
5:E:232:ASP:HB2	5:E:235:LYS:H	1.78	0.49
26:U:230:GLN:HE22	27:O:356:ARG:H	1.60	0.49
15:W:64:THR:HG22	15:W:65:PHE:H	1.77	0.49
20:Z:748:LEU:HG	29:I:85:PHE:HD2	1.76	0.49
29:I:315:GLY:O	29:I:316:PHE:C	2.50	0.49
6:F:3:ARG:HA	6:F:4:ASN:HB3	1.93	0.49
20:Z:728:LYS:CB	29:I:58:LYS:O	2.51	0.49
21:N:812:ALA:HB3	29:I:65:ILE:HD11	1.95	0.49
15:W:163:ASN:HB2	15:W:164:PRO:HD2	1.95	0.48
21:N:395:ALA:HA	21:N:401:LYS:HD3	1.94	0.48
24:Q:125:ALA:HB1	24:Q:133:LEU:HD23	1.94	0.48
7:G:204:HIS:O	7:G:204:HIS:CG	2.66	0.48
26:U:36:VAL:HG21	26:U:89:LEU:HD12	1.95	0.48
28:H:273:ARG:CZ	29:I:316:PHE:CD1	2.96	0.48
3:c:150:THR:HG22	3:c:160:TRP:HE1	1.78	0.48
13:6:20:ILE:HD12	13:6:118:ILE:HD12	1.96	0.48
20:Z:249:MET:HE3	20:Z:268:ALA:HB2	1.95	0.48
15:W:165:GLN:HE21	15:W:167:GLU:HB2	1.77	0.48
16:V:254:ARG:HE	16:V:272:GLY:HA2	1.77	0.48
20:Z:728:LYS:CA	29:I:62:MET:SD	3.01	0.48
20:Z:747:ALA:C	29:I:84:PRO:HG2	2.38	0.48
6:f:104:ALA:HB3	6:f:107:ARG:HG3	1.95	0.48
6:f:171:TYR:HA	6:f:174:ARG:HH21	1.78	0.48
8:1:133:TYR:CE2	8:1:147:CYS:HB3	2.49	0.48
20:Z:253:VAL:HG21	20:Z:287:ARG:HH12	1.79	0.48
20:Z:741:LEU:HD12	29:I:70:LEU:HD11	1.95	0.48
8:1:68:VAL:HG11	8:1:91:PHE:CE2	2.49	0.48
20:Z:255:LEU:CB	21:N:816:LYS:HZ3	2.27	0.48
20:Z:747:ALA:C	20:Z:748:LEU:HG	2.37	0.48
11:k:174:MET:HB2	11:k:176:PHE:CZ	2.48	0.48
2:B:68:THR:HB	2:B:69:PRO:CD	2.44	0.48
21:N:83:LEU:HD21	21:N:133:LEU:HB2	1.96	0.48
21:N:150:LEU:O	21:N:154:LEU:HG	2.14	0.48
20:Z:741:LEU:HD11	29:I:74:GLU:OE1	2.13	0.48
21:N:474:SER:HB2	21:N:477:SER:HB2	1.96	0.48
22:S:33:GLU:HG3	22:S:57:LEU:HD13	1.96	0.48
2:B:17:LYS:HZ1	33:J:405:LYS:HG3	1.40	0.48
20:Z:748:LEU:CB	29:I:89:GLN:OE1	2.62	0.48
20:Z:728:LYS:CE	29:I:62:MET:HE2	2.43	0.47
12:5:111:GLU:HG2	12:5:260:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:292:ILE:HG23	17:T:263:ALA:HB1	1.96	0.47
20:Z:732:ILE:HB	20:Z:771:HIS:CE1	2.49	0.47
20:Z:748:LEU:HD22	29:I:89:GLN:OE1	2.15	0.47
3:c:68:LYS:HG2	3:c:227:GLN:HE22	1.80	0.47
4:d:70:HIS:HE1	4:d:104:VAL:HB	1.79	0.47
29:I:292:TYR:CE1	33:J:267:GLU:HB2	2.50	0.47
7:G:187:LEU:HD11	7:G:191:GLU:HB2	1.96	0.47
12:5:130:TRP:CE2	12:5:161:LEU:HD11	2.50	0.47
32:M:369:THR:HG23	32:M:410:VAL:HG12	1.97	0.47
1:a:14:ARG:CZ	7:g:7:GLY:HA2	2.44	0.47
2:b:218:ASN:HD21	2:b:236:ARG:HB2	1.79	0.47
21:N:162:ARG:HG3	21:N:165:ILE:HD12	1.97	0.47
21:N:469:VAL:HG12	21:N:469:VAL:O	2.15	0.46
21:N:530:GLU:CD	21:N:530:GLU:H	2.23	0.46
16:V:271:VAL:HG12	16:V:271:VAL:O	2.15	0.46
33:J:220:GLN:HG2	33:J:224:GLY:H	1.80	0.46
33:J:331:HIS:CE1	33:J:359:LYS:HD2	2.50	0.46
9:i:126:TYR:HB3	9:i:156:LEU:HD21	1.97	0.46
2:B:17:LYS:HG2	33:J:405:LYS:HD3	1.37	0.46
20:Z:738:TYR:CE1	29:I:69:LEU:C	2.94	0.46
20:Z:739:ALA:CB	20:Z:764:LEU:HD13	2.39	0.46
9:2:32:ILE:HG21	9:2:73:ALA:HB3	1.97	0.46
20:Z:744:ALA:C	20:Z:747:ALA:H	2.24	0.46
21:N:518:ALA:HB1	21:N:550:GLY:HA3	1.97	0.46
31:L:429:GLU:HG2	32:M:330:VAL:HG22	1.98	0.46
2:B:68:THR:HB	2:B:69:PRO:HD2	1.98	0.46
5:e:113:THR:HG23	5:e:144:ILE:HD13	1.98	0.45
20:Z:255:LEU:HD13	21:N:816:LYS:CE	2.42	0.45
20:Z:738:TYR:HH	29:I:69:LEU:HB3	1.79	0.45
28:H:318:ARG:CZ	28:H:331:ARG:HH22	2.29	0.45
11:4:128:LEU:HD12	11:4:129:PRO:HD2	1.98	0.45
13:6:146:ALA:H	13:6:155:MET:HE2	1.81	0.45
18:X:125:MET:HA	18:X:125:MET:HE2	1.98	0.45
28:H:365:LEU:HD23	28:H:370:ARG:HH12	1.81	0.45
31:L:54:ASN:HD22	31:L:54:ASN:H	1.62	0.45
27:O:330:ARG:HE	27:O:334:LEU:HG	1.81	0.45
2:b:227:ILE:HD11	9:i:215:TYR:CD2	2.51	0.45
5:e:214:GLU:CD	5:e:214:GLU:H	2.24	0.45
9:2:221:THR:HG21	9:2:224:VAL:HG12	1.97	0.45
28:H:390:ARG:HG3	28:H:404:TRP:CZ3	2.51	0.45
13:m:188:VAL:O	13:m:192:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:248:TYR:HA	29:I:54:ARG:NH1	2.32	0.45
20:Z:255:LEU:CB	21:N:816:LYS:CE	2.94	0.45
3:c:211:LEU:HD23	3:c:211:LEU:HA	1.71	0.45
20:Z:728:LYS:HG3	29:I:62:MET:N	2.23	0.45
20:Z:741:LEU:HD23	20:Z:744:ALA:CB	2.46	0.45
11:k:9:VAL:HG11	11:k:157:GLY:HA3	1.99	0.45
8:1:47:HIS:CD2	8:1:48:ASP:H	2.35	0.45
20:Z:255:LEU:HB3	21:N:816:LYS:NZ	2.32	0.45
20:Z:748:LEU:HB3	29:I:89:GLN:OE1	2.17	0.45
25:R:101:GLU:O	25:R:105:LYS:HG3	2.17	0.45
15:W:125:LEU:HB2	15:W:157:PHE:CE1	2.52	0.45
15:W:26:PHE:HA	15:W:29:GLN:HE21	1.83	0.44
21:N:809:ARG:HD2	29:I:68:HIS:HB3	1.98	0.44
27:O:192:SER:HB2	27:O:217:LEU:HD21	1.98	0.44
14:n:84:VAL:HG21	14:n:125:ILE:HG21	1.99	0.44
30:K:235:ILE:HG22	30:K:236:ARG:N	2.33	0.44
10:3:187:VAL:HG21	10:3:200:LEU:HD21	1.98	0.44
20:Z:734:ASP:HB2	29:I:66:LYS:HB3	2.00	0.44
23:P:361:THR:HG22	23:P:363:LEU:H	1.82	0.44
28:H:337:ILE:HG23	28:H:370:ARG:HH22	1.83	0.44
33:J:11:VAL:H	33:J:14:THR:HB	1.81	0.44
23:P:393:VAL:HG22	23:P:400:VAL:HG23	2.00	0.44
13:6:154:ILE:HG23	13:6:195:SER:HB2	1.99	0.44
22:S:352:VAL:HA	22:S:387:VAL:HG22	2.00	0.44
12:5:147:GLU:HB3	12:5:148:ARG:H	1.54	0.44
21:N:885:ILE:HG22	21:N:887:ASP:H	1.81	0.44
4:D:70:HIS:HB3	4:D:219:SER:HA	2.00	0.44
6:F:69:HIS:CD2	6:F:102:LYS:HE3	2.52	0.44
28:H:271:PHE:CD1	28:H:273:ARG:NH1	2.86	0.44
1:A:126:GLN:HB3	2:B:84:VAL:HG21	1.99	0.44
20:Z:728:LYS:HG3	29:I:61:ARG:C	2.40	0.44
11:k:8:ARG:HH11	11:k:115:GLU:HA	1.82	0.43
11:k:8:ARG:HH21	11:k:129:PRO:HB3	1.83	0.43
7:G:109:ILE:H	7:G:109:ILE:HD12	1.82	0.43
20:Z:248:TYR:HA	29:I:54:ARG:CZ	2.47	0.43
5:e:205:LYS:HB3	5:e:212:LEU:HD22	2.00	0.43
20:Z:253:VAL:CG2	20:Z:287:ARG:HH12	2.32	0.43
20:Z:748:LEU:HD22	29:I:89:GLN:CD	2.43	0.43
22:S:109:GLU:O	22:S:109:GLU:HG2	2.18	0.43
27:O:218:SER:HB2	27:O:251:LEU:HD21	2.00	0.43
29:I:299:GLU:CD	29:I:299:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:163:ASN:HB2	15:W:164:PRO:CD	2.48	0.43
16:V:186:GLN:HG2	33:J:118:ASP:HA	2.01	0.43
23:P:193:TYR:CE2	23:P:230:HIS:CG	3.06	0.43
23:P:307:GLU:O	23:P:352:VAL:HG21	2.17	0.43
32:M:196:ALA:HB2	32:M:345:ARG:HG3	2.01	0.43
3:C:120:GLN:NE2	4:D:81:ASP:HA	2.33	0.43
17:T:251:HIS:CG	17:T:251:HIS:O	2.69	0.43
20:Z:745:LEU:HD13	29:I:80:GLU:CD	2.43	0.43
28:H:152:ILE:O	28:H:152:ILE:HG22	2.19	0.43
3:C:51:LYS:H	3:C:51:LYS:HD3	1.83	0.43
20:Z:248:TYR:CA	29:I:54:ARG:HH22	2.31	0.43
21:N:102:VAL:H	21:N:102:VAL:HG23	1.54	0.43
20:Z:728:LYS:CB	29:I:62:MET:CE	2.91	0.43
20:Z:748:LEU:CG	29:I:85:PHE:HB2	2.49	0.43
27:O:168:THR:O	27:O:172:TYR:CD2	2.72	0.43
4:d:70:HIS:CE1	4:d:104:VAL:HB	2.53	0.43
4:d:192:VAL:O	4:d:196:VAL:HG23	2.19	0.43
6:F:166:GLN:N	6:F:166:GLN:CD	2.77	0.43
8:1:101:ASN:O	8:1:102:LEU:HD23	2.19	0.43
19:Y:11:GLN:HB2	24:Q:427:PHE:CZ	2.54	0.43
19:Y:30:GLU:HA	22:S:239:ARG:HH22	1.84	0.43
20:Z:632:GLU:HA	21:N:792:SER:CB	2.49	0.43
30:K:74:HIS:CE1	30:K:77:ARG:NH2	2.87	0.43
10:j:18:LYS:H	10:j:158:LEU:H	1.66	0.43
26:U:194:LEU:HD22	27:O:392:TRP:CH2	2.54	0.43
31:L:98:LEU:HD23	31:L:98:LEU:HA	1.85	0.43
16:V:224:GLY:O	16:V:297:THR:HG23	2.19	0.43
30:K:192:LEU:HD23	30:K:192:LEU:C	2.44	0.42
8:h:168:LEU:HD23	8:h:168:LEU:HA	1.81	0.42
12:5:189:TYR:CE1	12:5:204:VAL:HG11	2.54	0.42
20:Z:146:PHE:CE1	20:Z:149:TRP:HB3	2.54	0.42
31:L:187:THR:HA	31:L:190:ILE:HD12	2.01	0.42
9:2:62:LYS:HD3	9:2:62:LYS:HA	1.89	0.42
20:Z:254:PRO:O	21:N:813:ARG:NH1	2.52	0.42
27:O:356:ARG:HH12	27:O:362:GLN:CD	2.28	0.42
1:A:101:ALA:HA	1:A:112:MET:SD	2.60	0.42
20:Z:746:ILE:O	29:I:84:PRO:HG3	2.19	0.42
23:P:122:ILE:HA	23:P:125:VAL:HG22	2.02	0.42
32:M:301:VAL:H	32:M:301:VAL:HG23	1.65	0.42
20:Z:728:LYS:CG	20:Z:728:LYS:CD	2.98	0.42
33:J:220:GLN:CG	33:J:224:GLY:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:581:ASP:HB3	21:N:616:HIS:CD2	2.54	0.42
22:S:330:LEU:O	22:S:334:HIS:CD2	2.72	0.42
32:M:140:LEU:HD23	32:M:140:LEU:HA	1.87	0.42
22:S:360:PHE:CD1	22:S:387:VAL:HG21	2.55	0.42
9:i:167:LEU:O	9:i:171:TRP:HB2	2.19	0.42
27:O:211:GLN:HE21	27:O:242:ILE:HD12	1.84	0.42
32:M:98:GLU:CD	32:M:98:GLU:H	2.27	0.42
20:Z:741:LEU:CB	29:I:73:GLU:OE2	2.68	0.42
20:Z:748:LEU:HD23	29:I:85:PHE:HB2	2.01	0.42
28:H:282:LYS:HD2	29:I:257:LEU:HB3	2.02	0.42
20:Z:748:LEU:HD23	29:I:85:PHE:CB	2.50	0.42
27:O:230:PHE:CZ	27:O:258:LEU:HD13	2.55	0.42
30:K:235:ILE:HG22	30:K:236:ARG:H	1.84	0.42
6:f:190:ILE:HG23	6:f:213:ILE:HD13	2.02	0.41
20:Z:738:TYR:CE2	29:I:69:LEU:HD23	2.55	0.41
20:Z:741:LEU:HA	20:Z:744:ALA:HB3	2.01	0.41
20:Z:257:PRO:HG2	21:N:820:GLU:OE2	2.20	0.41
20:Z:728:LYS:CG	29:I:62:MET:CA	2.90	0.41
21:N:186:ILE:HD13	21:N:214:LEU:CD2	2.50	0.41
22:S:143:GLN:HE22	22:S:187:ILE:HG12	1.84	0.41
28:H:457:PHE:CE1	29:I:347:LYS:HB2	2.55	0.41
4:D:33:ALA:HA	4:D:46:CYS:HA	2.03	0.41
2:b:118:MET:SD	2:b:150:VAL:HG12	2.61	0.41
8:h:61:THR:HG22	8:h:104:ALA:HB1	2.03	0.41
13:m:95:ASN:H	13:m:95:ASN:HD22	1.68	0.41
14:n:186:PRO:HG2	9:2:162:ALA:HA	2.02	0.41
10:3:53:ILE:HB	10:3:60:VAL:HG13	2.02	0.41
20:Z:248:TYR:N	29:I:54:ARG:HH22	2.18	0.41
21:N:647:ASP:HA	21:N:648:PRO:HD3	1.83	0.41
28:H:402:ILE:HD11	28:H:439:THR:HA	2.02	0.41
32:M:283:LEU:O	32:M:283:LEU:HG	2.21	0.41
5:e:107:ILE:HG21	5:e:112:LEU:HD23	2.02	0.41
1:A:87:ILE:HD12	7:G:158:TRP:CH2	2.56	0.41
8:1:151:PHE:HB2	8:1:163:PHE:CZ	2.55	0.41
20:Z:255:LEU:HD23	21:N:813:ARG:HD2	2.02	0.41
20:Z:748:LEU:CD2	29:I:85:PHE:HB2	2.51	0.41
24:Q:264:TYR:CD1	24:Q:330:LEU:HD23	2.56	0.41
1:a:41:ASN:HD21	1:a:174:LYS:H	1.69	0.41
7:g:70:VAL:HG11	7:g:112:PHE:CZ	2.56	0.41
11:k:37:GLN:HG2	11:k:189:ILE:HD12	2.03	0.41
4:D:155:ILE:HG23	5:E:82:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:739:ALA:HB2	20:Z:764:LEU:CD1	2.43	0.41
20:Z:748:LEU:O	29:I:84:PRO:HA	2.20	0.41
30:K:182:GLN:HA	30:K:185:ARG:HE	1.86	0.41
2:b:85:LEU:HD23	2:b:134:LEU:HD11	2.03	0.41
4:d:212:ILE:H	4:d:229:ILE:HD11	1.86	0.41
9:i:139:LEU:HD12	9:i:139:LEU:HA	1.98	0.41
9:i:177:LYS:O	9:i:181:ILE:HG13	2.21	0.41
6:F:71:GLY:HA3	6:F:222:PHE:CZ	2.57	0.40
28:H:271:PHE:CD1	28:H:273:ARG:CZ	3.04	0.40
20:Z:24:THR:HB	20:Z:25:PRO:CD	2.51	0.40
29:I:316:PHE:O	29:I:317:ASP:C	2.64	0.40
5:e:221:CYS:HB3	5:e:231:TYR:OH	2.21	0.40
9:i:196:LEU:HD13	13:6:204:ILE:HD12	2.04	0.40
14:n:158:GLN:CD	14:n:158:GLN:H	2.28	0.40
20:Z:738:TYR:CZ	29:I:69:LEU:C	3.00	0.40
3:c:174:THR:HA	3:c:177:GLN:HE21	1.87	0.40
14:n:133:MET:HG2	14:n:143:LEU:HB2	2.03	0.40
3:C:80:LEU:HD12	3:C:80:LEU:H	1.85	0.40
21:N:9:LEU:HD13	21:N:28:ILE:HA	2.02	0.40
23:P:281:ILE:HD13	23:P:281:ILE:HG21	1.91	0.40
26:U:194:LEU:HD22	27:O:392:TRP:CZ2	2.56	0.40
1:a:40:ILE:HD13	1:a:71:TYR:CE1	2.57	0.40
2:b:160:LYS:HD3	2:b:179:TRP:CZ2	2.57	0.40
3:C:15:PRO:HA	4:D:22:TYR:CD1	2.57	0.40
5:E:217:ALA:O	5:E:218:GLN:HB2	2.22	0.40
18:X:72:GLU:HB3	18:X:92:SER:O	2.21	0.40
20:Z:253:VAL:CG2	20:Z:287:ARG:HH22	2.35	0.40
20:Z:254:PRO:C	29:I:61:ARG:HH21	2.28	0.40
20:Z:724:GLU:HB3	29:I:66:LYS:HZ3	1.86	0.40
24:Q:352:GLU:HB3	24:Q:353:PRO:HD3	2.04	0.40
28:H:271:PHE:HD1	28:H:273:ARG:CZ	2.35	0.40
31:L:299:ARG:HH11	31:L:299:ARG:HD2	1.71	0.40
33:J:98:VAL:HG12	33:J:122:LEU:HD13	2.02	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	240/242 (99%)	230 (96%)	7 (3%)	3 (1%)	9 41
1	a	240/242 (99%)	230 (96%)	10 (4%)	0	100 100
2	B	244/246 (99%)	230 (94%)	10 (4%)	4 (2%)	7 37
2	b	244/246 (99%)	229 (94%)	11 (4%)	4 (2%)	7 37
3	C	239/241 (99%)	223 (93%)	12 (5%)	4 (2%)	7 35
3	c	239/241 (99%)	220 (92%)	16 (7%)	3 (1%)	9 41
4	D	236/252 (94%)	225 (95%)	8 (3%)	3 (1%)	9 41
4	d	250/252 (99%)	238 (95%)	9 (4%)	3 (1%)	10 42
5	E	242/244 (99%)	229 (95%)	10 (4%)	3 (1%)	10 42
5	e	242/244 (99%)	229 (95%)	9 (4%)	4 (2%)	7 35
6	F	230/232 (99%)	222 (96%)	7 (3%)	1 (0%)	30 67
6	f	230/232 (99%)	221 (96%)	8 (4%)	1 (0%)	30 67
7	G	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	7 35
7	g	242/244 (99%)	227 (94%)	13 (5%)	2 (1%)	16 52
8	1	194/196 (99%)	188 (97%)	6 (3%)	0	100 100
8	h	194/196 (99%)	183 (94%)	11 (6%)	0	100 100
9	2	224/226 (99%)	214 (96%)	7 (3%)	3 (1%)	9 41
9	i	224/226 (99%)	218 (97%)	6 (3%)	0	100 100
10	3	202/204 (99%)	186 (92%)	12 (6%)	4 (2%)	6 31
10	j	202/204 (99%)	190 (94%)	10 (5%)	2 (1%)	12 47
11	4	193/195 (99%)	182 (94%)	10 (5%)	1 (0%)	24 63
11	k	193/195 (99%)	177 (92%)	13 (7%)	3 (2%)	7 37
12	5	210/212 (99%)	200 (95%)	10 (5%)	0	100 100
12	l	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24 63
13	6	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	m	220/222 (99%)	202 (92%)	15 (7%)	3 (1%)	9 39
14	7	227/232 (98%)	212 (93%)	13 (6%)	2 (1%)	14 49
14	n	230/232 (99%)	212 (92%)	17 (7%)	1 (0%)	30 67
15	W	195/197 (99%)	180 (92%)	10 (5%)	5 (3%)	4 25
16	V	287/289 (99%)	260 (91%)	15 (5%)	12 (4%)	2 17
17	T	264/266 (99%)	238 (90%)	19 (7%)	7 (3%)	4 25
18	X	125/127 (98%)	108 (86%)	11 (9%)	6 (5%)	2 16
19	Y	87/89 (98%)	76 (87%)	8 (9%)	3 (3%)	3 20
20	Z	902/970 (93%)	821 (91%)	61 (7%)	20 (2%)	5 28
21	N	920/922 (100%)	863 (94%)	45 (5%)	12 (1%)	9 41
22	S	473/475 (100%)	442 (93%)	21 (4%)	10 (2%)	5 29
23	P	438/440 (100%)	416 (95%)	14 (3%)	8 (2%)	6 33
24	Q	432/434 (100%)	396 (92%)	24 (6%)	12 (3%)	4 24
25	R	403/405 (100%)	379 (94%)	19 (5%)	5 (1%)	10 42
26	U	302/304 (99%)	284 (94%)	15 (5%)	3 (1%)	12 47
27	O	386/388 (100%)	370 (96%)	12 (3%)	4 (1%)	12 47
28	H	424/426 (100%)	384 (91%)	26 (6%)	14 (3%)	3 20
29	I	383/385 (100%)	342 (89%)	30 (8%)	11 (3%)	3 23
30	K	392/394 (100%)	347 (88%)	37 (9%)	8 (2%)	6 31
31	L	386/388 (100%)	353 (92%)	24 (6%)	9 (2%)	5 28
32	M	419/421 (100%)	376 (90%)	34 (8%)	9 (2%)	5 29
33	J	403/405 (100%)	357 (89%)	32 (8%)	14 (4%)	3 20
All	All	13924/14101 (99%)	12941 (93%)	749 (5%)	234 (2%)	9 35

All (234) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	PHE
3	C	14	SER
4	D	166	ARG
15	W	165	GLN
16	V	112	PRO
16	V	176	ASN
17	T	43	ASP

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Mol	Chain	Res	Type
17	T	134	LYS
17	T	251	HIS
18	X	29	VAL
19	Y	44	ALA
20	Z	24	THR
20	Z	85	VAL
20	Z	870	ALA
21	N	790	GLU
22	S	97	THR
22	S	98	SER
22	S	116	ALA
22	S	118	PHE
24	Q	67	THR
24	Q	68	MET
24	Q	253	ASN
25	R	71	LEU
27	O	183	ASN
28	H	71	GLU
28	H	138	GLU
28	H	190	ARG
28	H	273	ARG
28	H	323	ALA
29	I	116	ASP
29	I	125	MET
29	I	213	ILE
30	K	236	ARG
30	K	398	ASN
31	L	343	LEU
32	M	315	PHE
32	M	317	SER
32	M	339	ARG
33	J	284	THR
2	b	52	SER
4	d	40	ASN
4	d	204	GLN
5	e	12	VAL
6	f	7	ASP
7	g	10	LEU
10	j	32	GLN
10	j	192	LYS
11	k	131	GLY
13	m	138	SER

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Mol	Chain	Res	Type
14	n	114	ALA
2	B	52	SER
3	C	64	GLU
4	D	70	HIS
9	2	235	PRO
9	2	249	ILE
10	3	6	SER
10	3	40	PHE
14	7	252	TRP
15	W	179	ARG
15	W	190	ILE
18	X	116	ALA
20	Z	728	LYS
20	Z	729	GLU
21	N	175	ASP
21	N	725	LEU
22	S	44	THR
22	S	69	LEU
23	P	2	SER
23	P	209	LYS
23	P	397	ALA
23	P	403	GLU
24	Q	46	VAL
24	Q	128	GLU
24	Q	252	HIS
24	Q	353	PRO
24	Q	405	GLN
25	R	263	ARG
25	R	375	LYS
26	U	218	GLU
28	H	194	SER
29	I	115	ASP
29	I	344	ILE
30	K	331	PRO
30	K	366	ALA
30	K	423	LYS
31	L	52	ALA
31	L	406	ASP
33	J	110	SER
33	J	287	ASN
33	J	320	SER
5	e	73	HIS

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Mol	Chain	Res	Type
5	e	126	GLY
11	k	132	ALA
1	A	11	GLY
1	A	37	GLN
1	A	49	ASP
3	C	184	MET
3	C	221	ASN
5	E	126	GLY
10	3	182	GLY
13	6	138	SER
15	W	136	ASN
17	T	135	ASN
17	T	141	LEU
17	T	173	GLU
18	X	19	GLU
18	X	115	SER
19	Y	35	PHE
20	Z	825	ALA
20	Z	887	GLY
20	Z	940	GLY
20	Z	947	GLY
21	N	148	SER
21	N	393	SER
21	N	395	ALA
21	N	777	ALA
21	N	781	ALA
21	N	831	GLU
22	S	84	ASP
22	S	108	ALA
22	S	132	ALA
23	P	131	PHE
23	P	328	ALA
23	P	331	GLY
24	Q	42	ALA
26	U	133	PRO
28	H	75	GLY
28	H	315	GLY
28	H	325	GLY
28	H	368	PRO
28	H	370	ARG
30	K	36	ASN
31	L	319	GLY

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Mol	Chain	Res	Type
32	M	179	THR
32	M	367	LYS
33	J	352	GLY
33	J	353	CYS
2	b	98	LYS
5	e	151	ASP
7	g	63	LYS
2	B	51	SER
4	D	40	ASN
7	G	13	SER
7	G	187	LEU
10	3	32	GLN
11	4	132	ALA
13	6	27	ASP
13	6	47	TYR
14	7	111	ASN
16	V	175	SER
16	V	183	ALA
16	V	186	GLN
16	V	223	SER
16	V	259	LYS
16	V	262	THR
16	V	275	ASP
18	X	78	ILE
18	X	113	GLU
20	Z	82	MET
20	Z	142	ASP
20	Z	233	LEU
20	Z	578	GLY
20	Z	926	ASN
21	N	832	HIS
22	S	327	ILE
23	P	126	THR
24	Q	149	LYS
24	Q	170	ASP
25	R	280	ILE
28	H	70	LYS
28	H	466	TYR
29	I	289	THR
29	I	298	GLY
29	I	375	VAL
31	L	330	PRO

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Mol	Chain	Res	Type
31	L	432	ILE
32	M	99	SER
32	M	240	ASN
33	J	141	LYS
33	J	252	SER
33	J	337	LEU
33	J	340	GLY
33	J	398	ILE
2	b	41	ASN
3	c	70	ASN
4	d	70	HIS
11	k	129	PRO
13	m	40	ASP
2	B	203	GLU
5	E	13	SER
6	F	59	TYR
7	G	63	LYS
7	G	73	HIS
15	W	180	LEU
16	V	102	GLN
16	V	185	ILE
17	T	227	PRO
19	Y	31	GLU
20	Z	25	PRO
20	Z	65	GLU
20	Z	463	HIS
20	Z	513	ALA
20	Z	557	GLU
25	R	125	GLU
27	O	119	SER
27	O	226	LYS
29	I	143	PRO
29	I	164	ALA
30	K	125	THR
30	K	314	VAL
31	L	289	ARG
31	L	374	PHE
32	M	94	LYS
32	M	109	ASP
33	J	311	ASP
33	J	341	ILE
33	J	373	ARG

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Mol	Chain	Res	Type
3	c	132	GLY
12	l	173	GLY
9	2	209	ILE
20	Z	802	ASP
21	N	123	PHE
21	N	894	ARG
24	Q	386	PHE
26	U	42	ASN
31	L	350	PRO
2	b	228	PRO
13	m	137	GLY
16	V	143	PRO
3	c	14	SER
27	O	305	ILE
5	E	12	VAL
28	H	152	ILE
29	I	297	GLY

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	206/206 (100%)	201 (98%)	5 (2%)	43	63
1	a	206/206 (100%)	204 (99%)	2 (1%)	68	76
2	B	205/205 (100%)	200 (98%)	5 (2%)	43	63
2	b	205/205 (100%)	202 (98%)	3 (2%)	57	71
3	C	201/201 (100%)	195 (97%)	6 (3%)	36	57
3	c	201/201 (100%)	196 (98%)	5 (2%)	42	62
4	D	210/224 (94%)	203 (97%)	7 (3%)	33	55
4	d	224/224 (100%)	221 (99%)	3 (1%)	61	72
5	E	200/200 (100%)	192 (96%)	8 (4%)	28	49
5	e	200/200 (100%)	196 (98%)	4 (2%)	48	66
6	F	191/191 (100%)	183 (96%)	8 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	191/191 (100%)	185 (97%)	6 (3%)	35	56
7	G	201/201 (100%)	195 (97%)	6 (3%)	36	57
7	g	201/201 (100%)	199 (99%)	2 (1%)	68	76
8	1	162/162 (100%)	157 (97%)	5 (3%)	35	56
8	h	162/162 (100%)	157 (97%)	5 (3%)	35	56
9	2	185/185 (100%)	180 (97%)	5 (3%)	39	60
9	i	185/185 (100%)	180 (97%)	5 (3%)	39	60
10	3	172/172 (100%)	168 (98%)	4 (2%)	44	63
10	j	172/172 (100%)	168 (98%)	4 (2%)	44	63
11	4	173/173 (100%)	168 (97%)	5 (3%)	37	58
11	k	173/173 (100%)	165 (95%)	8 (5%)	24	46
12	5	169/169 (100%)	166 (98%)	3 (2%)	51	67
12	l	169/169 (100%)	163 (96%)	6 (4%)	31	52
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%)	189 (97%)	6 (3%)	35	56
14	n	198/198 (100%)	193 (98%)	5 (2%)	42	62
15	W	171/171 (100%)	167 (98%)	4 (2%)	44	63
16	V	253/253 (100%)	244 (96%)	9 (4%)	31	52
17	T	249/249 (100%)	242 (97%)	7 (3%)	38	59
18	X	116/116 (100%)	112 (97%)	4 (3%)	32	54
19	Y	81/81 (100%)	77 (95%)	4 (5%)	22	44
20	Z	773/828 (93%)	751 (97%)	22 (3%)	38	59
21	N	776/776 (100%)	759 (98%)	17 (2%)	45	64
22	S	447/447 (100%)	437 (98%)	10 (2%)	45	64
23	P	412/412 (100%)	406 (98%)	6 (2%)	57	71
24	Q	391/391 (100%)	378 (97%)	13 (3%)	33	55
25	R	356/356 (100%)	349 (98%)	7 (2%)	48	66
26	U	277/277 (100%)	269 (97%)	8 (3%)	37	58
27	O	363/363 (100%)	354 (98%)	9 (2%)	42	62
28	H	361/361 (100%)	347 (96%)	14 (4%)	28	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	I	342/342 (100%)	329 (96%)	13 (4%)	29	51
30	K	346/346 (100%)	332 (96%)	14 (4%)	28	49
31	L	332/332 (100%)	316 (95%)	16 (5%)	23	45
32	M	364/364 (100%)	354 (97%)	10 (3%)	39	60
33	J	352/352 (100%)	338 (96%)	14 (4%)	28	49
All	All	12089/12161 (99%)	11747 (97%)	342 (3%)	38	59

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	19	PHE
1	a	195	ASN
2	b	52	SER
2	b	74	VAL
2	b	146	SER
3	c	66	LEU
3	c	70	ASN
3	c	130	PRO
3	c	222	ASP
3	c	231	LYS
4	d	5	ASP
4	d	10	ILE
4	d	24	LEU
5	e	40	ILE
5	e	67	ILE
5	e	88	MET
5	e	208	MET
6	f	54	ASP
6	f	72	LEU
6	f	153	VAL
6	f	156	LEU
6	f	159	THR
6	f	219	ASP
7	g	107	ILE
7	g	224	THR
8	h	101	ASN
8	h	135	ILE
8	h	144	TYR
8	h	181	VAL
8	h	188	THR

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Mol	Chain	Res	Type
9	i	68	PRO
9	i	106	VAL
9	i	109	LEU
9	i	155	SER
9	i	196	LEU
10	j	13	VAL
10	j	49	VAL
10	j	176	ASP
10	j	190	ILE
11	k	4	ILE
11	k	7	ILE
11	k	39	SER
11	k	66	LEU
11	k	74	GLU
11	k	92	ILE
11	k	101	ASN
11	k	153	THR
12	l	79	LEU
12	l	83	PHE
12	l	92	ASP
12	l	157	ILE
12	l	161	LEU
12	l	204	VAL
13	m	73	VAL
13	m	95	ASN
13	m	115	VAL
13	m	136	VAL
13	m	155	MET
14	n	39	VAL
14	n	73	GLU
14	n	132	VAL
14	n	175	LEU
14	n	253	ASP
1	A	49	ASP
1	A	53	VAL
1	A	76	SER
1	A	176	GLN
1	A	245	LEU
2	B	43	VAL
2	B	96	SER
2	B	97	TYR
2	B	164	ILE

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Mol	Chain	Res	Type
2	B	225	THR
3	C	45	VAL
3	C	51	LYS
3	C	118	ILE
3	C	184	MET
3	C	231	LYS
3	C	232	PRO
4	D	5	ASP
4	D	59	ILE
4	D	68	ASP
4	D	73	LEU
4	D	126	VAL
4	D	168	SER
4	D	194	LEU
5	E	22	PHE
5	E	42	THR
5	E	78	MET
5	E	81	LEU
5	E	97	VAL
5	E	100	ASN
5	E	112	LEU
5	E	144	ILE
6	F	7	ASP
6	F	42	THR
6	F	45	VAL
6	F	72	LEU
6	F	153	VAL
6	F	198	SER
6	F	204	GLU
6	F	208	VAL
7	G	11	SER
7	G	18	ASP
7	G	46	VAL
7	G	100	LYS
7	G	109	ILE
7	G	224	THR
8	1	12	ILE
8	1	30	THR
8	1	90	VAL
8	1	135	ILE
8	1	162	ASP
9	2	137	SER

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Mol	Chain	Res	Type
9	2	161	LEU
9	2	230	LYS
9	2	236	ARG
9	2	252	ILE
10	3	13	VAL
10	3	18	LYS
10	3	26	ASP
10	3	71	THR
11	4	58	GLU
11	4	101	ASN
11	4	126	VAL
11	4	162	LYS
11	4	183	ILE
12	5	76	THR
12	5	79	LEU
12	5	151	VAL
13	6	30	VAL
13	6	42	SER
13	6	49	PRO
13	6	216	THR
13	6	217	LYS
14	7	37	PRO
14	7	53	VAL
14	7	101	LYS
14	7	165	LEU
14	7	173	PRO
14	7	205	VAL
15	W	14	GLU
15	W	79	THR
15	W	93	ILE
15	W	108	GLN
16	V	24	LYS
16	V	32	ILE
16	V	45	VAL
16	V	71	MET
16	V	98	THR
16	V	117	TRP
16	V	122	ASP
16	V	199	LEU
16	V	300	VAL
17	T	29	PRO
17	T	46	ILE

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Mol	Chain	Res	Type
17	T	106	ILE
17	T	150	ARG
17	T	172	SER
17	T	219	LYS
17	T	259	ILE
18	X	14	VAL
18	X	43	LEU
18	X	60	GLU
18	X	114	LEU
19	Y	19	LYS
19	Y	20	LYS
19	Y	59	ILE
19	Y	66	ASP
20	Z	27	LYS
20	Z	57	LYS
20	Z	64	TYR
20	Z	146	PHE
20	Z	171	LYS
20	Z	206	ASP
20	Z	221	VAL
20	Z	253	VAL
20	Z	255	LEU
20	Z	257	PRO
20	Z	386	VAL
20	Z	563	VAL
20	Z	566	LEU
20	Z	611	THR
20	Z	728	LYS
20	Z	734	ASP
20	Z	745	LEU
20	Z	748	LEU
20	Z	842	GLN
20	Z	918	ASP
20	Z	951	GLN
20	Z	970	TYR
21	N	57	ASP
21	N	59	GLU
21	N	102	VAL
21	N	118	THR
21	N	274	VAL
21	N	307	LYS
21	N	360	GLN

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Mol	Chain	Res	Type
21	N	385	VAL
21	N	599	TYR
21	N	623	PHE
21	N	634	LEU
21	N	681	ASN
21	N	703	GLN
21	N	821	LYS
21	N	832	HIS
21	N	852	ASN
21	N	885	ILE
22	S	75	CYS
22	S	89	LYS
22	S	113	SER
22	S	131	THR
22	S	155	LEU
22	S	163	VAL
22	S	370	LEU
22	S	373	LYS
22	S	471	LEU
22	S	475	TYR
23	P	100	VAL
23	P	110	LEU
23	P	124	VAL
23	P	298	SER
23	P	396	PRO
23	P	399	ILE
24	Q	8	LEU
24	Q	26	VAL
24	Q	83	GLU
24	Q	106	GLN
24	Q	120	LYS
24	Q	164	GLU
24	Q	209	TYR
24	Q	221	MET
24	Q	275	ILE
24	Q	343	LEU
24	Q	408	THR
24	Q	409	TYR
24	Q	426	LEU
25	R	71	LEU
25	R	92	ILE
25	R	94	PHE

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Mol	Chain	Res	Type
25	R	176	ARG
25	R	299	SER
25	R	317	ILE
25	R	395	ASN
26	U	37	ILE
26	U	71	ASN
26	U	74	GLU
26	U	89	LEU
26	U	127	GLN
26	U	143	VAL
26	U	190	LEU
26	U	261	LEU
27	O	6	GLU
27	O	26	PHE
27	O	237	PRO
27	O	258	LEU
27	O	270	ILE
27	O	327	LEU
27	O	343	GLN
27	O	359	SER
27	O	362	GLN
28	H	78	PRO
28	H	128	ASN
28	H	170	GLU
28	H	193	PRO
28	H	203	LYS
28	H	241	ASP
28	H	257	THR
28	H	304	CYS
28	H	367	ARG
28	H	370	ARG
28	H	394	LYS
28	H	423	CYS
28	H	436	LYS
28	H	442	ASP
29	I	71	LEU
29	I	127	ASP
29	I	147	VAL
29	I	184	ILE
29	I	199	GLU
29	I	247	ILE
29	I	253	ILE

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Mol	Chain	Res	Type
29	I	330	LYS
29	I	343	ARG
29	I	351	GLU
29	I	353	PRO
29	I	369	MET
29	I	385	ASP
30	K	81	ARG
30	K	89	ILE
30	K	125	THR
30	K	129	GLU
30	K	133	PRO
30	K	137	VAL
30	K	230	THR
30	K	237	VAL
30	K	264	ASN
30	K	274	VAL
30	K	292	VAL
30	K	329	LEU
30	K	335	ASP
30	K	422	ASP
31	L	54	ASN
31	L	66	GLU
31	L	70	TYR
31	L	107	GLU
31	L	112	LEU
31	L	131	VAL
31	L	148	LEU
31	L	158	ILE
31	L	177	GLU
31	L	178	ILE
31	L	196	VAL
31	L	229	THR
31	L	283	VAL
31	L	362	LYS
31	L	374	PHE
31	L	421	LYS
32	M	36	LEU
32	M	86	MET
32	M	157	ASP
32	M	168	LYS
32	M	253	GLN
32	M	291	PHE

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Mol	Chain	Res	Type
32	M	340	SER
32	M	351	LEU
32	M	403	LEU
32	M	409	SER
33	J	10	ILE
33	J	30	THR
33	J	34	ILE
33	J	36	SER
33	J	119	SER
33	J	142	VAL
33	J	155	LYS
33	J	179	ILE
33	J	186	ILE
33	J	236	MET
33	J	286	LYS
33	J	297	LEU
33	J	336	ASN
33	J	338	THR

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

Mol	Chain	Res	Type
1	a	41	ASN
1	a	56	GLN
1	a	126	GLN
1	a	130	GLN
1	a	184	ASN
2	b	94	HIS
2	b	123	GLN
2	b	143	ASN
2	b	218	ASN
3	c	21	GLN
3	c	70	ASN
3	c	89	ASN
3	c	152	ASN
3	c	177	GLN
3	c	227	GLN
4	d	19	GLN
4	d	96	HIS
4	d	149	GLN
4	d	167	ASN
4	d	209	ASN

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Mol	Chain	Res	Type
4	d	230	ASN
4	d	241	GLN
4	d	246	GLN
5	e	73	HIS
5	e	108	ASN
5	e	147	HIS
5	e	154	GLN
5	e	157	HIS
5	e	188	HIS
5	e	206	GLN
5	e	233	ASN
6	f	43	HIS
6	f	110	HIS
6	f	166	GLN
6	f	199	GLN
7	g	12	ASN
7	g	21	ASN
7	g	68	GLN
7	g	87	HIS
7	g	123	HIS
7	g	144	ASN
7	g	147	HIS
7	g	182	HIS
7	g	204	HIS
7	g	207	ASN
7	g	244	GLN
8	h	71	HIS
8	h	78	GLN
8	h	101	ASN
8	h	170	GLN
9	i	39	ASN
9	i	59	ASN
9	i	64	HIS
9	i	170	HIS
9	i	189	GLN
9	i	194	ASN
9	i	223	ASN
9	i	229	GLN
10	j	38	ASN
10	j	64	ASN
10	j	145	GLN
10	j	204	GLN

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Mol	Chain	Res	Type
11	k	86	GLN
11	k	101	ASN
11	k	112	ASN
11	k	133	HIS
11	k	146	HIS
11	k	166	GLN
12	l	241	HIS
12	l	254	HIS
12	l	263	HIS
13	m	16	ASN
13	m	44	ASN
13	m	95	ASN
13	m	100	ASN
13	m	116	HIS
13	m	166	ASN
14	n	70	ASN
14	n	94	GLN
14	n	95	HIS
14	n	145	ASN
14	n	182	HIS
14	n	185	ASN
14	n	212	ASN
14	n	236	ASN
1	A	27	GLN
1	A	41	ASN
1	A	56	GLN
1	A	92	ASN
1	A	123	ASN
1	A	193	HIS
1	A	209	HIS
2	B	139	HIS
2	B	149	GLN
3	C	31	HIS
3	C	103	ASN
3	C	156	ASN
3	C	221	ASN
4	D	55	GLN
4	D	117	GLN
4	D	122	GLN
4	D	178	ASN
5	E	99	HIS
5	E	147	HIS

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Mol	Chain	Res	Type
5	E	157	HIS
5	E	188	HIS
5	E	218	GLN
6	F	69	HIS
6	F	117	GLN
6	F	121	GLN
7	G	12	ASN
7	G	62	GLN
7	G	64	ASN
7	G	90	ASN
7	G	118	GLN
7	G	123	HIS
7	G	207	ASN
8	1	47	HIS
8	1	69	GLN
8	1	150	ASN
8	1	166	HIS
9	2	38	ASN
9	2	120	GLN
9	2	138	HIS
9	2	173	GLN
9	2	201	ASN
10	3	64	ASN
10	3	89	GLN
10	3	145	GLN
10	3	204	GLN
11	4	63	ASN
11	4	78	GLN
11	4	101	ASN
11	4	112	ASN
11	4	147	HIS
11	4	191	GLN
12	5	218	ASN
12	5	241	HIS
12	5	265	ASN
13	6	173	ASN
13	6	205	GLN
14	7	51	ASN
14	7	141	ASN
14	7	164	ASN
14	7	185	ASN
15	W	29	GLN

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Mol	Chain	Res	Type
15	W	47	ASN
15	W	77	HIS
15	W	86	HIS
15	W	100	HIS
15	W	102	GLN
15	W	162	ASN
15	W	165	GLN
16	V	64	ASN
16	V	73	GLN
16	V	102	GLN
16	V	124	ASN
16	V	126	GLN
16	V	204	HIS
16	V	222	GLN
16	V	250	GLN
16	V	274	GLN
17	T	17	ASN
17	T	47	GLN
17	T	74	ASN
17	T	84	GLN
17	T	112	ASN
17	T	116	GLN
17	T	204	ASN
17	T	225	ASN
17	T	230	ASN
17	T	236	ASN
18	X	38	ASN
18	X	130	ASN
19	Y	56	GLN
19	Y	75	ASN
20	Z	9	GLN
20	Z	10	GLN
20	Z	23	GLN
20	Z	214	HIS
20	Z	275	GLN
20	Z	396	ASN
20	Z	429	ASN
20	Z	434	GLN
20	Z	502	ASN
20	Z	532	HIS
20	Z	577	GLN
20	Z	622	HIS

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Mol	Chain	Res	Type
20	Z	760	HIS
20	Z	763	HIS
20	Z	766	HIS
20	Z	769	ASN
20	Z	789	GLN
20	Z	868	ASN
20	Z	897	HIS
20	Z	917	ASN
20	Z	931	GLN
21	N	17	GLN
21	N	41	ASN
21	N	187	ASN
21	N	216	ASN
21	N	226	ASN
21	N	231	ASN
21	N	267	GLN
21	N	306	ASN
21	N	308	ASN
21	N	329	HIS
21	N	360	GLN
21	N	525	ASN
21	N	564	ASN
21	N	607	GLN
21	N	613	HIS
21	N	616	HIS
21	N	672	ASN
21	N	681	ASN
21	N	688	ASN
21	N	712	ASN
21	N	716	GLN
21	N	719	ASN
21	N	824	ASN
21	N	877	GLN
21	N	922	GLN
22	S	32	GLN
22	S	79	ASN
22	S	99	ASN
22	S	122	ASN
22	S	135	ASN
22	S	143	GLN
22	S	205	ASN
22	S	206	GLN

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Mol	Chain	Res	Type
22	S	227	ASN
22	S	303	ASN
22	S	317	HIS
22	S	334	HIS
22	S	412	ASN
22	S	417	GLN
22	S	438	HIS
23	P	230	HIS
23	P	275	ASN
23	P	278	ASN
23	P	282	HIS
23	P	285	GLN
23	P	334	ASN
23	P	337	HIS
23	P	385	ASN
24	Q	16	ASN
24	Q	37	GLN
24	Q	145	HIS
24	Q	178	HIS
24	Q	190	ASN
24	Q	206	ASN
24	Q	273	ASN
24	Q	280	ASN
24	Q	283	ASN
24	Q	320	GLN
24	Q	361	HIS
24	Q	372	GLN
24	Q	392	GLN
24	Q	405	GLN
24	Q	420	ASN
24	Q	425	GLN
25	R	130	GLN
25	R	136	ASN
25	R	143	GLN
25	R	149	ASN
25	R	184	GLN
25	R	314	ASN
25	R	325	HIS
25	R	378	ASN
25	R	395	ASN
26	U	70	HIS
26	U	192	ASN

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Mol	Chain	Res	Type
26	U	223	HIS
26	U	230	GLN
26	U	234	ASN
26	U	252	HIS
26	U	260	ASN
27	O	186	ASN
27	O	211	GLN
27	O	235	HIS
27	O	244	ASN
27	O	289	GLN
27	O	318	HIS
27	O	345	ASN
27	O	354	GLN
28	H	128	ASN
28	H	130	ASN
28	H	148	ASN
28	H	151	GLN
28	H	182	ASN
28	H	392	HIS
28	H	413	ASN
29	I	78	ASN
29	I	150	HIS
29	I	161	GLN
29	I	254	GLN
29	I	274	ASN
29	I	410	GLN
29	I	431	ASN
30	K	35	ASN
30	K	42	ASN
30	K	64	GLN
30	K	98	GLN
30	K	140	HIS
30	K	194	GLN
30	K	200	GLN
30	K	264	ASN
31	L	54	ASN
31	L	67	HIS
31	L	73	GLN
31	L	76	GLN
31	L	99	GLN
31	L	103	GLN
31	L	133	ASN

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Mol	Chain	Res	Type
31	L	189	GLN
31	L	203	ASN
31	L	242	ASN
31	L	320	GLN
32	M	55	ASN
32	M	72	ASN
32	M	96	ASN
32	M	105	ASN
32	M	125	GLN
32	M	143	ASN
32	M	238	GLN
32	M	253	GLN
32	M	377	GLN
32	M	412	HIS
33	J	40	ASN
33	J	52	ASN
33	J	123	HIS
33	J	205	HIS
33	J	240	HIS
33	J	277	ASN
33	J	331	HIS
33	J	391	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ADP	J	501	35	28,29,29	2.15	4 (14%)	43,45,45	1.38	5 (11%)
34	ATP	M	501	35	32,33,33	3.01	4 (12%)	48,52,52	1.56	11 (22%)
34	ATP	L	501	35	32,33,33	3.90	7 (21%)	48,52,52	1.70	11 (22%)
34	ATP	K	501	35	32,33,33	3.22	7 (21%)	48,52,52	1.72	7 (14%)
34	ATP	I	501	35	32,33,33	4.11	6 (18%)	48,52,52	1.58	9 (18%)
34	ATP	H	501	35	32,33,33	3.29	8 (25%)	48,52,52	1.56	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	J	501	35	-	6/16/32/32	0/3/3/3
34	ATP	M	501	35	-	9/22/38/38	0/3/3/3
34	ATP	L	501	35	-	5/22/38/38	0/3/3/3
34	ATP	K	501	35	-	2/22/38/38	0/3/3/3
34	ATP	I	501	35	-	9/22/38/38	0/3/3/3
34	ATP	H	501	35	-	9/22/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	L	501	ATP	PB-O3B	16.28	1.77	1.59
34	I	501	ATP	PB-O3A	14.72	1.75	1.59
34	I	501	ATP	PB-O3B	14.13	1.74	1.59
34	H	501	ATP	PB-O3A	13.29	1.73	1.59
34	L	501	ATP	PB-O3A	13.07	1.73	1.59
34	M	501	ATP	PB-O3B	10.35	1.70	1.59
34	K	501	ATP	PB-O3A	10.26	1.70	1.59
34	H	501	ATP	PA-O3A	9.48	1.69	1.59
34	K	501	ATP	PA-O3A	9.44	1.69	1.59
34	M	501	ATP	PB-O3A	9.39	1.69	1.59
34	K	501	ATP	PB-O3B	9.14	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	501	ADP	PA-O3A	8.93	1.69	1.59
34	M	501	ATP	PA-O3A	7.75	1.67	1.59
34	I	501	ATP	PA-O3A	7.54	1.67	1.59
34	I	501	ATP	C5-N7	-4.93	1.30	1.39
34	H	501	ATP	PB-O3B	4.32	1.64	1.59
36	J	501	ADP	C5-C4	3.70	1.45	1.39
34	H	501	ATP	C4-N3	3.50	1.41	1.34
34	L	501	ATP	C2'-C1'	-3.22	1.43	1.53
34	K	501	ATP	C3'-C4'	3.12	1.60	1.53
34	H	501	ATP	C5-N7	-2.78	1.34	1.39
34	K	501	ATP	C5-C6	2.74	1.48	1.41
34	M	501	ATP	C1'-N9	-2.71	1.38	1.46
36	J	501	ADP	C4-N3	2.68	1.39	1.34
34	L	501	ATP	O4'-C4'	-2.62	1.39	1.45
34	I	501	ATP	O4'-C1'	2.51	1.47	1.42
34	I	501	ATP	C4-N3	2.49	1.39	1.34
34	H	501	ATP	O4'-C4'	2.38	1.50	1.45
34	K	501	ATP	C4-N9	2.31	1.42	1.37
34	L	501	ATP	PA-O2A	-2.27	1.44	1.55
34	L	501	ATP	C6-N6	2.25	1.40	1.34
34	K	501	ATP	C2-N3	2.24	1.37	1.33
34	H	501	ATP	C2-N1	2.12	1.37	1.33
36	J	501	ADP	C1'-N9	2.08	1.52	1.46
34	H	501	ATP	C8-N9	-2.05	1.34	1.37
34	L	501	ATP	C6-N1	2.03	1.41	1.35

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	K	501	ATP	N6-C6-N1	6.21	132.21	118.38
34	H	501	ATP	C6-C5-C4	5.26	124.36	117.18
34	K	501	ATP	O4'-C1'-N9	4.66	117.04	108.09
34	M	501	ATP	N3-C2-N1	4.39	135.22	128.58
34	L	501	ATP	O4'-C1'-N9	4.33	116.41	108.09
36	J	501	ADP	O4'-C1'-N9	4.06	115.88	108.09
34	I	501	ATP	N6-C6-N1	3.87	127.00	118.38
34	L	501	ATP	C5'-C4'-C3'	3.80	128.89	115.21
36	J	501	ADP	C1'-N9-C8	3.78	135.49	127.09
34	I	501	ATP	O4'-C4'-C3'	-3.69	97.82	105.15
34	I	501	ATP	C5-N7-C8	3.65	109.19	103.45
34	K	501	ATP	C5-C6-N6	-3.44	114.78	123.29
36	J	501	ADP	C4-N9-C1'	-3.36	118.76	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	501	ATP	N6-C6-N1	3.36	125.86	118.38
34	M	501	ATP	N6-C6-N1	3.20	125.50	118.38
34	K	501	ATP	O3B-PB-O1B	-3.14	101.27	110.70
34	L	501	ATP	N6-C6-N1	3.10	125.29	118.38
34	M	501	ATP	C6-C5-C4	3.08	121.38	117.18
34	H	501	ATP	C1'-N9-C8	3.07	133.91	127.09
34	K	501	ATP	C6-C5-C4	3.03	121.31	117.18
34	L	501	ATP	O3B-PB-O1B	-2.91	101.94	110.70
34	L	501	ATP	O3A-PA-O1A	-2.90	102.00	110.70
34	M	501	ATP	O2B-PB-O3A	2.87	115.03	107.27
34	L	501	ATP	C4-N9-C1'	2.77	133.10	126.63
34	L	501	ATP	C4-N9-C8	-2.76	102.84	105.74
34	K	501	ATP	C4-N9-C8	-2.72	102.88	105.74
34	M	501	ATP	O3B-PB-O1B	-2.63	102.78	110.70
34	H	501	ATP	C4-N9-C1'	-2.61	120.53	126.63
34	I	501	ATP	C6-C5-C4	2.60	120.73	117.18
36	J	501	ADP	N3-C2-N1	2.58	132.48	128.58
34	I	501	ATP	N3-C2-N1	2.47	132.32	128.58
34	H	501	ATP	C5-C4-N3	-2.47	123.31	126.72
34	L	501	ATP	C5-C6-N6	-2.42	117.31	123.29
34	H	501	ATP	C4-C5-N7	-2.39	107.85	110.58
34	M	501	ATP	O4'-C4'-C3'	-2.37	100.45	105.15
34	L	501	ATP	O2B-PB-O1B	2.37	123.46	112.44
34	L	501	ATP	C2'-C1'-N9	-2.37	107.43	113.30
34	H	501	ATP	C6-C5-N7	-2.36	127.55	132.09
34	I	501	ATP	N9-C8-N7	-2.36	110.59	113.94
34	I	501	ATP	O3B-PG-O1G	-2.30	98.95	111.04
34	M	501	ATP	O3A-PA-O1A	-2.23	104.00	110.70
34	K	501	ATP	C5-N7-C8	2.21	106.93	103.45
34	H	501	ATP	C5-C6-N1	-2.21	111.89	117.51
34	M	501	ATP	C2-N1-C6	-2.17	115.16	118.73
36	J	501	ADP	C2'-C1'-N9	-2.15	107.95	113.30
34	I	501	ATP	O4'-C1'-N9	2.15	112.21	108.09
34	L	501	ATP	N9-C8-N7	2.13	116.97	113.94
34	I	501	ATP	C1'-N9-C8	2.12	131.80	127.09
34	H	501	ATP	O2B-PB-O3B	-2.11	101.56	107.27
34	M	501	ATP	C5'-C4'-C3'	2.04	122.56	115.21
34	H	501	ATP	C5-N7-C8	2.02	106.63	103.45
34	M	501	ATP	C2-N3-C4	-2.02	106.89	111.83
34	M	501	ATP	O3G-PG-O2G	2.01	115.35	107.80

There are no chirality outliers.

All (40) torsion outliers are listed below:

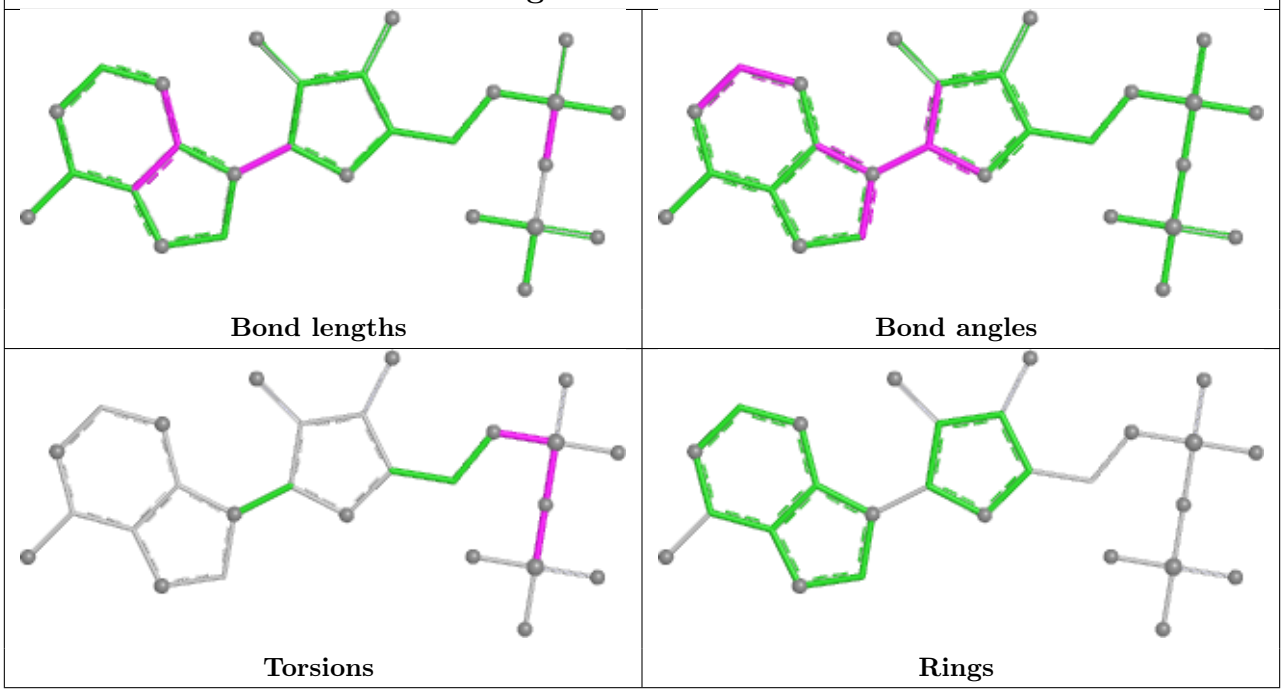
Mol	Chain	Res	Type	Atoms
34	H	501	ATP	PB-O3B-PG-O2G
34	H	501	ATP	C5'-O5'-PA-O1A
34	H	501	ATP	C5'-O5'-PA-O2A
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O3A
34	L	501	ATP	PB-O3B-PG-O2G
34	L	501	ATP	C5'-O5'-PA-O1A
34	L	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
34	M	501	ATP	PB-O3B-PG-O3G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

There are no ring outliers.

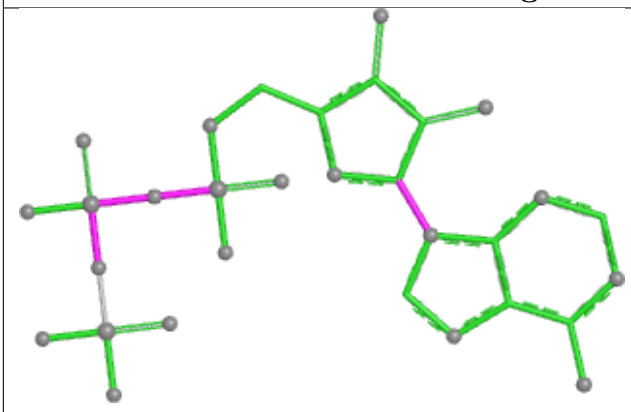
No monomer is involved in short contacts.

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.

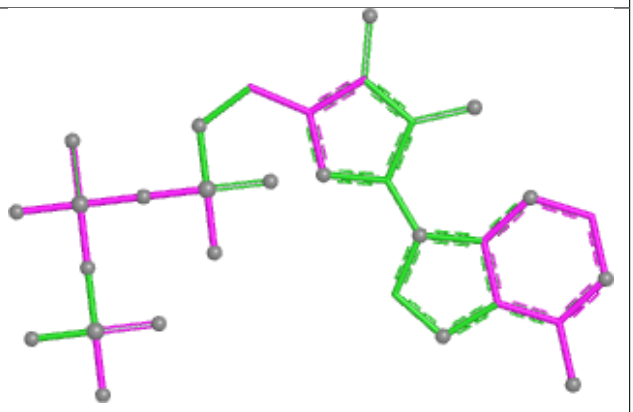
Ligand ADP J 501



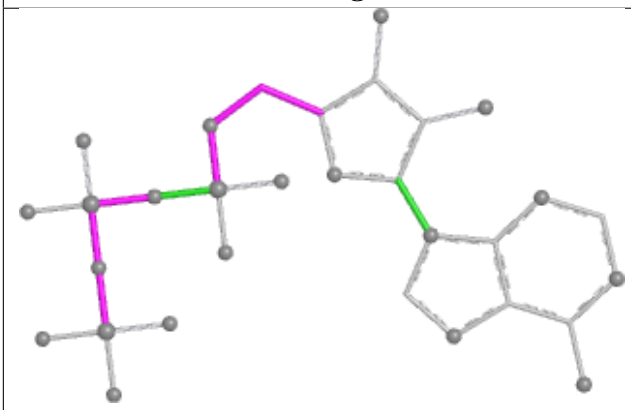
Ligand ATP M 501



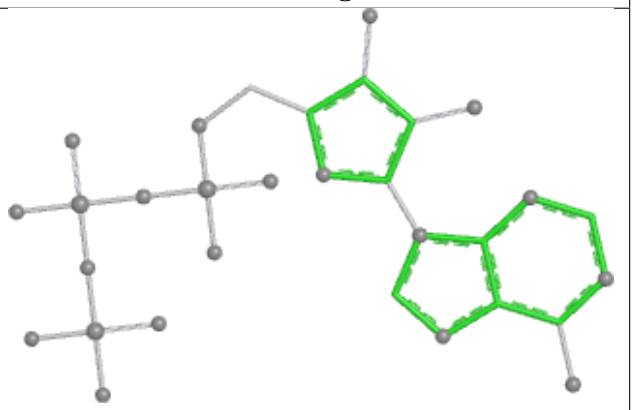
Bond lengths



Bond angles

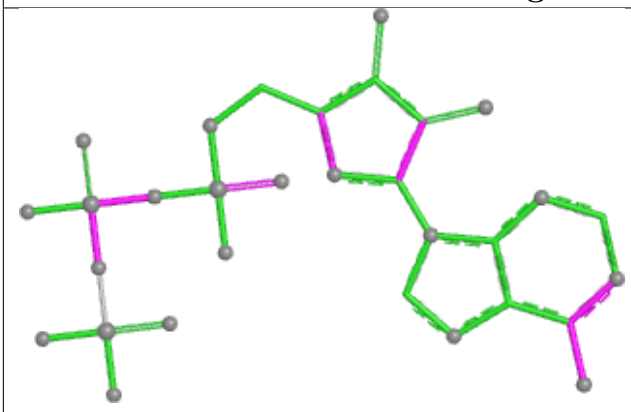


Torsions

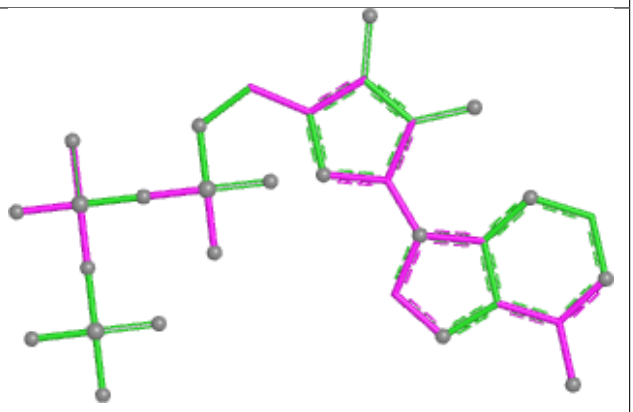


Rings

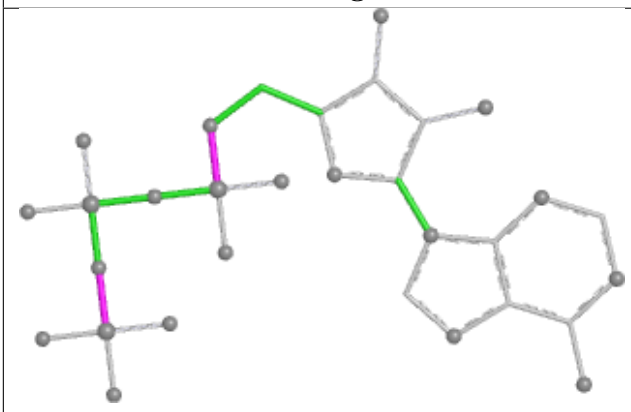
Ligand ATP L 501



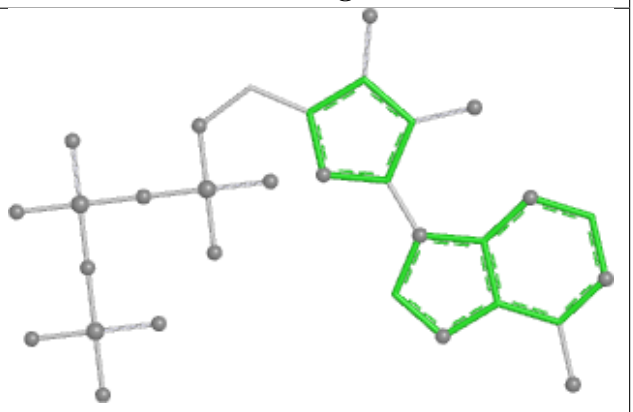
Bond lengths



Bond angles

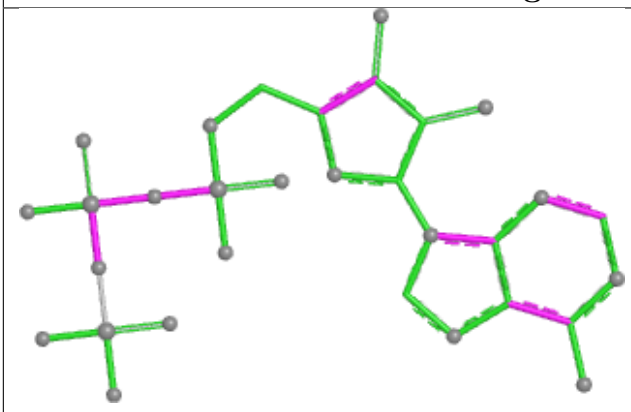


Torsions

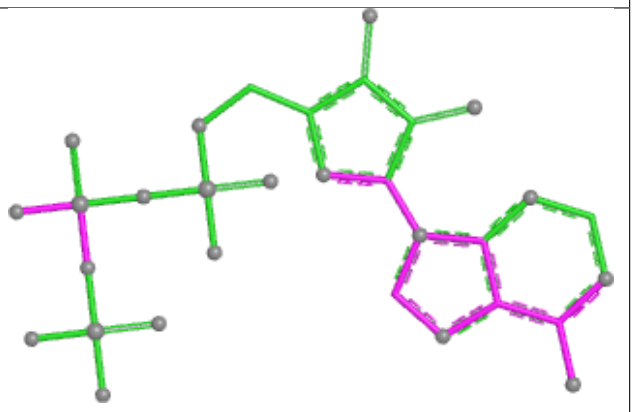


Rings

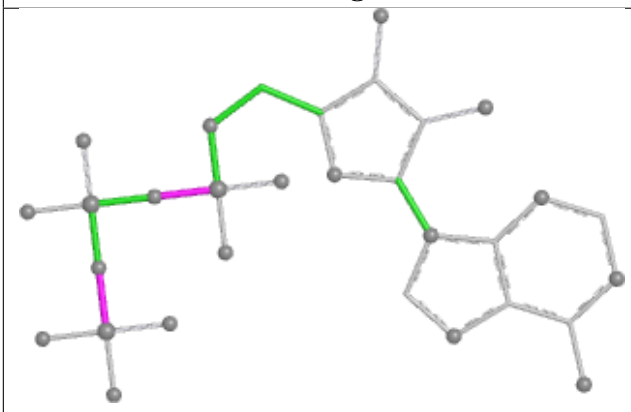
Ligand ATP K 501



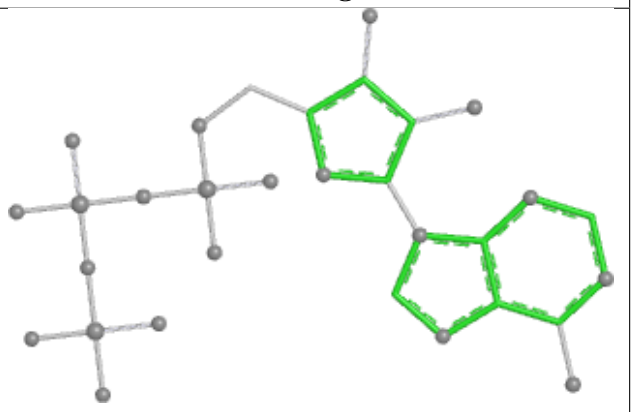
Bond lengths



Bond angles

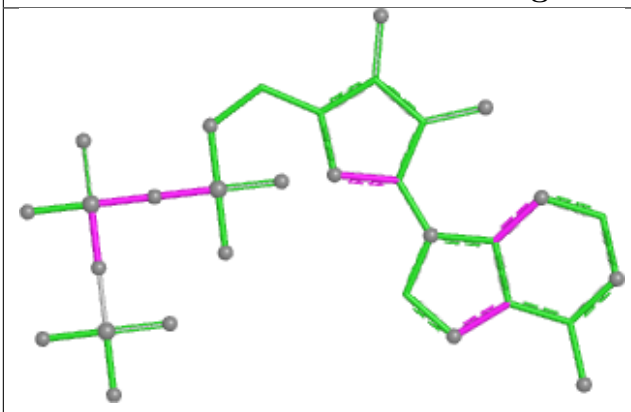


Torsions

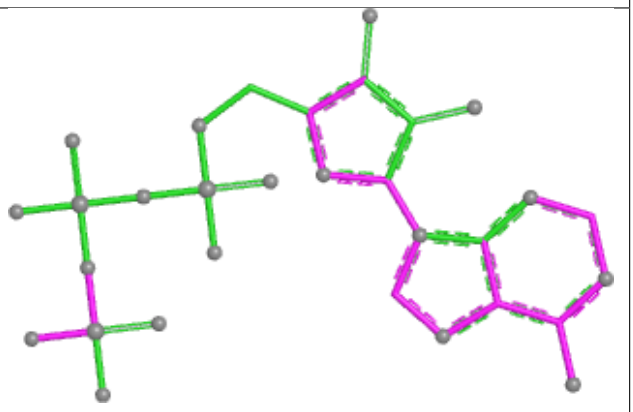


Rings

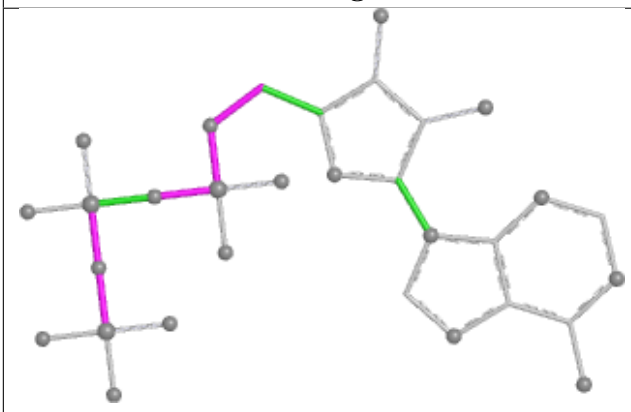
Ligand ATP I 501



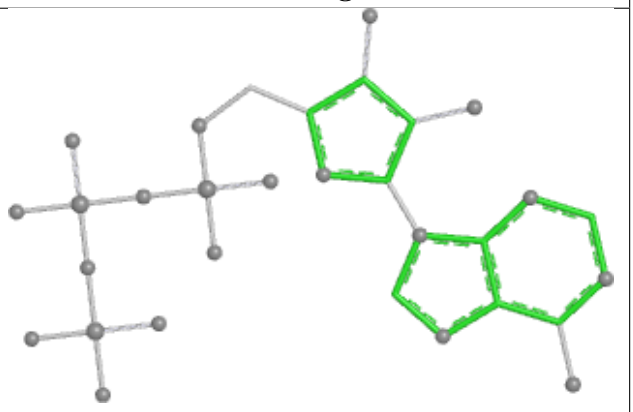
Bond lengths



Bond angles

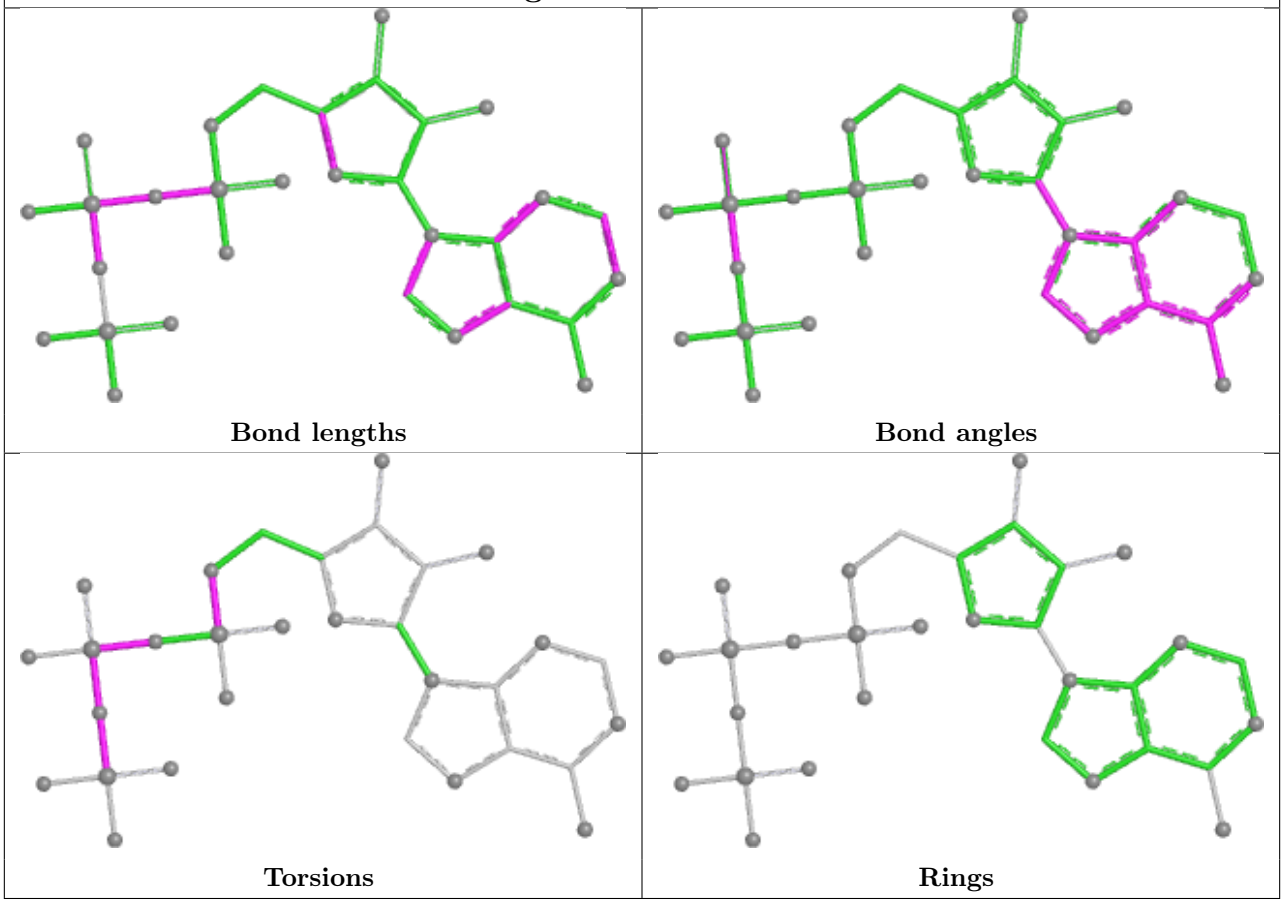


Torsions



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.

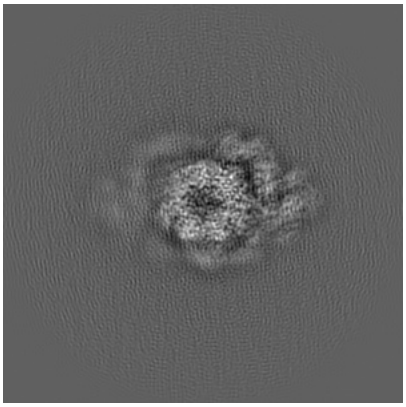
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4323. 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



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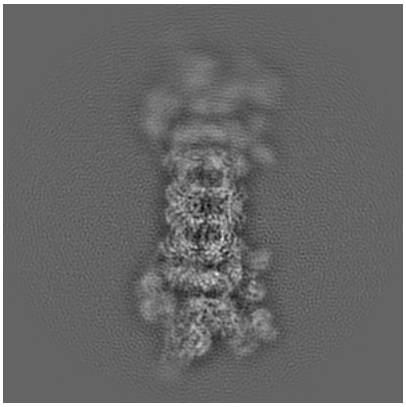
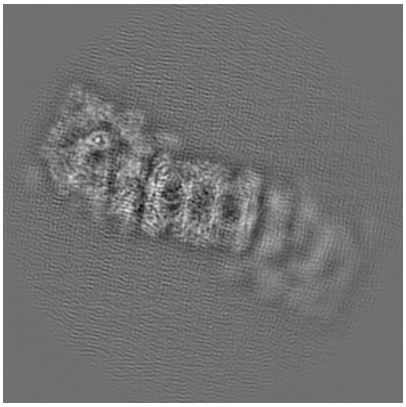


Y

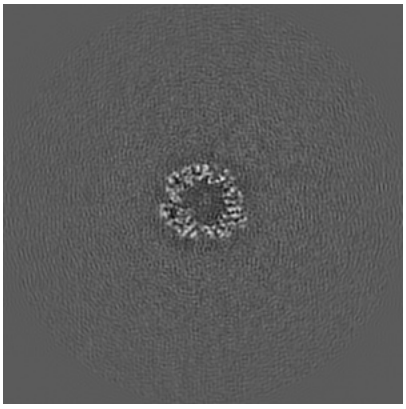


Z

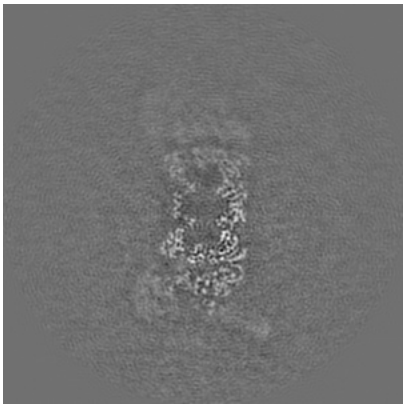
The images above show the map projected in three orthogonal directions.

6.2 Central slices

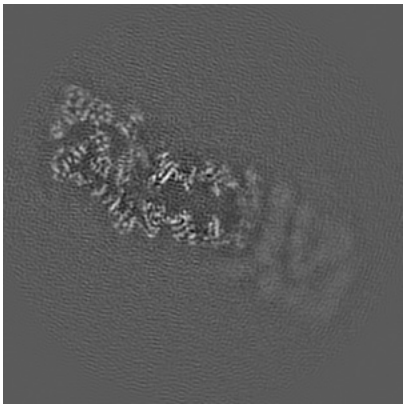
6.2.1 Primary map



X Index: 192



Y Index: 192

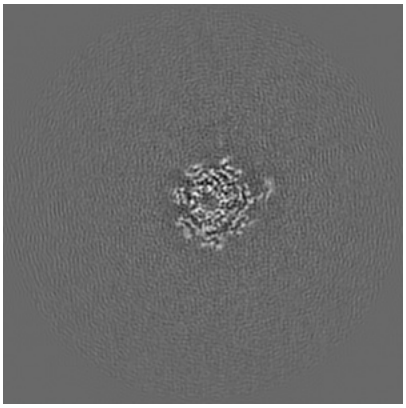


Z Index: 192

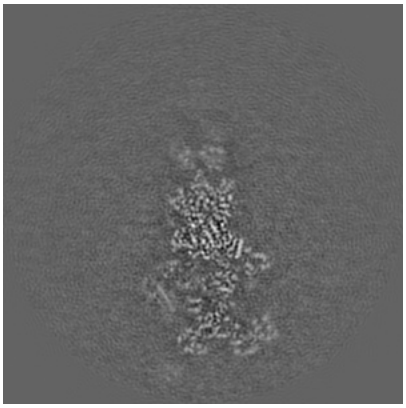
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

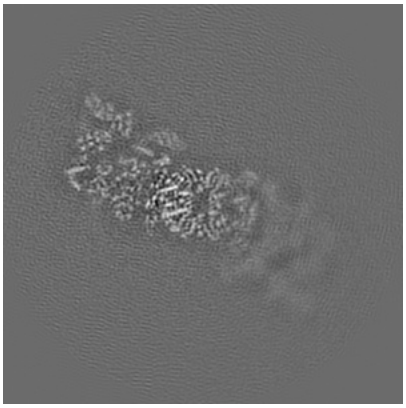
6.3.1 Primary map



X Index: 149



Y Index: 216

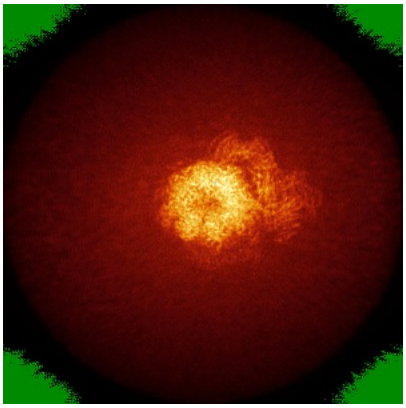


Z Index: 210

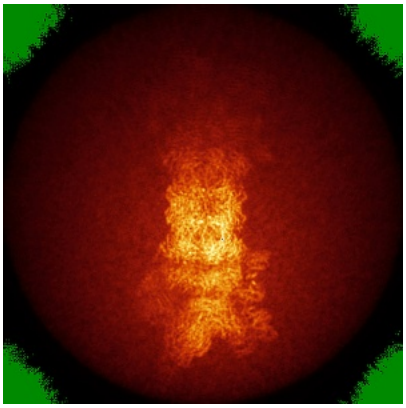
The images above show the largest variance slices of the map in three orthogonal directions.

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

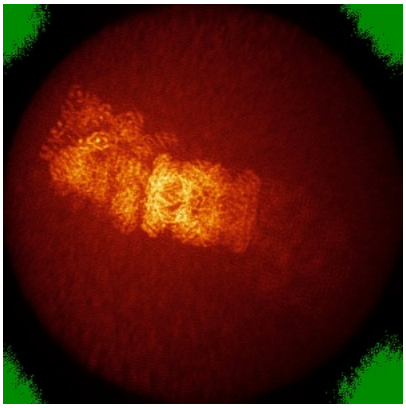
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

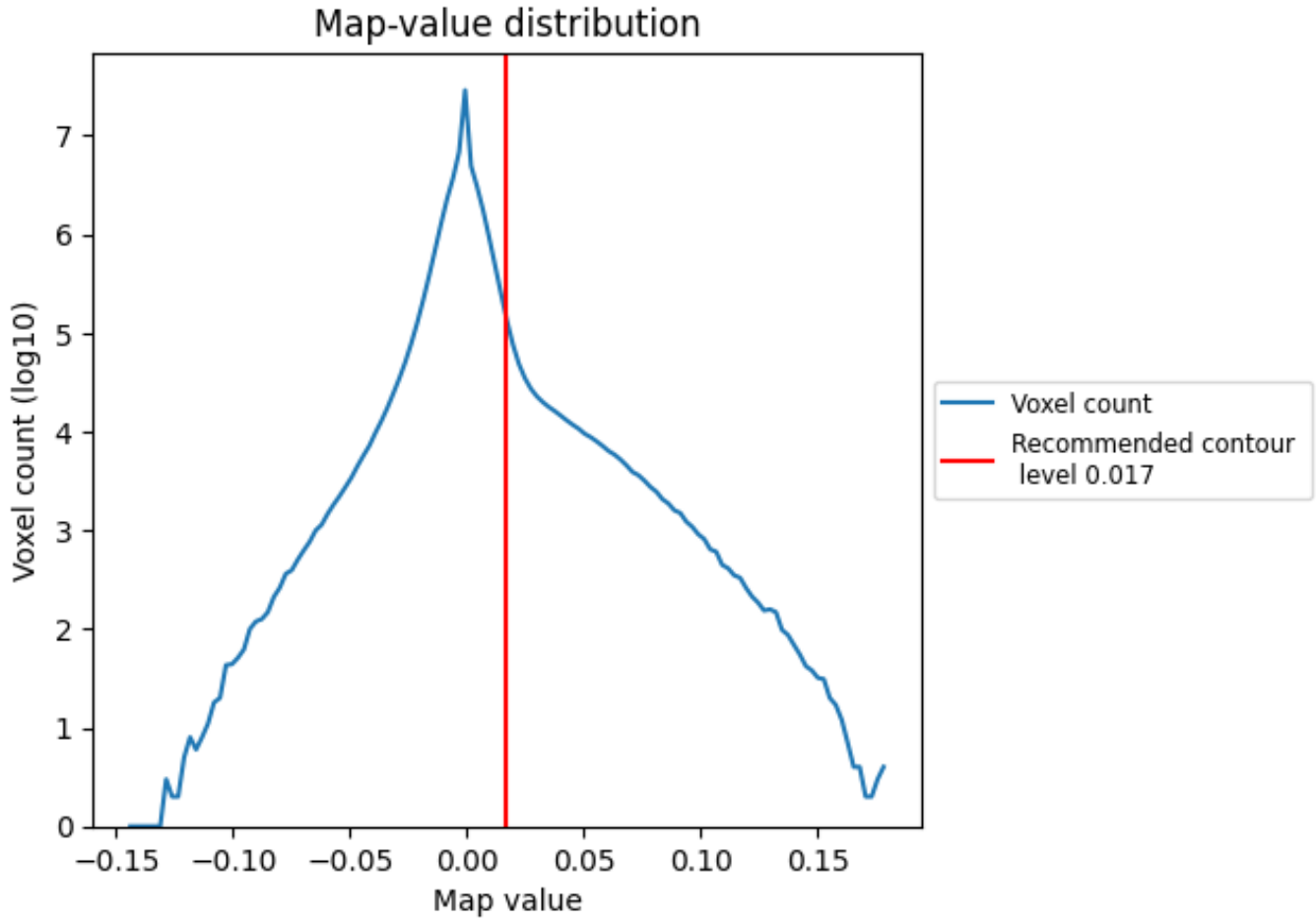
6.6 Mask visualisation (i)

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

7 Map analysis

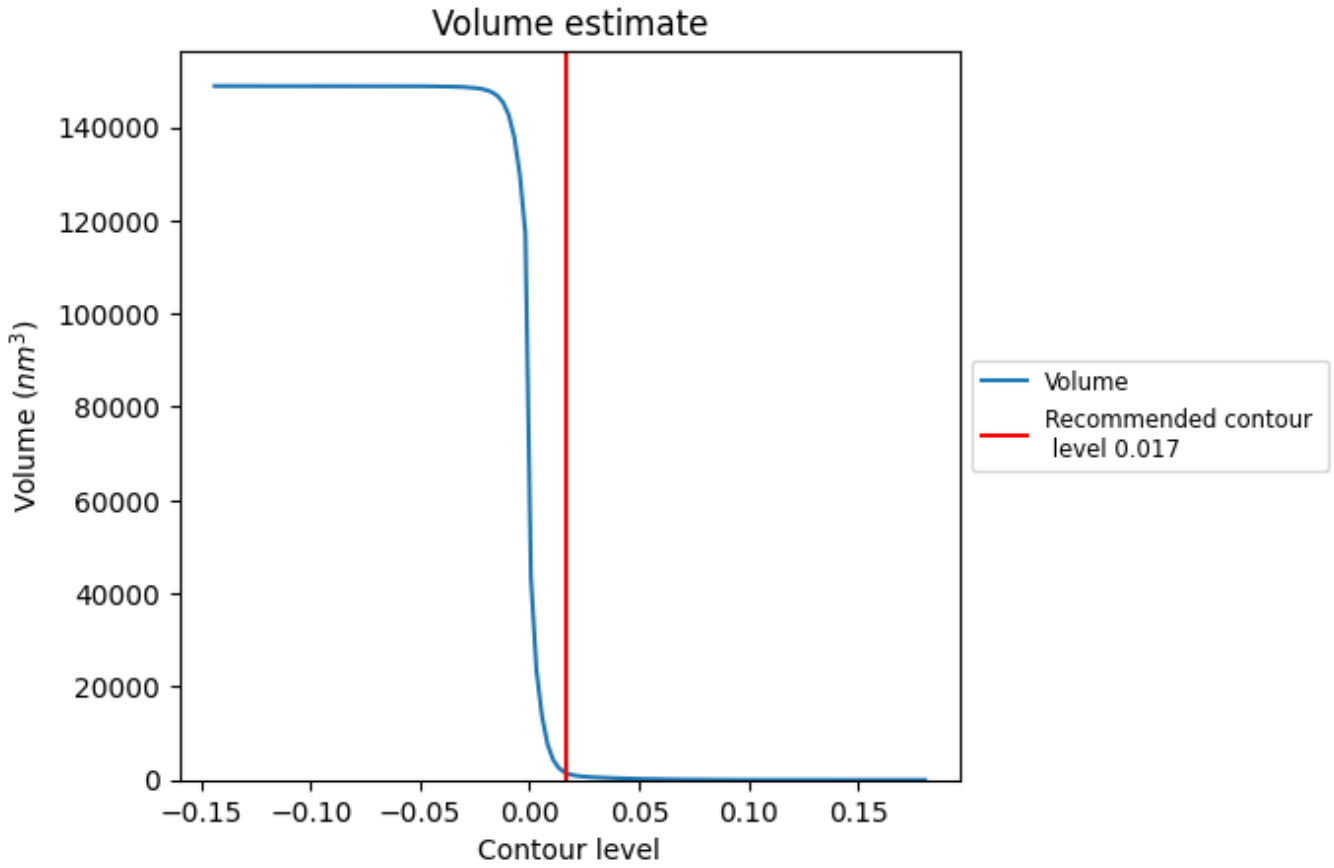
This section contains the results of statistical analysis of the map.

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.

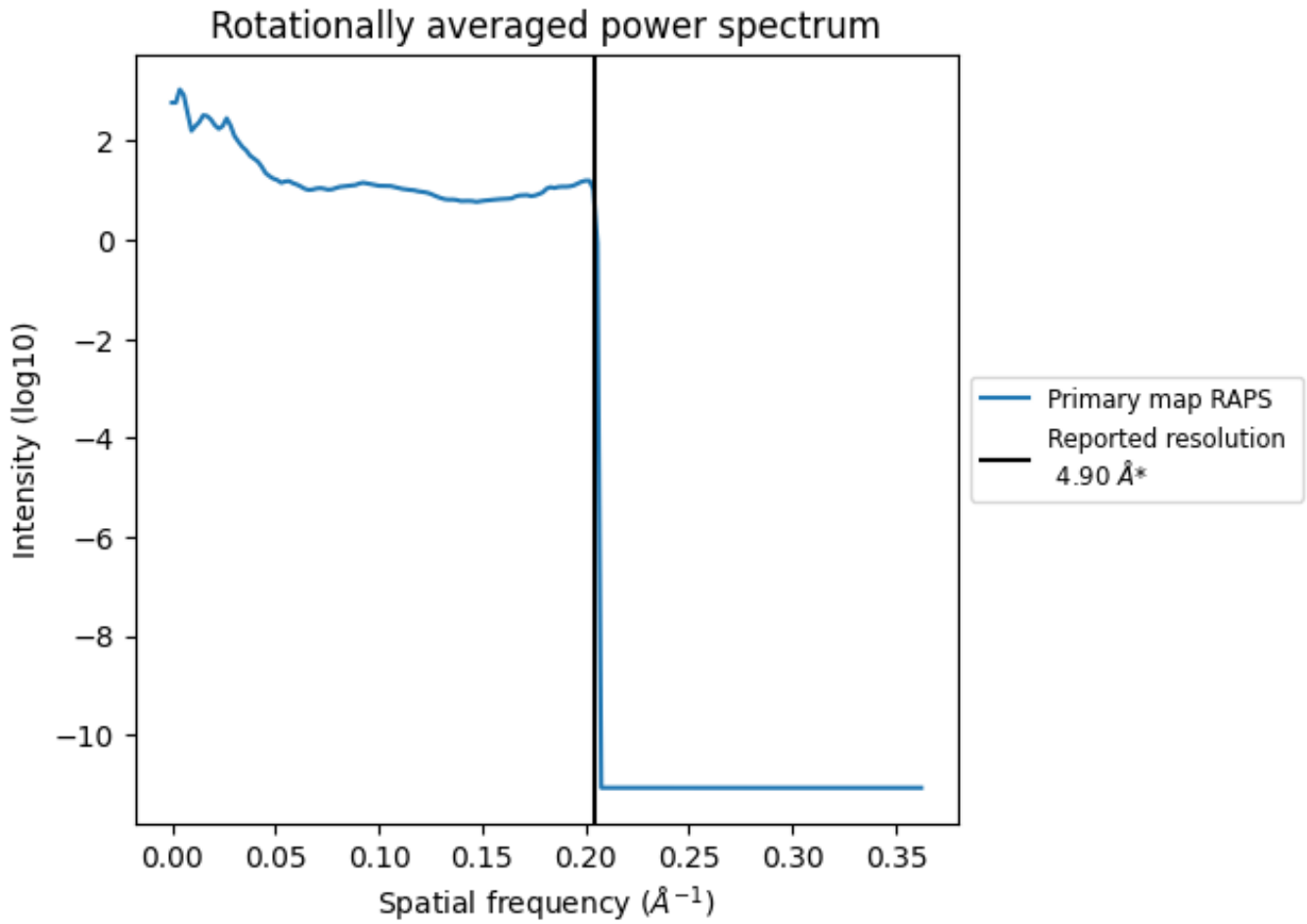
7.2 Volume estimate



The volume at the recommended contour level is 1456 nm^3; this corresponds to an approximate mass of 1315 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 0.204 Å^{-1}

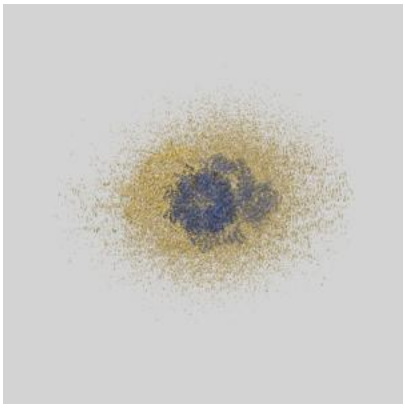
8 Fourier-Shell correlation

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

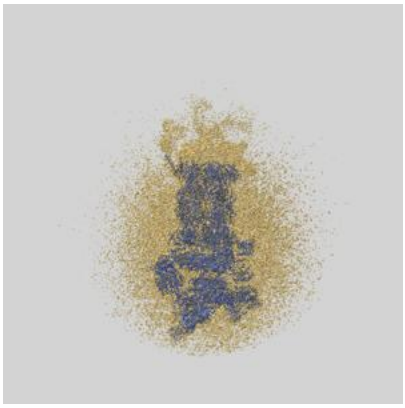
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4323 and PDB model 6FVX. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay



X

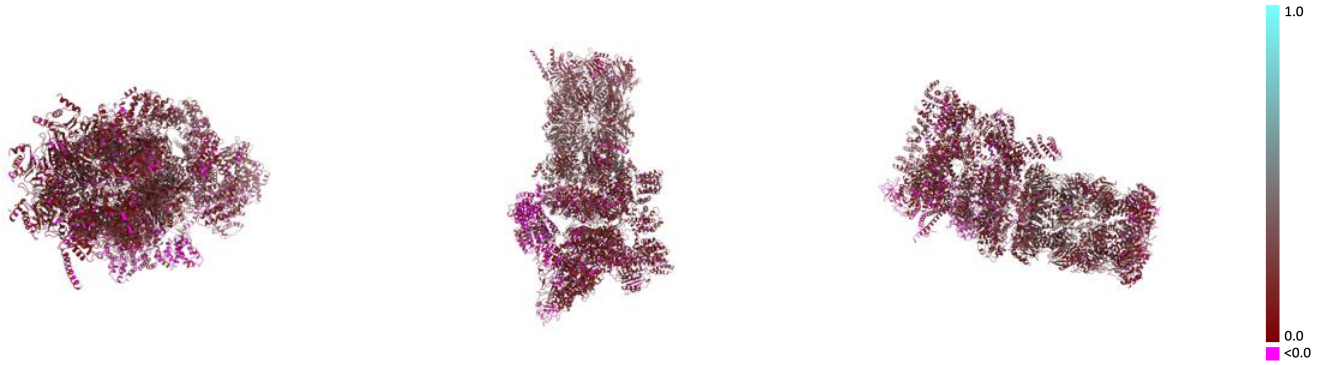


Y

Z

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

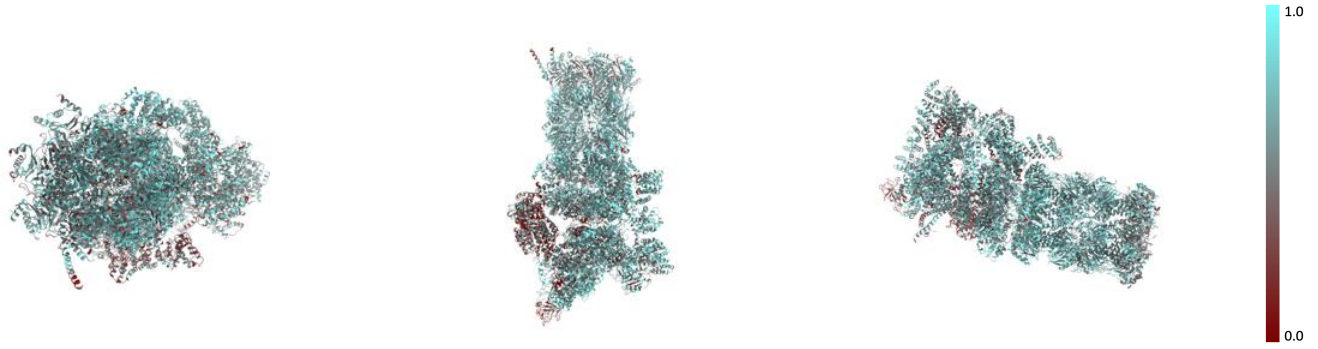
9.2 Q-score mapped to coordinate model



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.

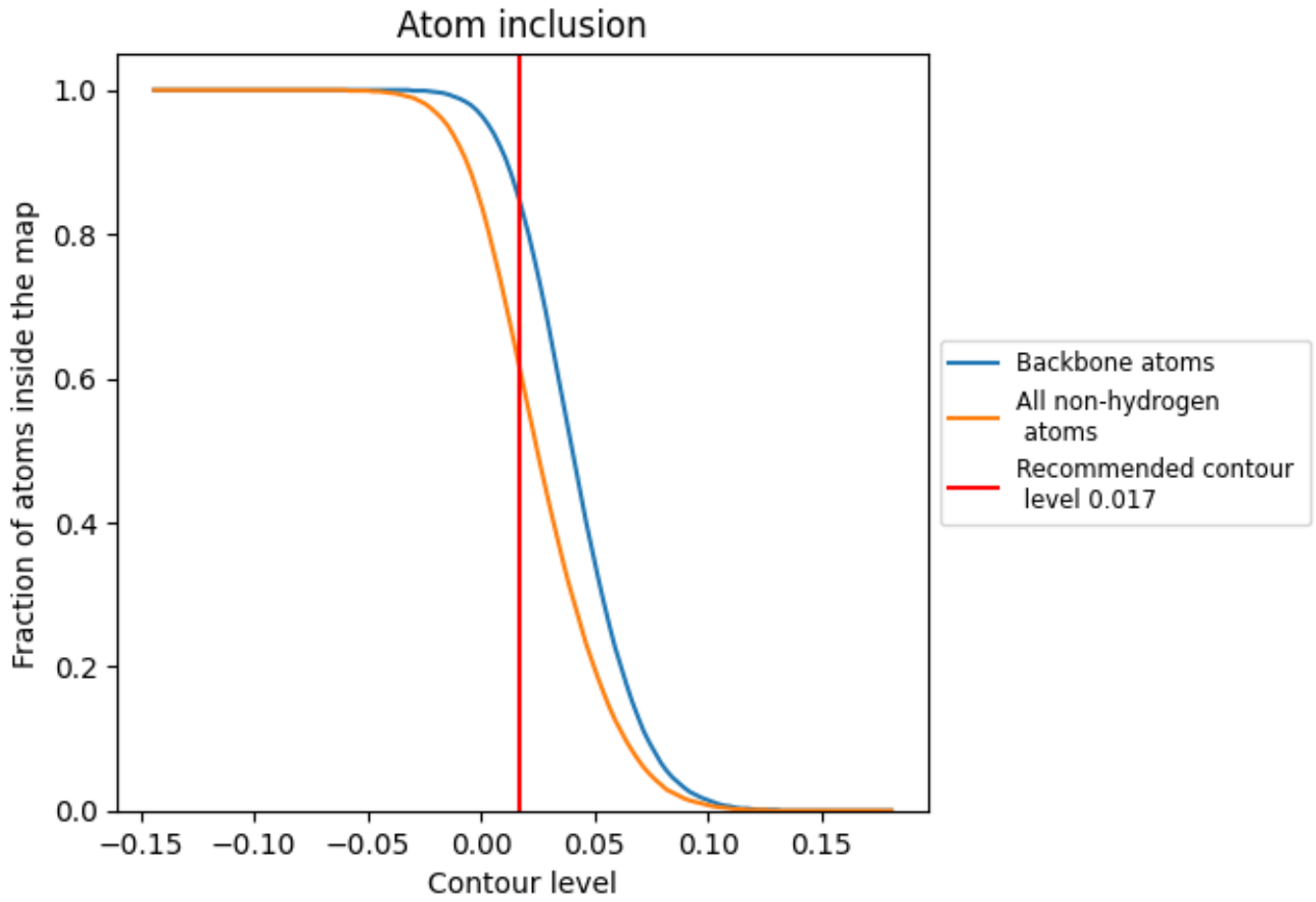
9.3 Atom inclusion mapped to coordinate model



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 (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.6130	0.1870
1	0.7530	0.2680
2	0.7290	0.2690
3	0.7100	0.2560
4	0.7180	0.2530
5	0.7560	0.2600
6	0.7200	0.2540
7	0.7220	0.2600
A	0.7240	0.2630
B	0.7050	0.2620
C	0.7020	0.2480
D	0.7030	0.2350
E	0.6920	0.2330
F	0.7260	0.2510
G	0.7390	0.2710
H	0.5590	0.1620
I	0.5780	0.1670
J	0.5240	0.1580
K	0.5910	0.1820
L	0.6350	0.2030
M	0.5980	0.1750
N	0.6180	0.1780
O	0.6560	0.1730
P	0.6930	0.1880
Q	0.6550	0.1650
R	0.6290	0.1630
S	0.5600	0.1480
T	0.5710	0.1520
U	0.6140	0.1930
V	0.6650	0.2110
W	0.6010	0.1530
X	0.1440	0.0360
Y	0.3690	0.0970
Z	0.3070	0.0310
a	0.5770	0.1750

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Chain	Atom inclusion	Q-score
b	0.5490	0.1700
c	0.5820	0.1820
d	0.5310	0.1640
e	0.5540	0.1620
f	0.5790	0.1590
g	0.5890	0.1740
h	0.7060	0.2410
i	0.6870	0.2290
j	0.6730	0.2330
k	0.6820	0.2260
l	0.7060	0.2340
m	0.6930	0.2240
n	0.6990	0.2390