



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:54 AM UTC

PDB ID : 6HE9 / pdb_00006he9
EMDB ID : EMD-0213
Title : PAN-proteasome in state 2
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 6.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

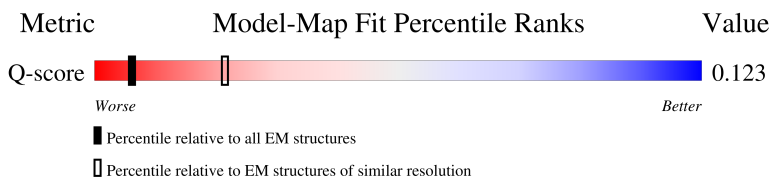
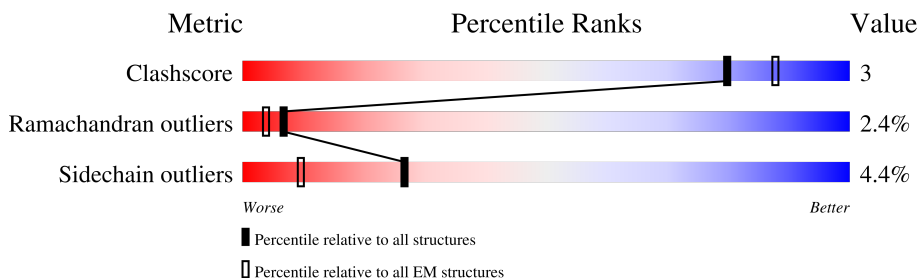
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.35 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	512 (5.85 - 6.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	 6% 42% 50% 7%
1	B	242	 7% 41% 52% 7%
1	C	242	 7% 43% 48% 7%
1	D	242	 8% 43% 50% 7%

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Mol	Chain	Length	Quality of chain
1	E	242	
1	F	242	
1	G	242	
1	a	242	
1	b	242	
1	c	242	
1	d	242	
1	e	242	
1	f	242	
1	g	242	
2	1	202	
2	2	202	
2	3	202	
2	4	202	
2	5	202	
2	6	202	
2	7	202	
2	h	202	
2	i	202	
2	j	202	
2	k	202	
2	l	202	
2	m	202	
2	n	202	
3	H	390	

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Mol	Chain	Length	Quality of chain
3	I	390	18% 43% 46% 10%
3	J	390	19% 38% 52% 8%
3	K	390	21% 41% 51% 8%
3	L	390	22% 41% 49% 10%
3	M	390	22% 40% 51% 8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 66909 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	a	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	B	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	b	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	C	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	c	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	D	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	d	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	E	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	e	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	F	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	f	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		
1	G	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	g	237	Total	C	N	O	S	0	0
			1866	1186	315	359	6		

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		

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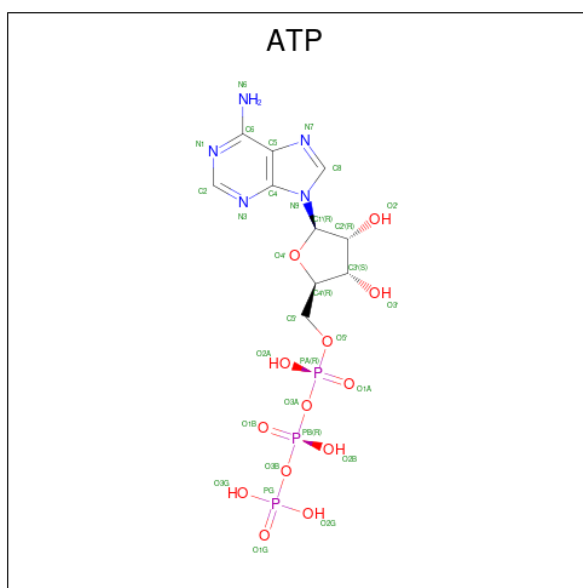
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	i	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	j	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	4	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	k	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	5	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	l	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	6	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	m	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	7	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	n	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		

- Molecule 3 is a protein called Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		
3	I	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		
3	K	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		
3	L	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		
3	M	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		
3	J	390	Total	C	N	O	S	0	0
			3100	1974	535	583	8		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

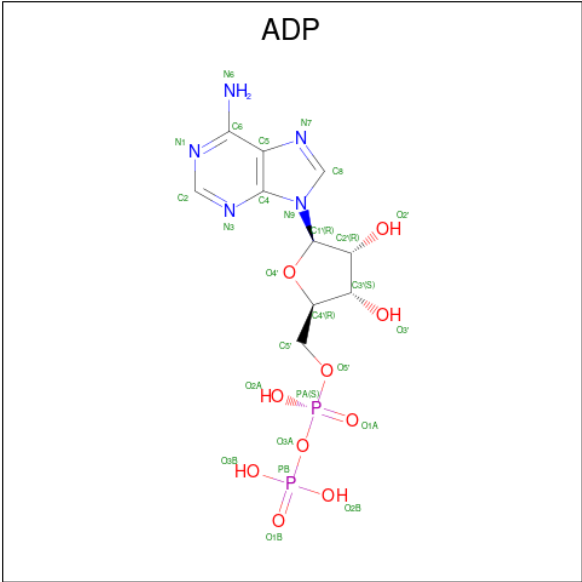


Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

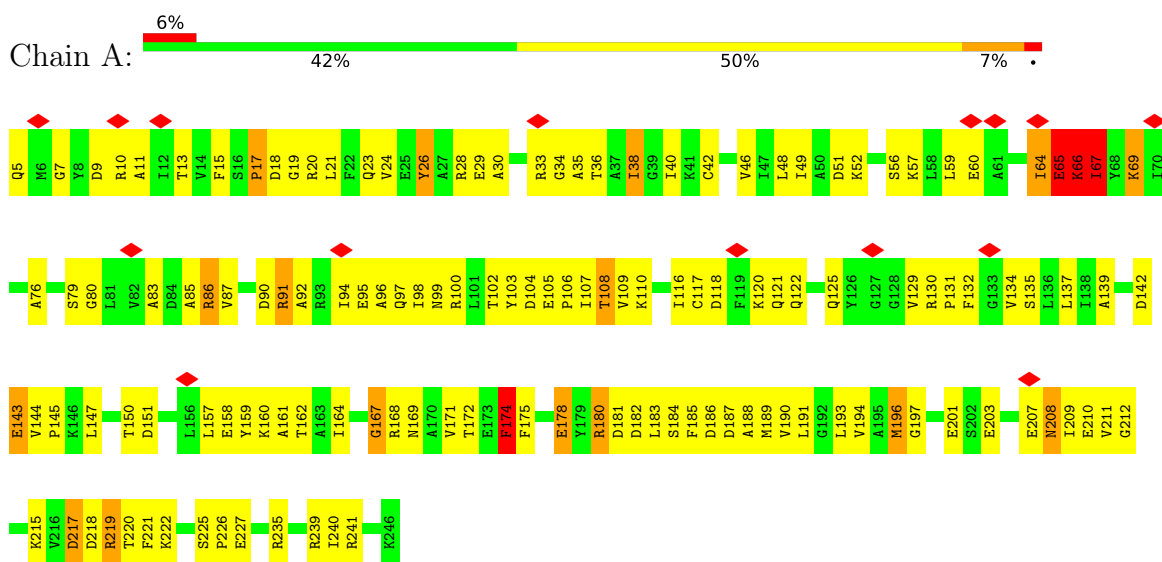


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	L	1	27	10	5	10	2	0

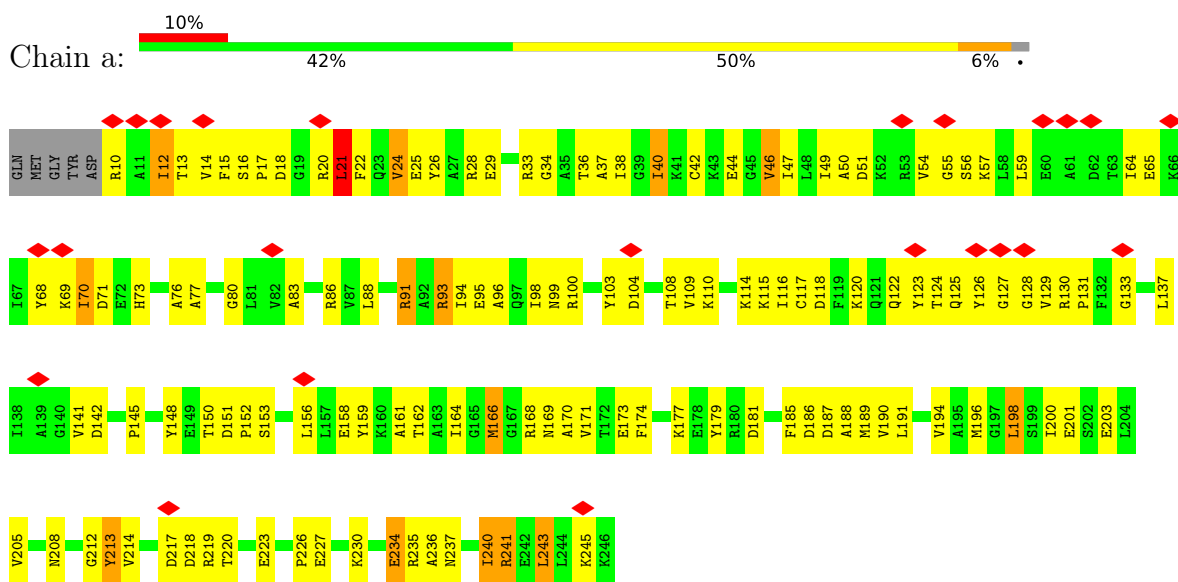
3 Residue-property plots

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

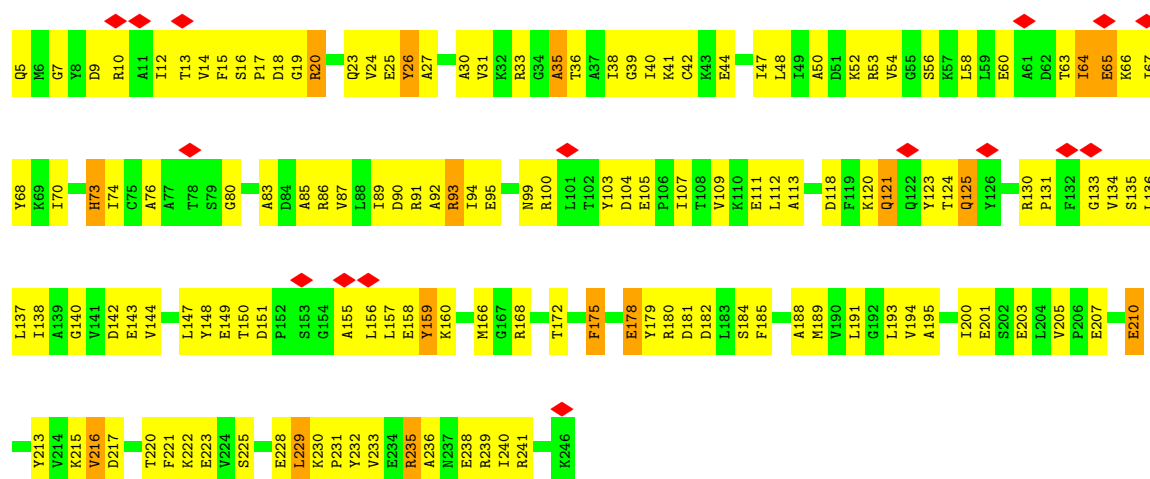
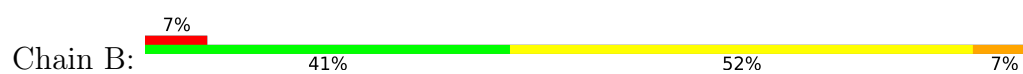
• Molecule 1: Proteasome subunit alpha



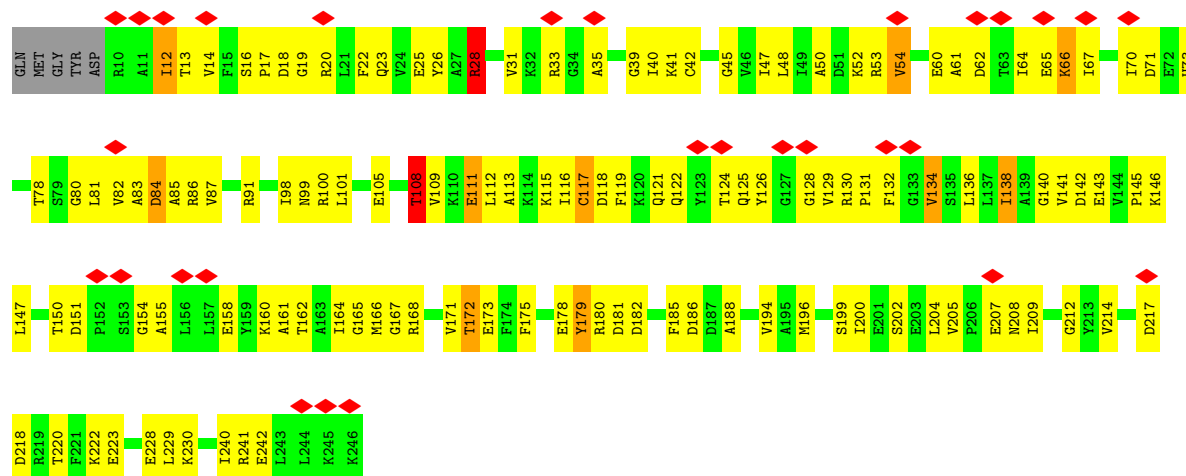
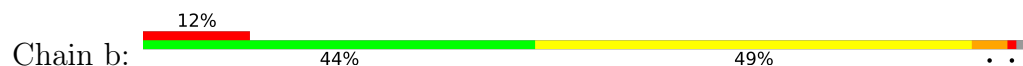
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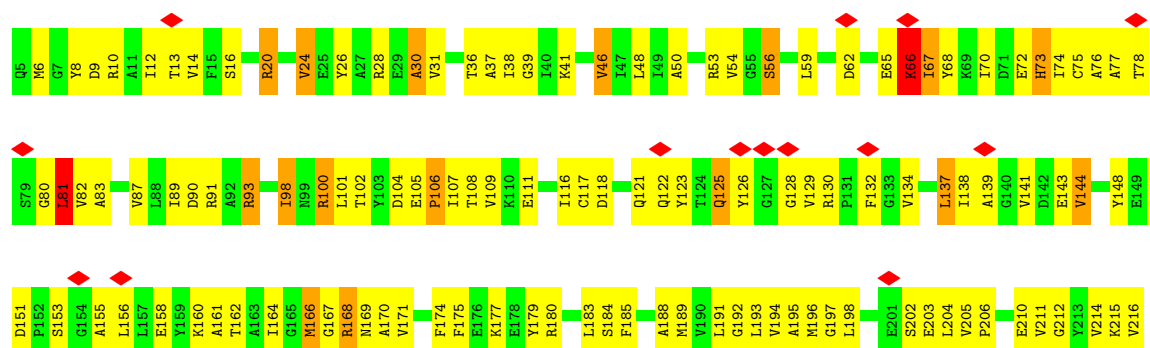
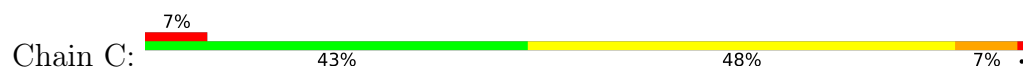
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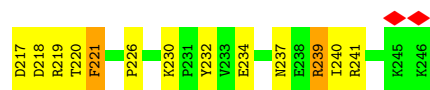


• Molecule 1: Proteasome subunit alpha

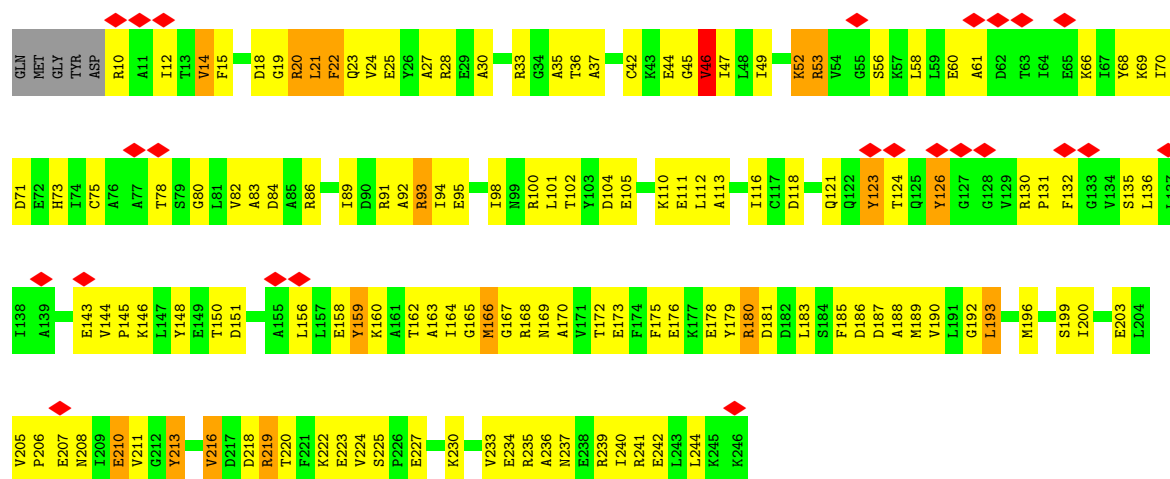
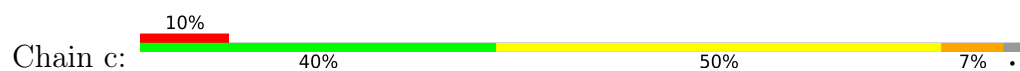


• Molecule 1: Proteasome subunit alpha

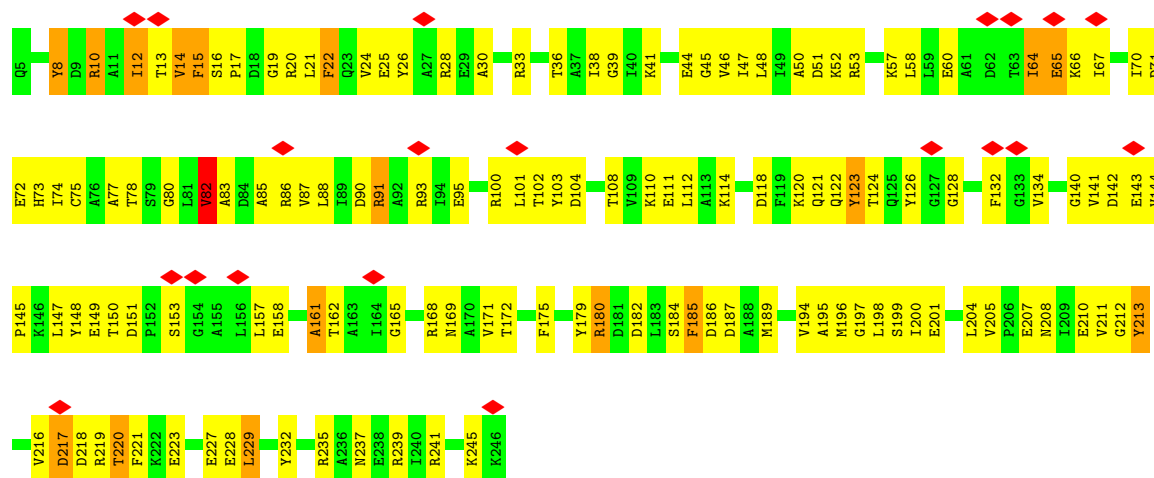
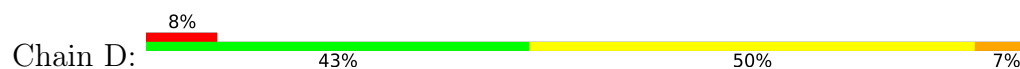




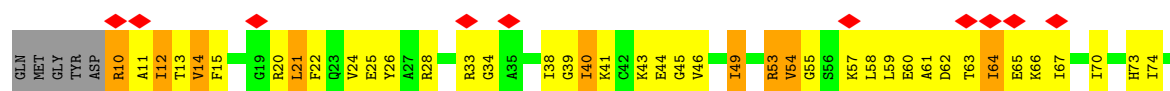
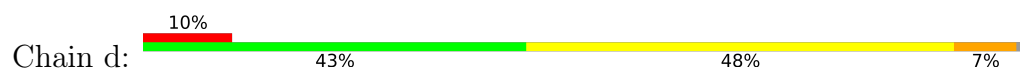
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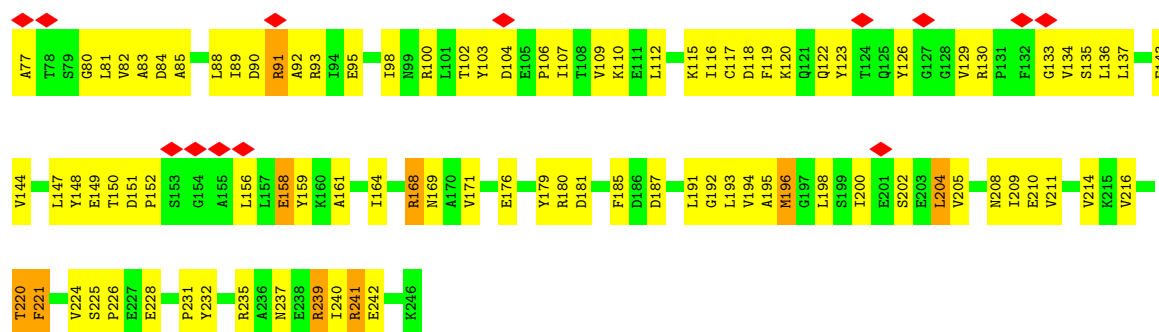


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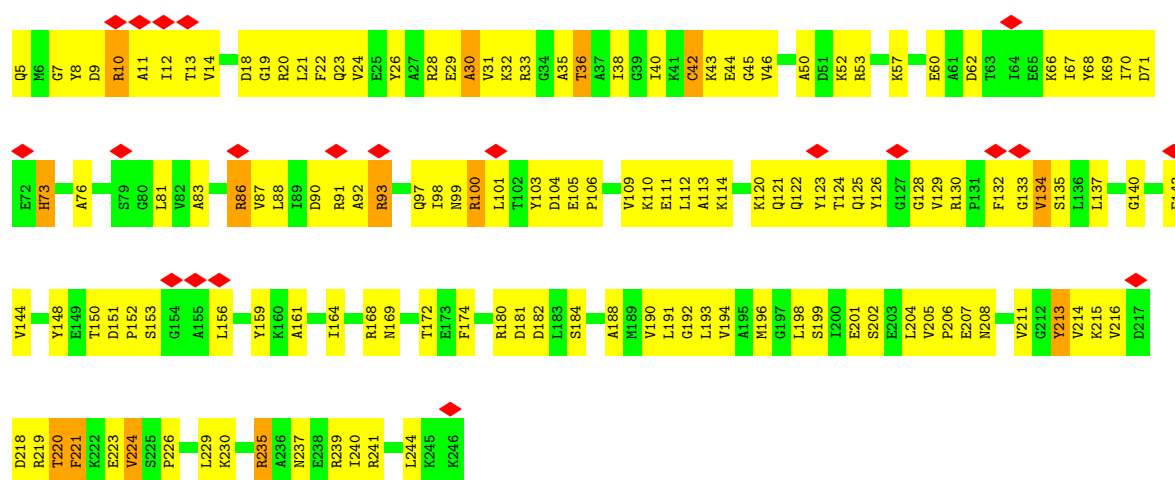


• Molecule 1: Proteasome subunit alpha

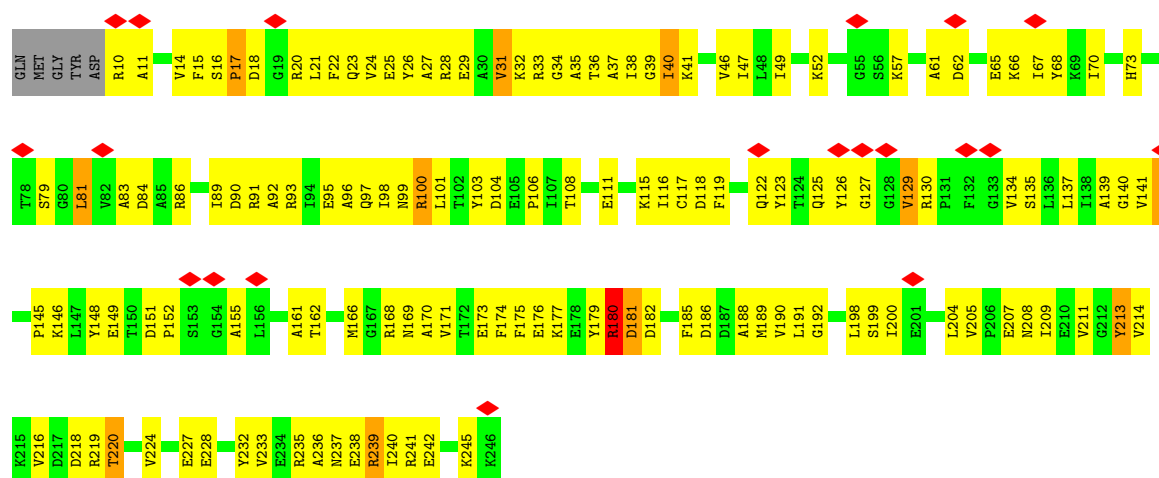




• Molecule 1: Proteasome subunit alpha

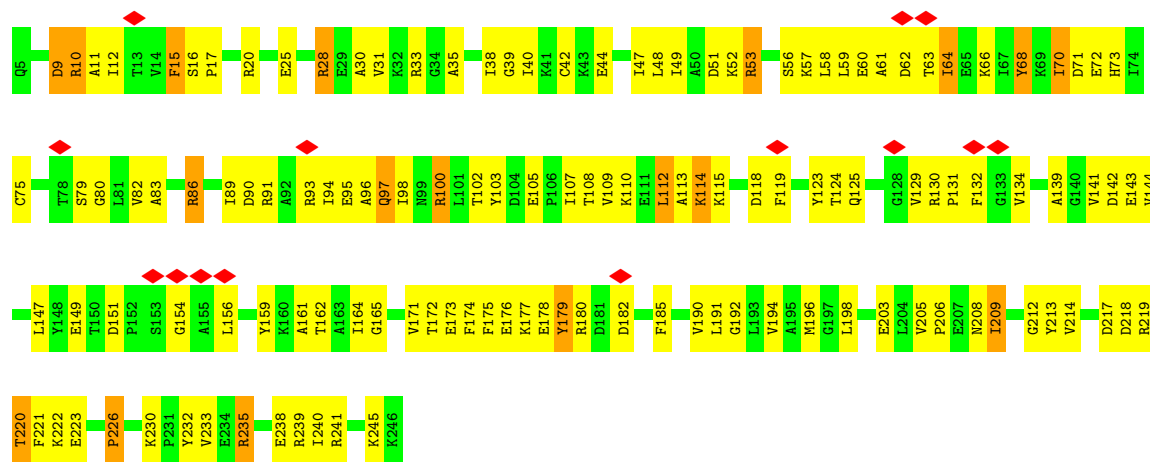


• Molecule 1: Proteasome subunit alpha

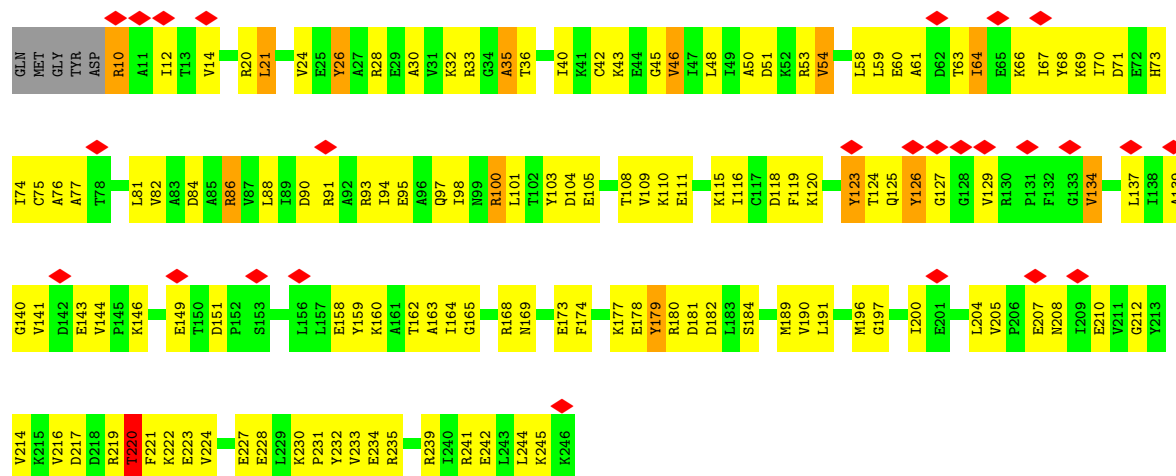


• Molecule 1: Proteasome subunit alpha

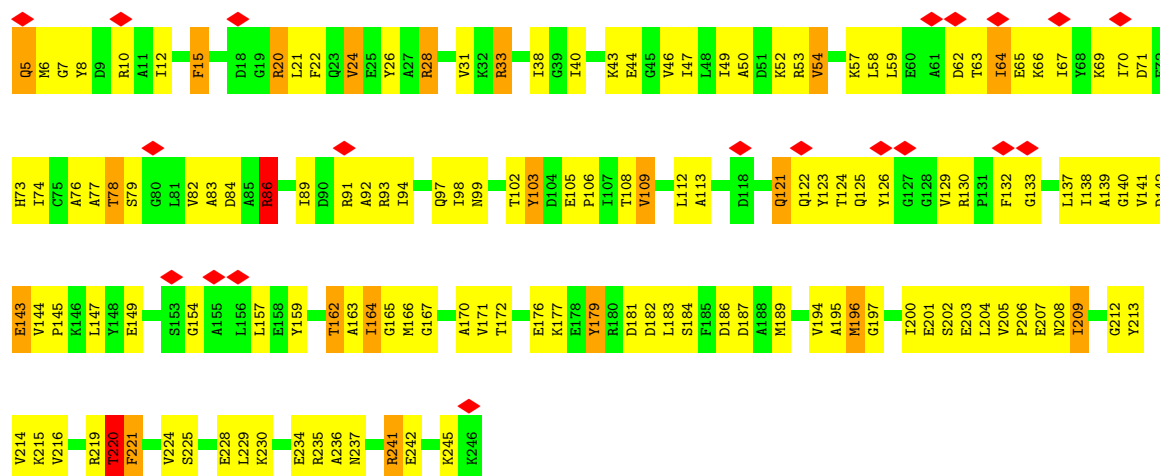
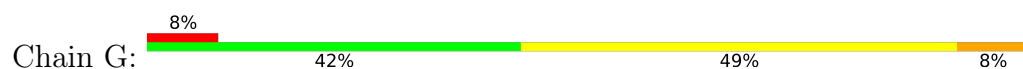




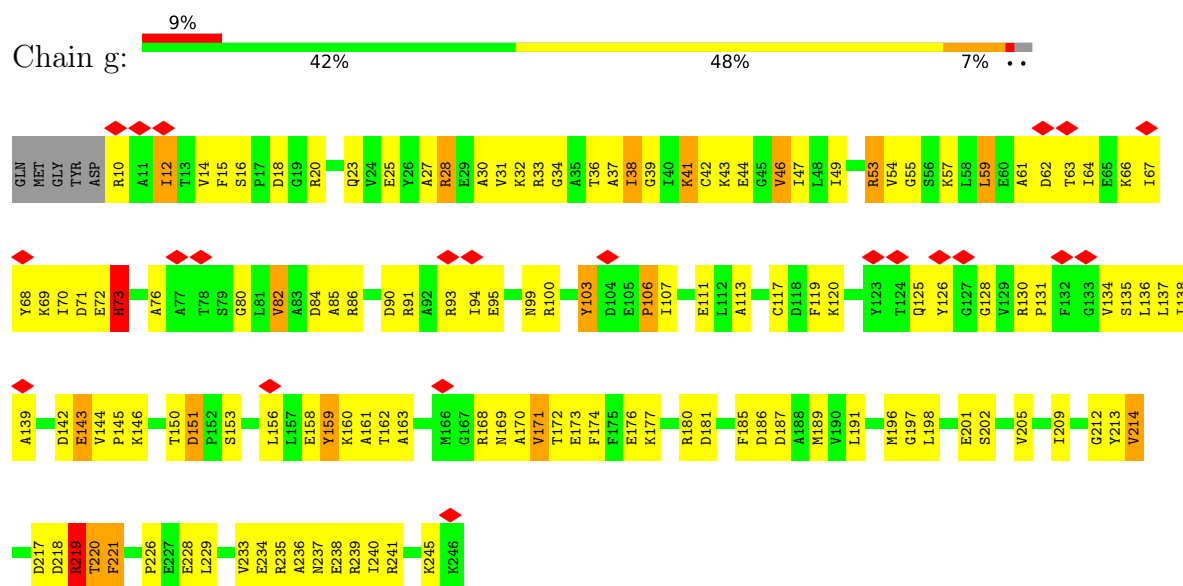
• Molecule 1: Proteasome subunit alpha



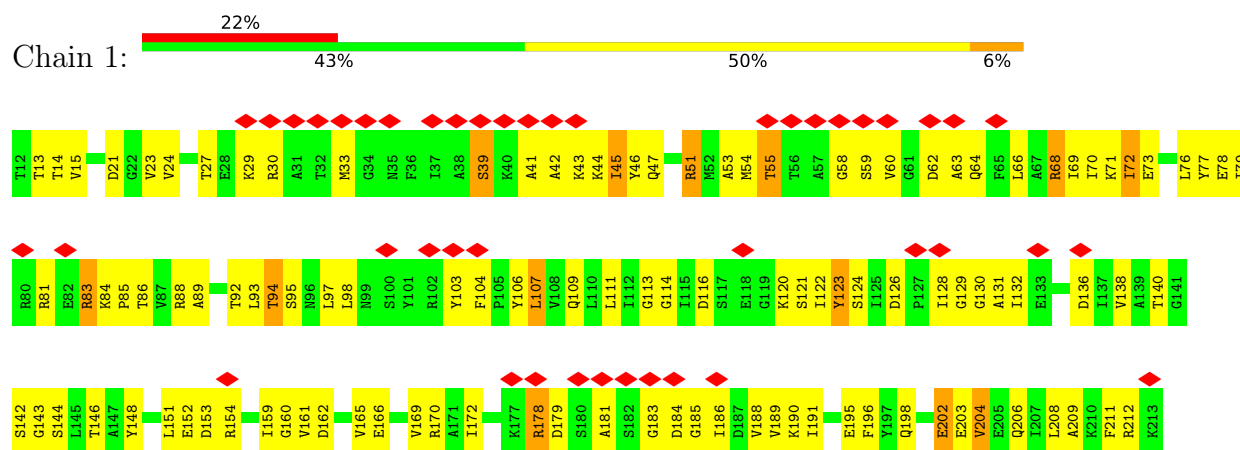
• Molecule 1: Proteasome subunit alpha



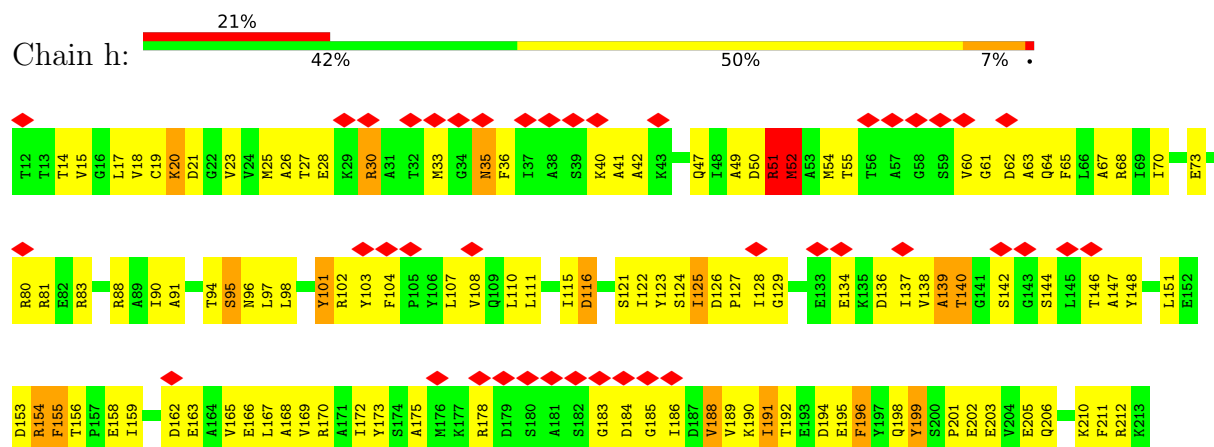
- Molecule 1: Proteasome subunit alpha



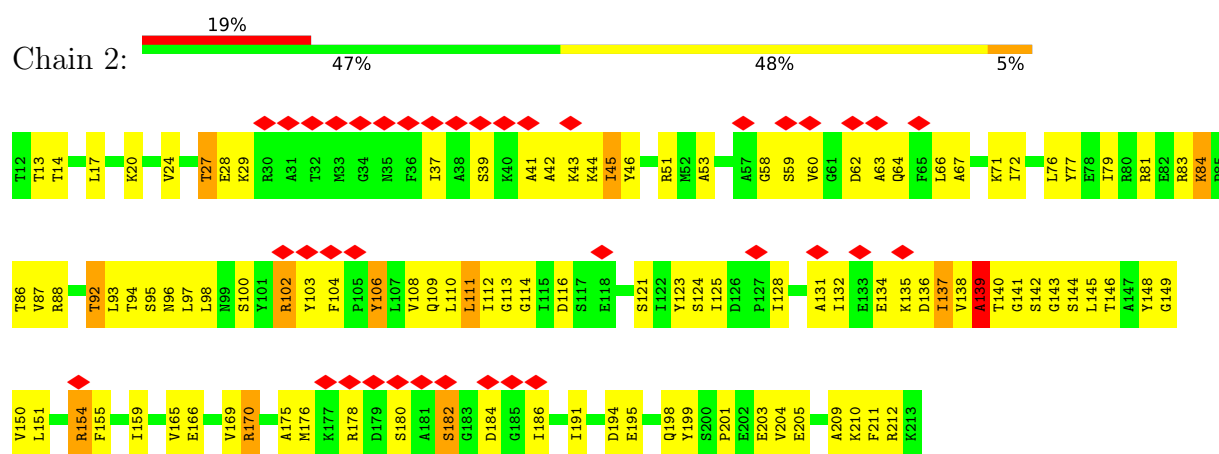
- Molecule 2: Proteasome subunit beta



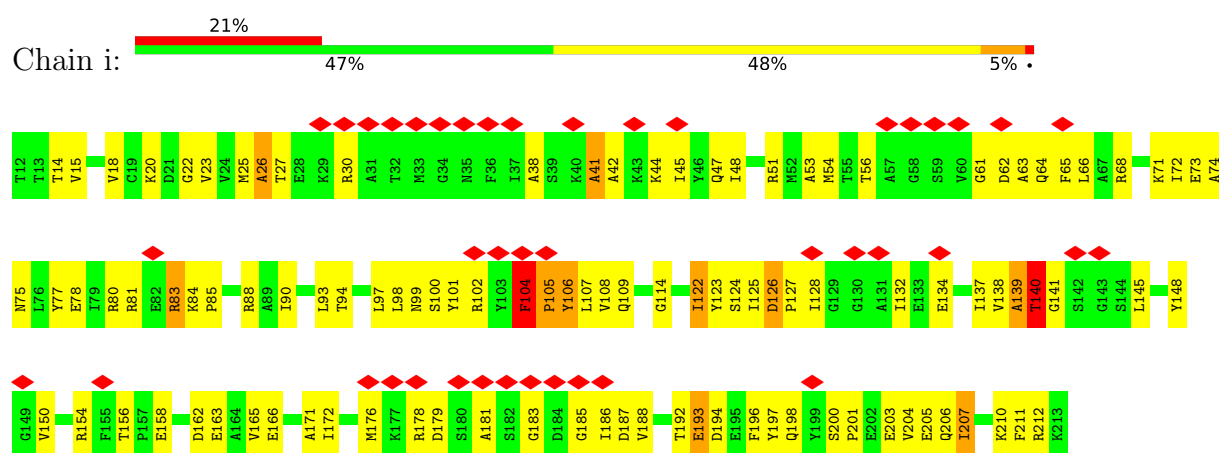
- Molecule 2: Proteasome subunit beta



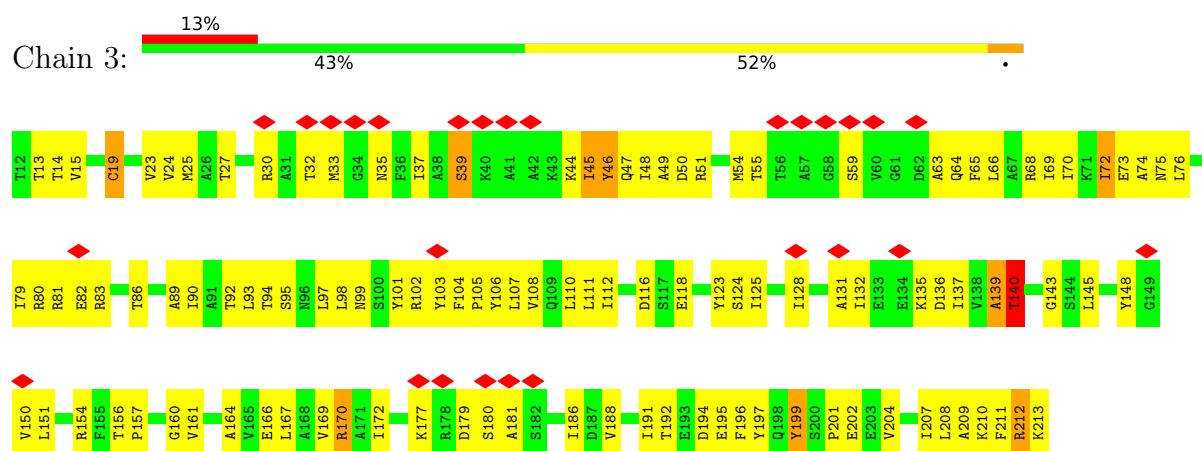
- Molecule 2: Proteasome subunit beta



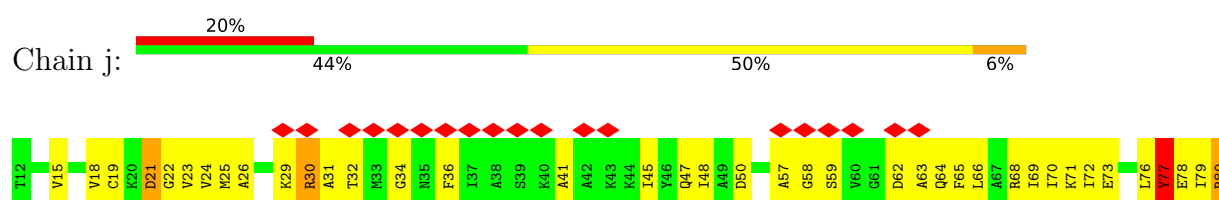
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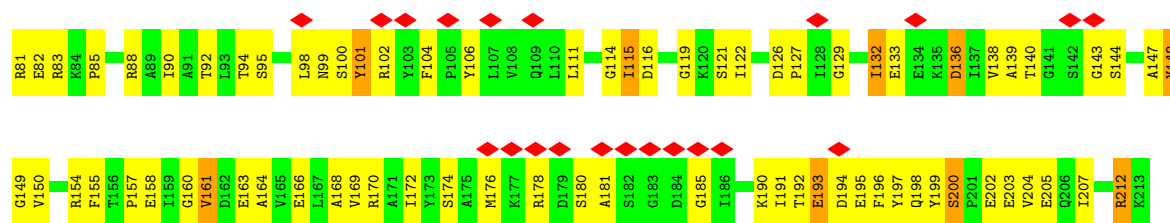


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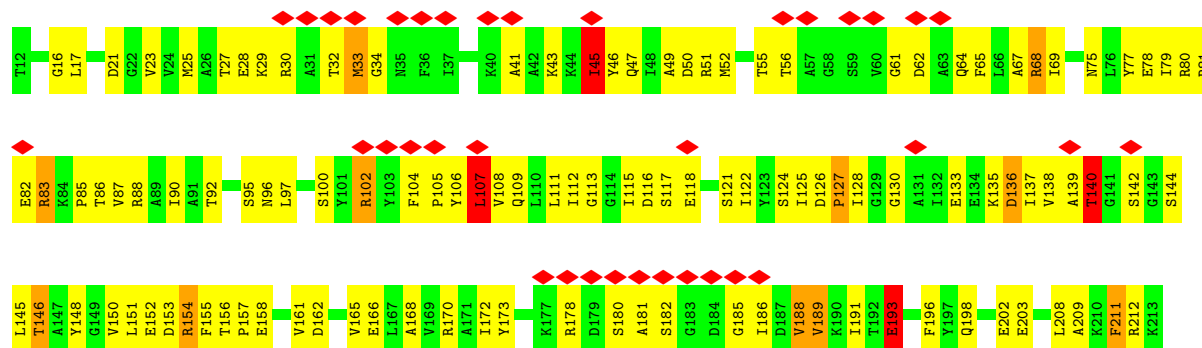
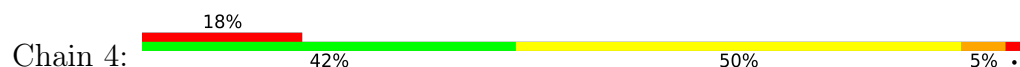


• Molecule 2: Proteasome subunit beta

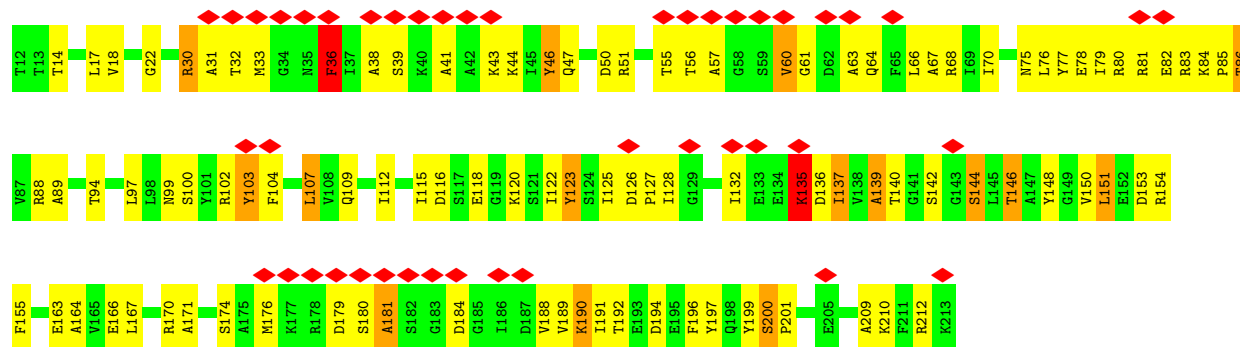




• Molecule 2: Proteasome subunit beta



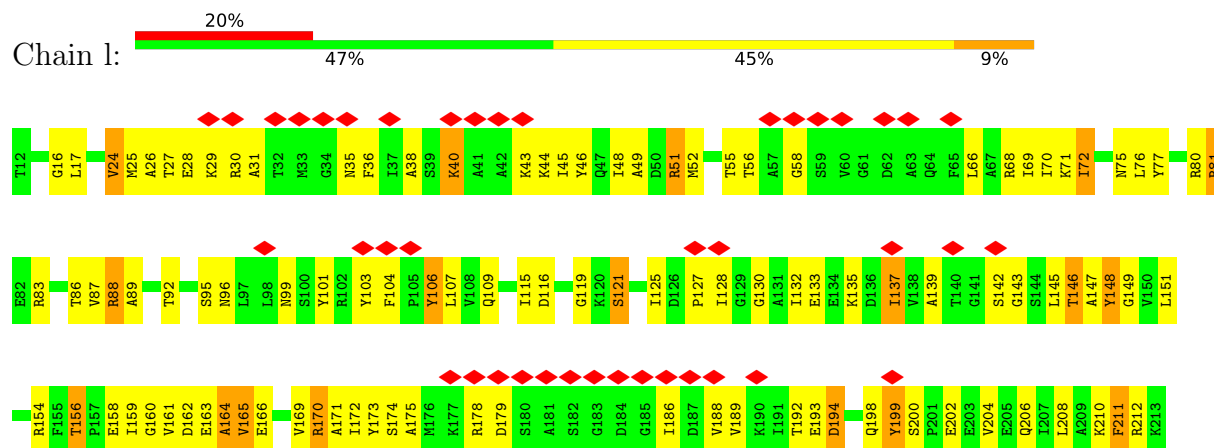
• Molecule 2: Proteasome subunit beta



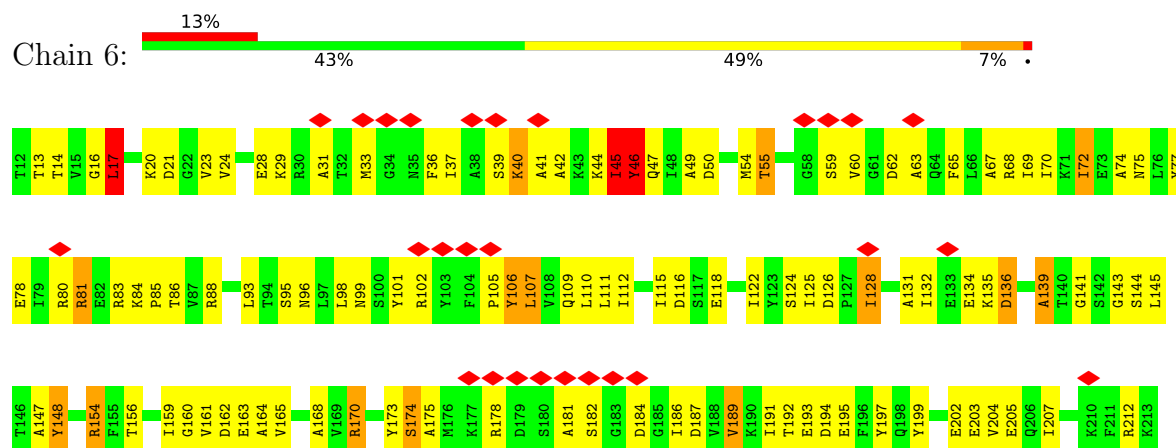
• Molecule 2: Proteasome subunit beta



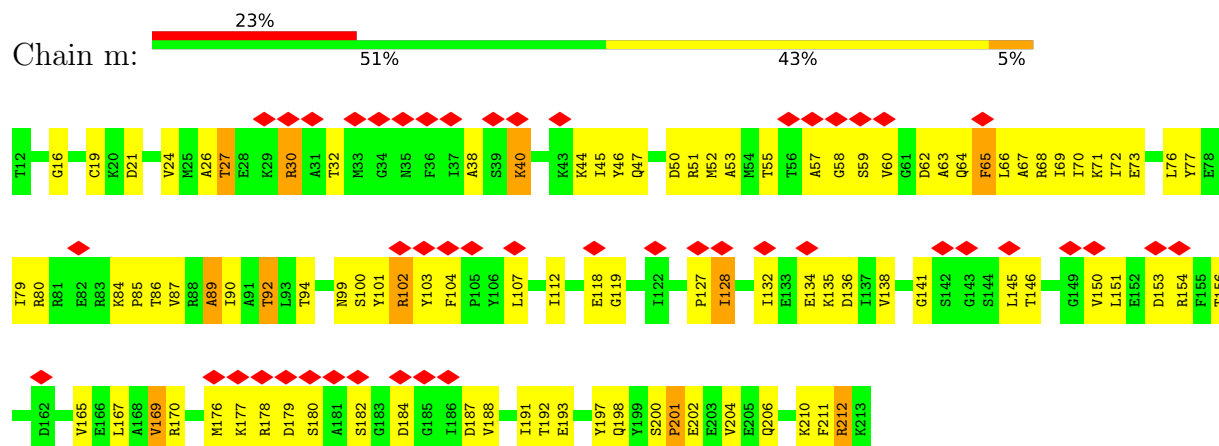
- Molecule 2: Proteasome subunit beta



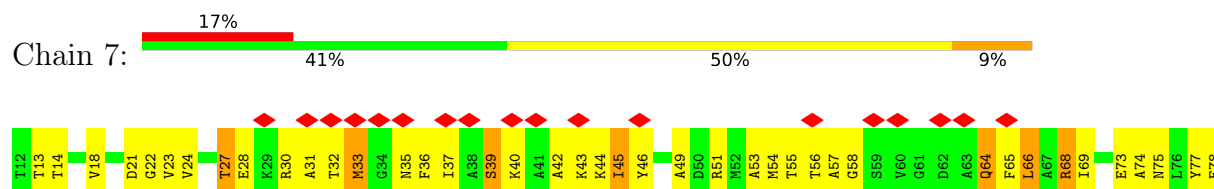
- Molecule 2: Proteasome subunit beta

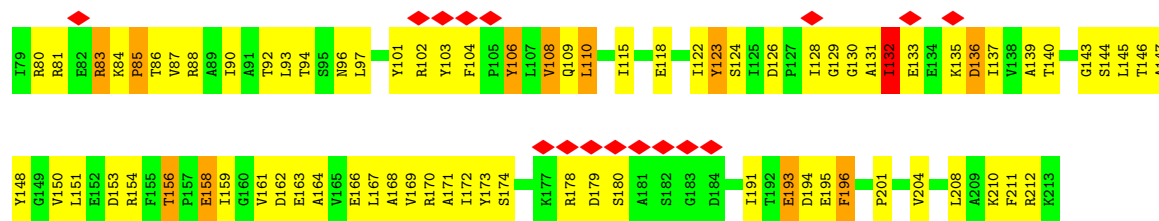


- Molecule 2: Proteasome subunit beta

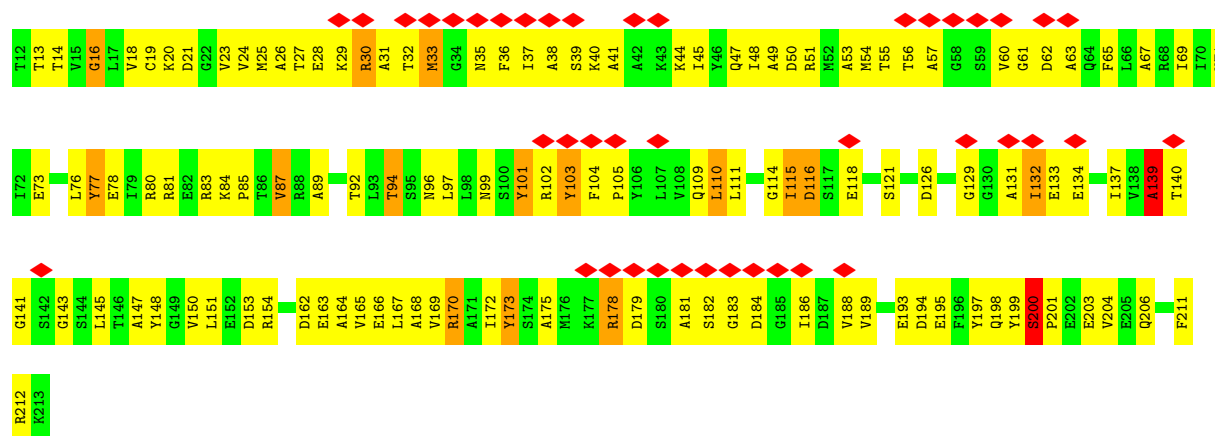


- Molecule 2: Proteasome subunit beta

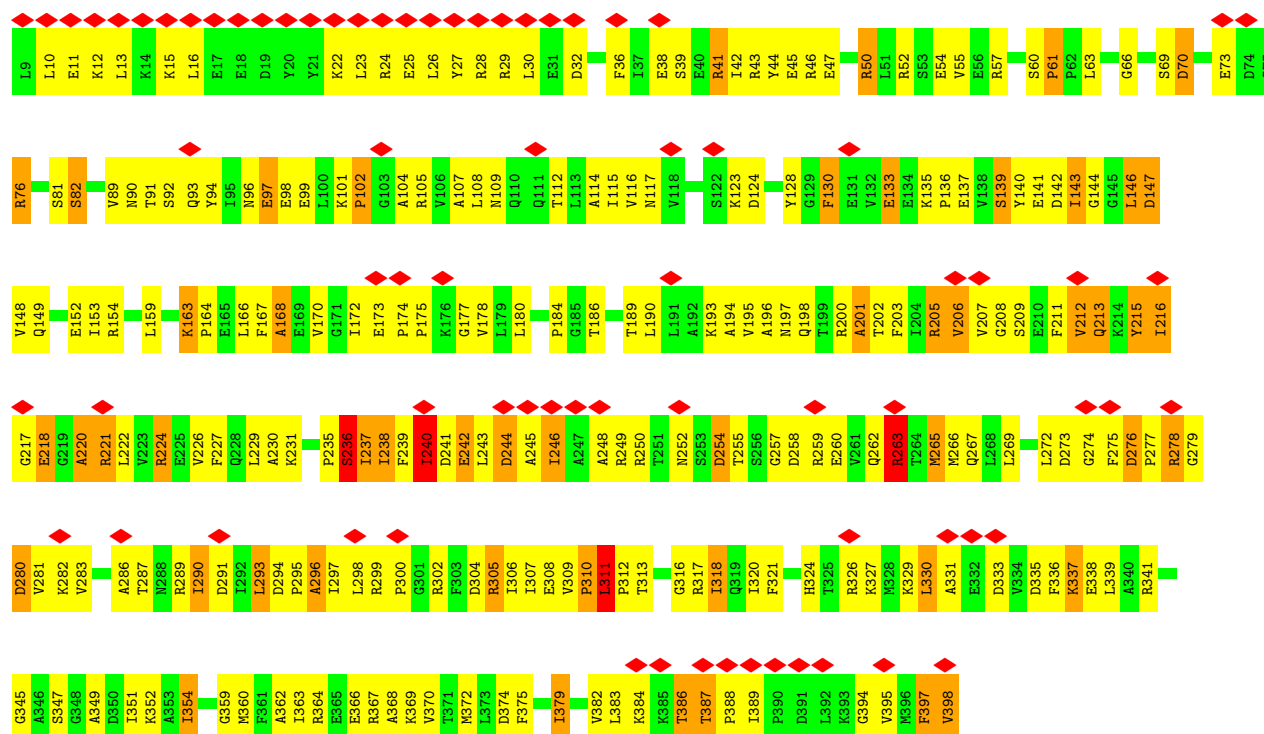




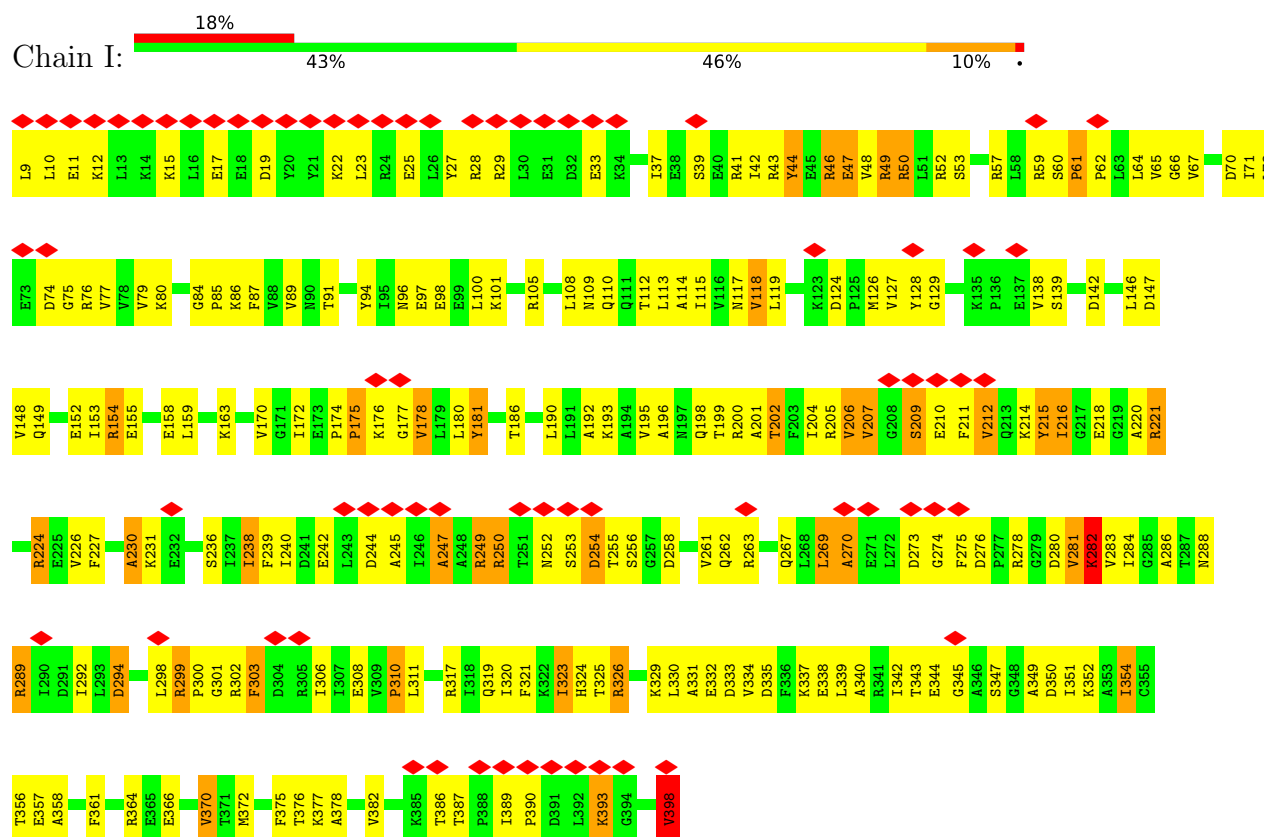
• Molecule 2: Proteasome subunit beta



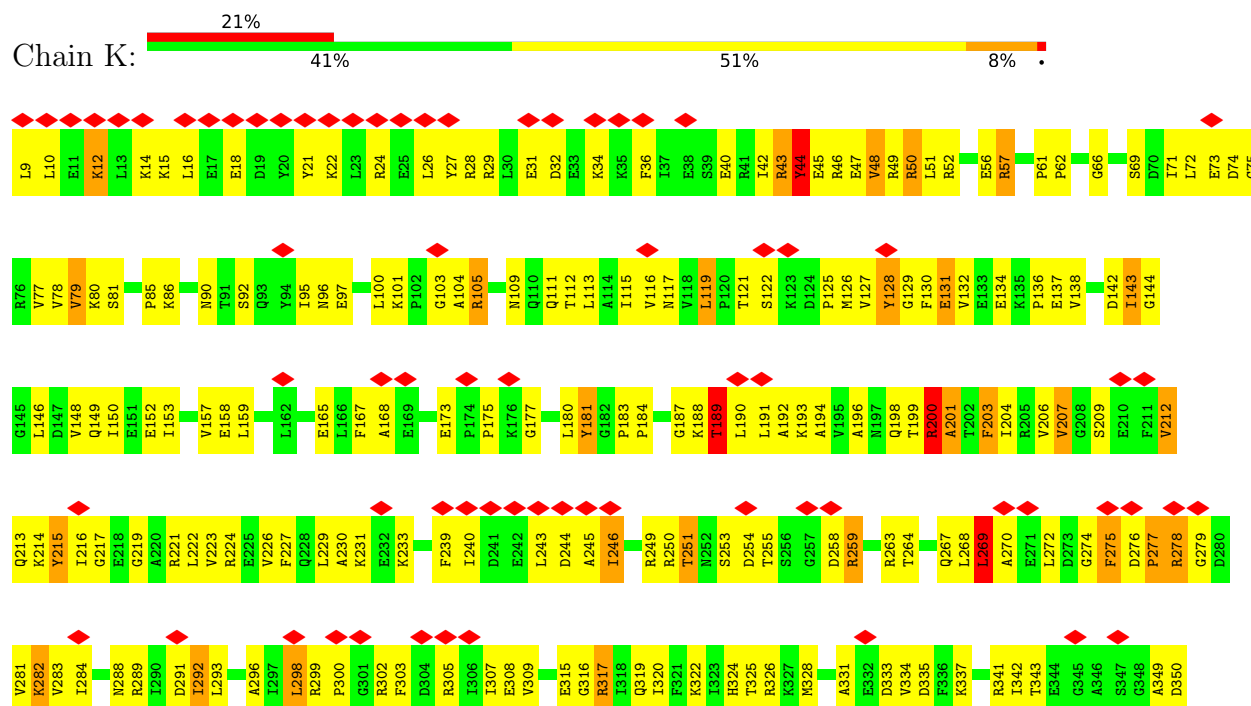
• Molecule 3: Proteasome-activating nucleotidase

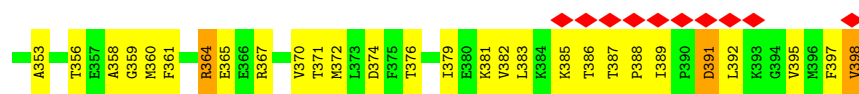


• Molecule 3: Proteasome-activating nucleotidase

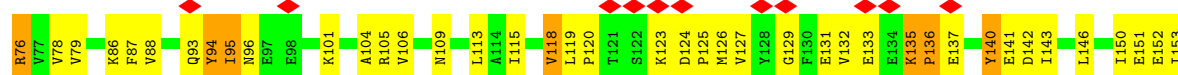
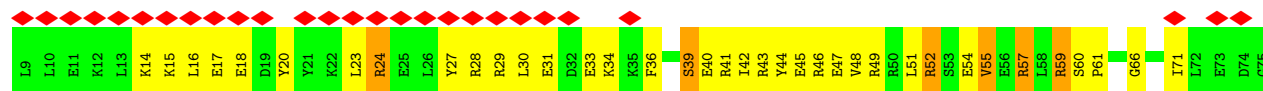


• Molecule 3: Proteasome-activating nucleotidase

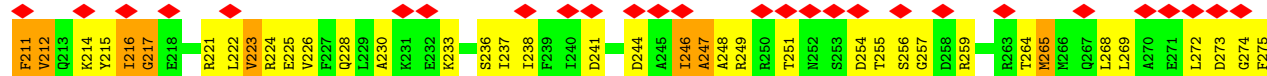
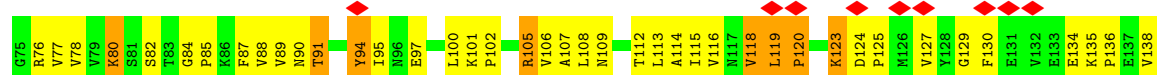
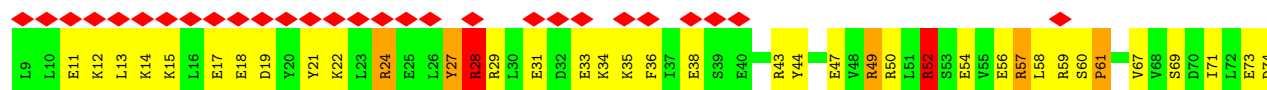


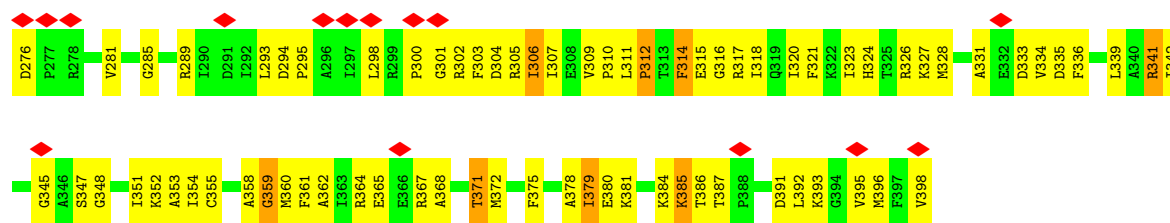


• Molecule 3: Proteasome-activating nucleotidase

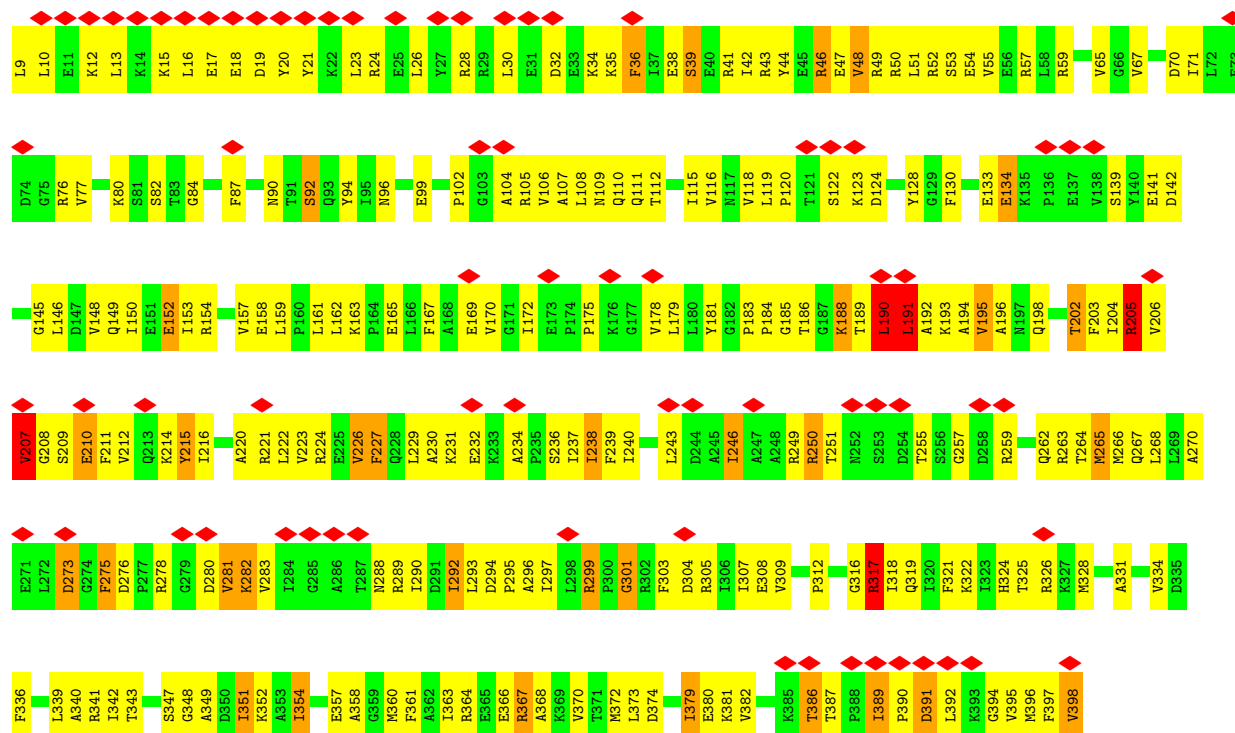


• Molecule 3: Proteasome-activating nucleotidase





• Molecule 3: Proteasome-activating nucleotidase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46148	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	0.061	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.24	67/1934 (3.5%)	2.48	141/2605 (5.4%)
1	B	2.32	92/1934 (4.8%)	2.43	116/2605 (4.5%)
1	C	2.27	81/1934 (4.2%)	2.43	121/2605 (4.6%)
1	D	2.28	81/1934 (4.2%)	2.42	126/2605 (4.8%)
1	E	2.29	84/1934 (4.3%)	2.45	135/2605 (5.2%)
1	F	2.21	65/1934 (3.4%)	2.46	135/2605 (5.2%)
1	G	2.30	69/1934 (3.6%)	2.47	136/2605 (5.2%)
1	a	2.29	71/1892 (3.8%)	2.52	134/2549 (5.3%)
1	b	2.32	73/1892 (3.9%)	2.45	124/2549 (4.9%)
1	c	2.32	91/1892 (4.8%)	2.47	126/2549 (4.9%)
1	d	2.31	73/1892 (3.9%)	2.43	113/2549 (4.4%)
1	e	2.32	83/1892 (4.4%)	2.50	144/2549 (5.6%)
1	f	2.28	83/1892 (4.4%)	2.41	120/2549 (4.7%)
1	g	2.35	77/1892 (4.1%)	2.39	124/2549 (4.9%)
2	1	2.24	58/1573 (3.7%)	2.46	111/2121 (5.2%)
2	2	2.23	57/1573 (3.6%)	2.38	99/2121 (4.7%)
2	3	2.29	62/1573 (3.9%)	2.43	115/2121 (5.4%)
2	4	2.31	66/1573 (4.2%)	2.40	88/2121 (4.1%)
2	5	3.16	74/1573 (4.7%)	2.52	95/2121 (4.5%)
2	6	2.28	68/1573 (4.3%)	2.54	105/2121 (5.0%)
2	7	2.34	73/1573 (4.6%)	2.51	108/2121 (5.1%)
2	h	2.28	53/1573 (3.4%)	2.51	115/2121 (5.4%)
2	i	2.27	54/1573 (3.4%)	2.55	103/2121 (4.9%)
2	j	2.25	57/1573 (3.6%)	2.44	97/2121 (4.6%)
2	k	2.17	51/1573 (3.2%)	2.37	95/2121 (4.5%)
2	l	3.17	60/1573 (3.8%)	2.44	90/2121 (4.2%)
2	m	2.30	48/1573 (3.1%)	2.38	95/2121 (4.5%)
2	n	2.33	72/1573 (4.6%)	2.46	113/2121 (5.3%)
3	H	2.31	142/3146 (4.5%)	2.46	222/4240 (5.2%)
3	I	2.27	110/3146 (3.5%)	2.45	209/4240 (4.9%)
3	J	2.28	135/3146 (4.3%)	2.47	228/4240 (5.4%)
3	K	2.26	124/3146 (3.9%)	2.46	226/4240 (5.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	L	2.35	132/3146 (4.2%)	2.51	235/4240 (5.5%)
3	M	2.28	118/3146 (3.8%)	2.44	205/4240 (4.8%)
All	All	2.34	2704/67680 (4.0%)	2.46	4549/91212 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	11
1	C	0	8
1	D	0	11
1	E	0	10
1	F	0	13
1	G	0	10
1	a	0	6
1	b	0	4
1	c	0	7
1	d	0	9
1	e	0	9
1	f	0	6
1	g	0	8
2	1	0	4
2	2	0	6
2	3	0	4
2	4	0	6
2	5	0	7
2	6	0	8
2	7	0	7
2	h	0	12
2	i	0	6
2	j	0	3
2	k	0	6
2	l	0	7
2	m	0	2
2	n	0	7
3	H	0	20
3	I	0	13
3	J	0	9
3	K	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	10
3	M	0	14
All	All	0	286

All (2704) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	CZ-NH1	56.45	2.11	1.32
2	5	170	ARG	CZ-NH1	54.70	2.09	1.32
2	l	211	PHE	CG-CD2	34.98	2.12	1.38
2	5	211	PHE	CG-CD2	33.60	2.09	1.38
2	l	211	PHE	CG-CD1	31.74	2.05	1.38
2	5	211	PHE	CG-CD1	31.52	2.05	1.38
2	5	211	PHE	CD1-CE1	24.27	2.11	1.38
2	5	211	PHE	CE1-CZ	23.84	2.10	1.38
2	l	211	PHE	CE1-CZ	22.86	2.07	1.38
2	5	211	PHE	CE2-CZ	22.35	2.05	1.38
2	l	211	PHE	CE2-CZ	22.08	2.04	1.38
2	l	211	PHE	CD2-CE2	21.17	2.02	1.38
2	5	211	PHE	CD2-CE2	20.12	1.99	1.38
2	l	211	PHE	CD1-CE1	19.93	1.98	1.38
2	3	19	CYS	CA-C	-15.95	1.32	1.52
3	L	333	ASP	CA-CB	13.64	1.63	1.53
2	m	16	GLY	CA-C	-12.91	1.39	1.51
2	j	63	ALA	CA-C	-12.45	1.37	1.52
2	7	68	ARG	CD-NE	11.74	1.62	1.46
3	J	398	VAL	C-O	-11.58	1.00	1.23
3	I	398	VAL	C-O	-11.56	1.00	1.23
3	L	398	VAL	C-O	-11.56	1.00	1.23
3	M	398	VAL	C-O	-11.56	1.00	1.23
3	H	398	VAL	C-OXT	-11.55	1.00	1.23
3	I	398	VAL	C-OXT	-11.55	1.00	1.23
3	M	398	VAL	C-OXT	-11.54	1.00	1.23
3	L	398	VAL	C-OXT	-11.54	1.00	1.23
3	K	398	VAL	C-OXT	-11.53	1.00	1.23
3	H	398	VAL	C-O	-11.53	1.00	1.23
3	K	398	VAL	C-O	-11.53	1.00	1.23
3	J	398	VAL	C-OXT	-11.53	1.00	1.23
2	m	53	ALA	N-CA	-11.30	1.32	1.46
1	E	109	VAL	C-N	11.15	1.47	1.33
2	l	131	ALA	CA-C	-11.08	1.39	1.52
1	b	45	GLY	CA-C	-10.86	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	194	VAL	CA-C	-10.67	1.39	1.52
1	d	28	ARG	CD-NE	10.66	1.61	1.46
1	C	41	LYS	CA-C	-10.44	1.40	1.52
1	D	73	HIS	N-CA	-10.42	1.36	1.46
3	M	106	VAL	CA-C	-10.34	1.40	1.52
3	L	278	ARG	C-N	10.24	1.45	1.33
3	K	245	ALA	N-CA	-10.22	1.38	1.47
1	a	212	GLY	CA-C	-10.21	1.43	1.52
1	b	179	TYR	CA-C	-10.16	1.40	1.52
2	3	104	PHE	CA-C	-10.16	1.42	1.52
2	n	39	SER	CA-C	-9.92	1.40	1.52
1	g	139	ALA	N-CA	-9.90	1.33	1.46
1	g	144	VAL	CA-C	9.89	1.61	1.52
2	h	188	VAL	CA-C	-9.84	1.41	1.52
1	d	106	PRO	N-CA	-9.74	1.35	1.47
2	5	45	ILE	CA-C	-9.66	1.40	1.52
2	h	110	LEU	CA-C	-9.51	1.41	1.52
1	e	134	VAL	CA-CB	-9.49	1.45	1.55
2	m	191	ILE	CA-C	-9.48	1.43	1.53
1	D	195	ALA	CA-C	-9.48	1.40	1.52
2	n	111	LEU	CA-C	-9.47	1.41	1.52
1	D	73	HIS	ND1-CE1	9.45	1.42	1.32
1	g	126	TYR	CA-CB	9.41	1.66	1.53
1	D	78	THR	CA-C	-9.41	1.41	1.52
2	4	126	ASP	CA-C	-9.38	1.41	1.53
1	C	241	ARG	CD-NE	9.37	1.59	1.46
2	l	160	GLY	CA-C	9.35	1.62	1.52
2	l	101	TYR	CA-C	-9.33	1.40	1.53
2	7	21	ASP	CA-C	-9.32	1.42	1.53
2	7	30	ARG	NE-CZ	9.28	1.43	1.33
1	D	223	GLU	N-CA	-9.22	1.34	1.46
1	G	139	ALA	CA-C	-9.21	1.41	1.52
1	B	238	GLU	CA-C	-9.10	1.41	1.52
3	H	92	SER	CA-C	-9.10	1.48	1.53
3	L	316	GLY	CA-C	-9.09	1.42	1.52
2	5	88	ARG	CD-NE	9.08	1.58	1.46
2	7	101	TYR	CA-CB	9.08	1.65	1.53
2	h	127	PRO	CA-CB	9.07	1.60	1.53
2	n	212	ARG	CD-NE	9.05	1.58	1.46
1	G	91	ARG	NE-CZ	9.02	1.43	1.33
1	f	100	ARG	NE-CZ	9.01	1.43	1.33
1	g	95	GLU	CA-CB	9.00	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	69	LYS	CA-C	-8.96	1.41	1.52
3	J	158	GLU	CA-C	-8.95	1.41	1.52
2	4	117	SER	N-CA	-8.92	1.34	1.46
2	3	199	TYR	CA-C	-8.90	1.41	1.53
1	B	94	ILE	CA-CB	8.90	1.65	1.54
2	h	42	ALA	CA-C	-8.90	1.41	1.52
1	c	73	HIS	ND1-CE1	8.89	1.41	1.32
3	I	308	GLU	CA-CB	8.89	1.64	1.53
1	G	83	ALA	N-CA	-8.87	1.35	1.46
2	l	158	GLU	CA-C	-8.85	1.40	1.53
1	A	51	ASP	CA-C	-8.85	1.41	1.52
2	4	51	ARG	CD-NE	8.85	1.58	1.46
2	n	16	GLY	CA-C	-8.82	1.39	1.51
2	j	203	GLU	CA-C	-8.81	1.41	1.52
3	H	24	ARG	N-CA	-8.79	1.35	1.46
2	7	156	THR	CA-C	8.78	1.60	1.52
1	D	74	ILE	CA-CB	-8.77	1.43	1.54
1	c	205	VAL	N-CA	-8.75	1.38	1.46
2	5	210	LYS	CA-C	-8.71	1.40	1.52
2	5	137	ILE	N-CA	-8.70	1.36	1.46
1	G	163	ALA	CA-C	-8.69	1.41	1.52
1	g	23	GLN	CA-C	-8.64	1.41	1.52
2	4	81	ARG	NE-CZ	8.63	1.42	1.33
2	l	51	ARG	N-CA	-8.62	1.36	1.46
3	H	265	MET	CA-CB	8.61	1.67	1.53
2	h	20	LYS	N-CA	-8.56	1.35	1.46
2	l	52	MET	CA-C	-8.56	1.42	1.52
3	M	362	ALA	CA-C	-8.55	1.41	1.52
3	L	141	GLU	CA-C	-8.52	1.41	1.52
3	I	239	PHE	N-CA	-8.52	1.35	1.46
3	I	206	VAL	CA-C	-8.51	1.43	1.52
2	j	190	LYS	CA-C	-8.50	1.42	1.52
1	A	134	VAL	CA-C	-8.50	1.42	1.52
2	l	95	SER	N-CA	-8.50	1.36	1.46
1	G	50	ALA	CA-C	-8.49	1.42	1.52
3	K	177	GLY	CA-C	-8.47	1.41	1.51
2	3	75	ASN	CA-C	-8.45	1.41	1.52
3	M	29	ARG	NE-CZ	8.45	1.42	1.33
1	D	48	LEU	N-CA	-8.44	1.36	1.46
2	5	173	TYR	CA-C	-8.43	1.41	1.52
2	l	173	TYR	CA-C	-8.42	1.41	1.52
2	n	81	ARG	CD-NE	8.40	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	81	ARG	CA-C	-8.40	1.41	1.52
3	M	352	LYS	N-CA	8.38	1.56	1.46
1	G	182	ASP	CA-C	-8.36	1.41	1.52
1	F	203	GLU	CA-C	-8.36	1.41	1.52
1	A	164	ILE	CA-C	-8.35	1.42	1.52
1	b	161	ALA	CA-C	-8.34	1.41	1.52
1	f	86	ARG	CZ-NH1	8.33	1.44	1.32
1	b	158	GLU	CA-C	-8.32	1.42	1.52
1	e	96	ALA	CA-C	-8.30	1.42	1.52
3	I	108	LEU	CA-C	-8.28	1.42	1.52
2	m	51	ARG	NE-CZ	8.27	1.42	1.33
3	M	43	ARG	CD-NE	8.26	1.57	1.46
1	b	67	ILE	N-CA	-8.25	1.36	1.46
3	I	306	ILE	C-N	8.22	1.42	1.33
3	L	228	GLN	CA-C	-8.21	1.42	1.52
3	J	394	GLY	C-N	8.20	1.43	1.33
3	I	138	VAL	CA-CB	-8.19	1.44	1.54
1	F	235	ARG	NE-CZ	8.17	1.42	1.33
2	6	80	ARG	NE-CZ	8.17	1.42	1.33
3	H	250	ARG	CZ-NH2	8.15	1.44	1.33
2	k	210	LYS	CA-C	-8.15	1.42	1.52
1	G	10	ARG	CD-NE	8.14	1.57	1.46
1	f	241	ARG	CZ-NH1	8.13	1.44	1.32
1	b	212	GLY	N-CA	8.11	1.52	1.44
1	f	53	ARG	NE-CZ	8.12	1.42	1.33
1	e	218	ASP	CA-C	-8.11	1.42	1.52
3	H	89	VAL	CA-C	-8.10	1.43	1.52
2	7	64	GLN	N-CA	-8.09	1.36	1.46
1	e	135	SER	CA-C	-8.09	1.42	1.52
1	c	95	GLU	CA-C	-8.08	1.41	1.52
2	2	178	ARG	CD-NE	8.08	1.57	1.46
1	D	77	ALA	CA-C	-8.06	1.43	1.52
2	7	54	MET	CA-C	-8.06	1.42	1.52
1	F	17	PRO	CA-CB	-8.05	1.42	1.53
3	H	349	ALA	C-N	8.05	1.44	1.33
1	A	100	ARG	CD-NE	8.05	1.57	1.46
2	l	212	ARG	N-CA	-8.04	1.35	1.46
2	j	149	GLY	CA-C	-8.03	1.43	1.52
2	l	81	ARG	CD-NE	8.03	1.57	1.46
1	E	219	ARG	C-N	8.01	1.45	1.33
2	5	114	GLY	CA-C	-8.01	1.42	1.52
2	7	212	ARG	CA-C	-8.01	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	ARG	NE-CZ	8.01	1.41	1.33
2	k	171	ALA	C-N	8.00	1.43	1.33
3	K	382	VAL	N-CA	-8.00	1.37	1.46
1	D	213	TYR	C-N	8.00	1.43	1.33
1	C	211	VAL	CA-C	-7.99	1.42	1.52
3	J	207	VAL	N-CA	-7.99	1.36	1.46
1	b	40	ILE	CA-C	-7.98	1.42	1.52
2	n	63	ALA	N-CA	-7.98	1.36	1.46
3	J	231	LYS	C-N	7.97	1.44	1.33
1	E	168	ARG	CD-NE	7.97	1.57	1.46
1	f	139	ALA	CA-C	-7.96	1.43	1.52
3	L	316	GLY	C-N	7.93	1.44	1.33
2	h	49	ALA	CA-C	-7.92	1.43	1.52
1	A	52	LYS	CA-C	-7.91	1.43	1.52
3	J	308	GLU	CA-CB	7.90	1.64	1.53
1	e	46	VAL	N-CA	-7.90	1.36	1.46
2	5	85	PRO	N-CA	-7.90	1.38	1.46
1	d	237	ASN	CA-CB	7.89	1.65	1.53
3	J	191	LEU	N-CA	-7.89	1.36	1.46
2	1	190	LYS	CA-C	-7.88	1.43	1.52
1	F	162	THR	CA-C	-7.88	1.43	1.52
1	B	68	TYR	N-CA	-7.88	1.35	1.46
3	I	209	SER	N-CA	-7.88	1.35	1.46
1	B	74	ILE	CA-C	-7.87	1.42	1.52
3	H	289	ARG	CA-C	-7.87	1.43	1.52
2	n	80	ARG	CA-CB	7.86	1.65	1.53
1	D	100	ARG	CD-NE	7.86	1.57	1.46
1	d	106	PRO	CA-C	-7.86	1.43	1.52
1	g	187	ASP	CA-C	-7.85	1.43	1.52
3	L	302	ARG	CD-NE	7.85	1.57	1.46
1	f	163	ALA	CA-C	-7.84	1.43	1.52
1	B	137	LEU	CA-C	-7.83	1.43	1.52
3	J	49	ARG	CD-NE	7.83	1.57	1.46
1	D	95	GLU	CA-C	7.82	1.63	1.52
3	K	72	LEU	CA-C	-7.82	1.43	1.52
3	L	61	PRO	CA-C	7.82	1.56	1.51
2	4	198	GLN	CA-C	-7.81	1.43	1.52
1	E	110	LYS	CA-C	-7.81	1.42	1.52
2	6	95	SER	CA-C	-7.80	1.43	1.52
2	2	170	ARG	CD-NE	7.79	1.57	1.46
2	2	94	THR	C-N	7.79	1.43	1.33
1	e	93	ARG	CA-C	-7.78	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	LYS	C-N	7.78	1.43	1.33
3	L	361	PHE	N-CA	-7.78	1.36	1.46
1	g	38	ILE	CA-C	-7.78	1.43	1.52
2	k	125	ILE	CA-C	-7.77	1.43	1.52
2	l	15	VAL	CA-C	-7.77	1.43	1.52
3	L	119	LEU	C-N	7.77	1.42	1.33
1	d	235	ARG	NE-CZ	7.77	1.41	1.33
1	c	69	LYS	C-N	7.75	1.42	1.33
1	C	20	ARG	NE-CZ	7.74	1.41	1.33
2	5	106	TYR	CA-C	-7.74	1.43	1.52
1	E	140	GLY	CA-C	-7.74	1.43	1.51
1	g	170	ALA	CA-C	-7.73	1.43	1.52
1	C	39	GLY	N-CA	-7.72	1.38	1.45
1	b	117	CYS	CA-C	-7.72	1.42	1.52
1	C	241	ARG	NE-CZ	7.72	1.41	1.33
2	h	212	ARG	NE-CZ	7.72	1.41	1.33
1	E	106	PRO	CA-C	-7.72	1.43	1.52
3	K	104	ALA	CA-CB	7.72	1.64	1.53
1	A	147	LEU	N-CA	-7.71	1.36	1.46
1	F	59	LEU	C-N	7.71	1.44	1.33
3	M	59	ARG	CZ-NH1	7.71	1.43	1.32
3	L	239	PHE	CA-CB	7.71	1.64	1.53
2	6	124	SER	CA-C	-7.70	1.43	1.52
3	J	293	LEU	N-CA	-7.70	1.36	1.45
2	2	211	PHE	N-CA	-7.70	1.36	1.46
1	E	111	GLU	CA-C	-7.70	1.42	1.52
2	6	189	VAL	CA-C	-7.70	1.43	1.52
1	d	115	LYS	C-N	7.69	1.42	1.33
1	G	170	ALA	C-N	7.68	1.43	1.33
2	m	80	ARG	NE-CZ	7.68	1.41	1.33
2	i	23	VAL	CA-C	-7.67	1.43	1.52
3	J	70	ASP	CA-C	-7.67	1.43	1.52
2	l	33	MET	N-CA	-7.67	1.37	1.46
2	n	81	ARG	C-N	7.66	1.44	1.33
2	3	95	SER	C-N	7.64	1.43	1.33
2	i	68	ARG	NE-CZ	7.63	1.41	1.33
2	4	165	VAL	N-CA	-7.63	1.37	1.46
3	K	302	ARG	CA-C	-7.62	1.43	1.52
1	F	156	LEU	N-CA	-7.62	1.36	1.46
3	K	143	ILE	CA-C	-7.61	1.43	1.52
3	H	341	ARG	CD-NE	7.61	1.56	1.46
1	f	241	ARG	NE-CZ	7.61	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	183	PRO	CA-CB	-7.60	1.43	1.54
1	d	221	PHE	C-O	-7.60	1.14	1.24
3	K	92	SER	CA-C	-7.59	1.43	1.53
3	M	178	VAL	CA-C	-7.59	1.43	1.52
1	B	7	GLY	C-N	7.59	1.45	1.33
1	f	181	ASP	N-CA	-7.59	1.35	1.46
3	H	11	GLU	N-CA	-7.59	1.37	1.46
1	G	130	ARG	NE-CZ	7.58	1.41	1.33
1	g	156	LEU	CA-C	-7.58	1.43	1.52
1	D	45	GLY	C-N	7.58	1.42	1.33
1	f	189	MET	CA-C	-7.57	1.43	1.52
1	E	12	ILE	CA-C	-7.57	1.42	1.52
1	a	51	ASP	CA-C	-7.56	1.43	1.52
1	C	74	ILE	CA-C	-7.56	1.43	1.52
2	4	122	ILE	N-CA	-7.55	1.37	1.46
1	e	20	ARG	CA-CB	7.55	1.65	1.53
1	f	196	MET	CA-C	-7.55	1.43	1.52
1	g	37	ALA	CA-C	-7.55	1.43	1.52
2	l	174	SER	CA-C	-7.55	1.43	1.52
1	G	241	ARG	NE-CZ	7.54	1.41	1.33
2	k	81	ARG	CD-NE	7.54	1.56	1.46
1	A	24	VAL	CA-C	-7.53	1.43	1.52
1	E	240	ILE	CA-C	-7.52	1.43	1.52
1	e	73	HIS	N-CA	-7.52	1.39	1.46
1	B	147	LEU	N-CA	-7.51	1.36	1.46
1	b	181	ASP	CA-C	-7.51	1.42	1.52
3	I	335	ASP	CA-C	-7.51	1.43	1.52
3	L	367	ARG	CZ-NH2	7.50	1.43	1.33
1	b	23	GLN	N-CA	-7.50	1.37	1.46
2	l	170	ARG	CD-NE	7.47	1.56	1.46
2	7	83	ARG	N-CA	-7.46	1.36	1.46
1	c	91	ARG	CD-NE	7.46	1.56	1.46
1	e	177	LYS	N-CA	-7.46	1.36	1.46
1	g	33	ARG	CZ-NH1	7.45	1.43	1.32
2	6	78	GLU	CA-CB	7.44	1.65	1.53
3	L	299	ARG	CD-NE	7.44	1.56	1.46
1	a	91	ARG	CZ-NH1	7.44	1.43	1.32
2	h	190	LYS	CA-CB	7.44	1.65	1.53
3	M	154	ARG	NE-CZ	7.44	1.41	1.33
1	b	60	GLU	CA-C	-7.43	1.43	1.52
1	e	115	LYS	CA-C	-7.43	1.43	1.52
1	f	219	ARG	NE-CZ	7.43	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	111	LEU	N-CA	-7.42	1.36	1.46
2	5	104	PHE	CA-C	7.42	1.61	1.52
1	B	38	ILE	CA-C	-7.42	1.43	1.52
3	H	311	LEU	C-N	7.41	1.42	1.33
3	M	302	ARG	CD-NE	7.41	1.56	1.46
1	B	138	ILE	CA-C	-7.40	1.43	1.52
2	5	180	SER	C-N	7.40	1.44	1.33
2	6	88	ARG	NE-CZ	7.40	1.41	1.33
2	j	154	ARG	CZ-NH2	7.40	1.43	1.33
3	I	28	ARG	CD-NE	7.39	1.56	1.46
3	M	203	PHE	C-N	7.39	1.43	1.33
3	H	163	LYS	CA-CB	7.39	1.65	1.53
3	H	259	ARG	CZ-NH2	7.38	1.43	1.33
1	D	88	LEU	CA-C	-7.38	1.43	1.52
2	7	97	LEU	C-N	7.38	1.43	1.33
1	c	146	LYS	CA-C	-7.37	1.43	1.52
1	b	147	LEU	CA-C	-7.37	1.43	1.52
1	e	100	ARG	NE-CZ	7.37	1.41	1.33
1	d	221	PHE	CA-CB	7.37	1.66	1.53
2	1	24	VAL	CA-C	-7.37	1.43	1.52
3	M	172	ILE	N-CA	7.36	1.55	1.46
3	I	278	ARG	CZ-NH2	7.36	1.43	1.33
1	c	20	ARG	NE-CZ	7.36	1.41	1.33
1	b	208	ASN	CA-CB	7.35	1.63	1.53
1	c	205	VAL	CA-CB	7.35	1.60	1.54
1	G	207	GLU	CA-C	-7.35	1.43	1.52
2	1	47	GLN	N-CA	-7.35	1.37	1.46
2	3	124	SER	N-CA	-7.35	1.37	1.46
3	J	325	THR	C-N	7.34	1.43	1.33
3	K	359	GLY	CA-C	-7.34	1.43	1.52
2	i	212	ARG	CD-NE	7.34	1.56	1.46
2	m	51	ARG	CA-C	-7.34	1.43	1.53
1	c	52	LYS	C-N	7.33	1.43	1.33
3	M	49	ARG	NE-CZ	7.33	1.41	1.33
3	J	351	ILE	C-N	7.32	1.43	1.33
1	c	104	ASP	CA-C	-7.32	1.44	1.53
2	5	21	ASP	C-N	7.32	1.41	1.32
2	j	68	ARG	NE-CZ	7.32	1.41	1.33
1	d	112	LEU	CA-CB	7.31	1.65	1.53
1	g	30	ALA	C-N	7.31	1.43	1.33
1	C	138	ILE	CA-CB	-7.30	1.45	1.54
1	G	137	LEU	CA-C	-7.30	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	51	ARG	CD-NE	7.29	1.56	1.46
1	g	100	ARG	C-N	7.29	1.43	1.33
3	L	341	ARG	NE-CZ	7.28	1.41	1.33
1	f	140	GLY	C-N	7.28	1.42	1.33
3	I	77	VAL	C-N	7.28	1.43	1.33
1	A	118	ASP	C-N	7.27	1.43	1.33
1	c	239	ARG	CD-NE	7.27	1.56	1.46
2	5	132	ILE	C-O	-7.27	1.16	1.24
1	A	168	ARG	C-N	7.27	1.43	1.33
1	c	168	ARG	CD-NE	7.26	1.56	1.46
1	G	93	ARG	NE-CZ	7.26	1.41	1.33
3	H	226	VAL	CA-CB	-7.26	1.45	1.54
2	4	121	SER	CA-C	-7.26	1.44	1.52
2	l	81	ARG	C-N	7.25	1.43	1.33
3	M	315	GLU	C-N	7.25	1.42	1.33
3	M	384	LYS	N-CA	-7.25	1.37	1.46
3	H	24	ARG	CD-NE	7.23	1.56	1.46
2	n	32	THR	N-CA	-7.23	1.36	1.45
1	a	50	ALA	C-N	7.22	1.43	1.33
2	5	101	TYR	N-CA	-7.22	1.38	1.46
1	a	47	ILE	N-CA	-7.22	1.37	1.46
3	M	259	ARG	NE-CZ	7.22	1.41	1.33
3	L	346	ALA	CA-CB	7.21	1.65	1.53
1	B	200	ILE	C-N	7.21	1.44	1.33
3	L	55	VAL	CA-C	7.21	1.61	1.52
1	G	76	ALA	C-N	7.21	1.43	1.33
3	L	216	ILE	N-CA	-7.21	1.38	1.46
2	m	118	GLU	N-CA	-7.20	1.36	1.46
1	A	161	ALA	C-N	7.20	1.42	1.33
1	g	181	ASP	CA-C	-7.19	1.45	1.53
1	A	131	PRO	C-N	7.19	1.43	1.33
2	m	26	ALA	C-N	7.18	1.43	1.33
1	G	20	ARG	NE-CZ	7.18	1.41	1.33
1	g	235	ARG	NE-CZ	7.18	1.41	1.33
1	c	27	ALA	N-CA	-7.17	1.37	1.46
1	d	239	ARG	CD-NE	7.17	1.56	1.46
2	m	184	ASP	CA-C	-7.17	1.44	1.52
2	1	42	ALA	CA-C	-7.17	1.43	1.52
2	h	144	SER	C-N	7.16	1.43	1.33
1	e	66	LYS	C-N	7.16	1.42	1.33
2	7	131	ALA	N-CA	-7.15	1.37	1.46
1	F	130	ARG	CD-NE	7.15	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	128	GLY	CA-C	-7.15	1.40	1.51
3	K	191	LEU	CA-C	7.15	1.62	1.52
2	i	80	ARG	N-CA	-7.14	1.37	1.46
1	c	200	ILE	CA-CB	-7.14	1.45	1.54
1	D	39	GLY	CA-C	-7.14	1.45	1.51
3	J	181	TYR	CA-C	-7.14	1.43	1.52
1	C	78	THR	CA-C	-7.14	1.43	1.52
2	5	30	ARG	NE-CZ	7.13	1.40	1.33
3	L	119	LEU	CA-C	-7.13	1.42	1.53
3	I	215	TYR	CA-C	-7.13	1.44	1.52
1	g	177	LYS	CA-C	-7.12	1.43	1.52
2	5	65	PHE	CA-CB	7.12	1.64	1.53
1	G	197	GLY	CA-C	-7.12	1.43	1.51
1	A	222	LYS	CA-C	-7.12	1.43	1.52
1	A	189	MET	CA-C	7.12	1.62	1.52
2	h	151	LEU	N-CA	-7.11	1.37	1.46
3	H	32	ASP	CA-C	-7.11	1.43	1.52
1	b	131	PRO	C-O	-7.10	1.15	1.23
2	1	47	GLN	CA-CB	7.10	1.62	1.53
1	E	235	ARG	NE-CZ	7.09	1.40	1.33
3	J	105	ARG	CA-C	-7.09	1.43	1.52
3	J	309	VAL	CA-C	7.09	1.60	1.52
3	H	61	PRO	C-N	-7.09	1.24	1.33
3	L	137	GLU	C-N	7.09	1.41	1.33
1	c	242	GLU	CA-CB	7.09	1.64	1.53
2	i	107	LEU	CA-CB	7.09	1.64	1.53
1	e	67	ILE	CA-C	-7.08	1.43	1.52
1	g	119	PHE	CA-CB	7.08	1.64	1.53
3	K	85	PRO	CA-C	-7.08	1.44	1.52
3	L	46	ARG	CD-NE	7.08	1.56	1.46
3	M	241	ASP	C-N	7.08	1.43	1.33
2	4	64	GLN	N-CA	-7.07	1.37	1.46
1	D	14	VAL	CA-C	-7.07	1.43	1.52
2	j	82	GLU	CA-C	-7.07	1.44	1.53
3	H	200	ARG	NE-CZ	7.07	1.40	1.33
1	b	168	ARG	CA-CB	7.07	1.64	1.53
3	J	77	VAL	CA-C	-7.06	1.44	1.52
3	K	337	LYS	CA-C	-7.06	1.43	1.52
1	D	46	VAL	C-O	7.06	1.31	1.23
3	K	289	ARG	NE-CZ	7.06	1.40	1.33
2	l	104	PHE	CA-CB	7.05	1.62	1.53
1	b	146	LYS	CA-C	-7.05	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	154	ARG	NE-CZ	7.05	1.40	1.33
1	f	10	ARG	CZ-NH2	7.05	1.42	1.33
2	1	178	ARG	C-N	7.05	1.42	1.33
3	L	209	SER	CA-C	-7.04	1.43	1.52
1	A	10	ARG	NE-CZ	7.04	1.40	1.33
2	4	17	LEU	N-CA	-7.04	1.37	1.46
1	E	93	ARG	CD-NE	7.04	1.56	1.46
3	H	102	PRO	C-N	7.03	1.44	1.33
2	n	18	VAL	C-N	7.03	1.43	1.33
1	d	216	VAL	N-CA	-7.03	1.38	1.46
2	7	109	GLN	CA-C	-7.03	1.44	1.52
2	n	109	GLN	CA-C	-7.03	1.44	1.52
3	J	255	THR	CA-C	-7.02	1.43	1.52
2	2	53	ALA	CA-C	-7.02	1.43	1.52
3	I	66	GLY	CA-C	7.02	1.57	1.52
3	L	388	PRO	N-CA	-7.02	1.38	1.47
2	7	191	ILE	N-CA	-7.02	1.37	1.46
2	k	153	ASP	CA-C	-7.01	1.43	1.52
2	1	13	THR	CA-CB	7.01	1.65	1.53
1	g	93	ARG	CZ-NH1	7.01	1.42	1.32
2	2	66	LEU	C-N	7.00	1.43	1.33
1	e	241	ARG	CA-C	-7.00	1.44	1.52
1	G	26	TYR	CA-C	-7.00	1.42	1.52
1	B	239	ARG	CD-NE	6.99	1.56	1.46
1	A	207	GLU	C-N	6.99	1.43	1.33
2	n	21	ASP	CA-CB	6.99	1.64	1.54
3	H	96	ASN	C-N	6.98	1.44	1.33
1	a	151	ASP	CA-CB	6.97	1.64	1.54
2	4	154	ARG	NE-CZ	6.97	1.40	1.33
3	H	69	SER	C-N	6.97	1.42	1.33
1	B	168	ARG	CD-NE	6.97	1.56	1.46
1	E	44	GLU	C-N	6.97	1.40	1.32
1	d	180	ARG	CD-NE	6.96	1.56	1.46
1	c	189	MET	CA-C	6.96	1.61	1.52
3	K	364	ARG	NE-CZ	6.96	1.40	1.33
1	d	171	VAL	CA-CB	-6.96	1.45	1.54
2	6	105	PRO	CA-C	6.95	1.61	1.52
3	J	275	PHE	C-O	-6.95	1.15	1.24
3	K	131	GLU	CA-C	-6.95	1.43	1.52
3	K	100	LEU	C-N	6.95	1.41	1.33
2	j	30	ARG	CD-NE	6.94	1.55	1.46
1	C	162	THR	C-N	6.94	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	VAL	CA-CB	-6.94	1.44	1.54
1	f	227	GLU	CA-C	-6.94	1.43	1.52
2	1	109	GLN	CA-C	-6.94	1.44	1.52
3	J	141	GLU	C-N	6.94	1.41	1.33
3	K	96	ASN	CA-CB	6.93	1.64	1.53
3	J	326	ARG	CZ-NH2	6.93	1.42	1.33
1	G	44	GLU	CA-C	-6.93	1.43	1.52
2	k	88	ARG	NE-CZ	6.93	1.40	1.33
3	H	54	GLU	C-N	6.93	1.42	1.33
3	K	10	LEU	CA-C	-6.93	1.43	1.52
2	5	48	ILE	C-N	6.93	1.41	1.33
2	7	163	GLU	CA-C	-6.93	1.43	1.52
2	n	89	ALA	C-N	6.93	1.42	1.33
1	F	165	GLY	CA-C	-6.93	1.42	1.51
2	5	168	ALA	CA-CB	6.93	1.64	1.53
1	B	180	ARG	CD-NE	6.92	1.55	1.46
1	f	241	ARG	N-CA	-6.92	1.37	1.46
3	I	115	ILE	C-N	6.92	1.43	1.33
2	5	51	ARG	CA-CB	6.92	1.63	1.53
2	5	155	PHE	CA-CB	6.92	1.63	1.53
3	K	381	LYS	C-N	6.92	1.42	1.33
2	l	161	VAL	CA-C	-6.91	1.43	1.52
1	G	235	ARG	CZ-NH2	6.91	1.42	1.33
1	b	140	GLY	CA-C	-6.90	1.44	1.51
3	L	299	ARG	NE-CZ	6.90	1.40	1.33
1	C	221	PHE	CA-C	6.90	1.62	1.52
2	n	189	VAL	CA-C	-6.90	1.44	1.52
3	I	180	LEU	C-N	6.90	1.42	1.33
1	G	236	ALA	CA-C	-6.89	1.43	1.52
1	c	170	ALA	CA-CB	6.89	1.64	1.53
2	2	29	LYS	CA-CB	6.89	1.65	1.53
1	b	20	ARG	CD-NE	6.88	1.55	1.46
3	I	326	ARG	CZ-NH2	6.88	1.42	1.33
1	f	73	HIS	CD2-NE2	6.88	1.45	1.37
2	3	83	ARG	NE-CZ	6.88	1.40	1.33
1	g	241	ARG	NE-CZ	6.88	1.40	1.33
3	I	274	GLY	CA-C	-6.88	1.43	1.52
1	g	120	LYS	C-N	6.88	1.43	1.34
2	l	26	ALA	CA-C	-6.88	1.44	1.52
1	c	236	ALA	CA-C	-6.87	1.44	1.52
1	c	237	ASN	CA-C	-6.87	1.43	1.52
1	E	164	ILE	CA-C	-6.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	205	VAL	CA-CB	-6.87	1.49	1.54
3	M	177	GLY	C-N	6.87	1.42	1.33
1	c	163	ALA	CA-C	-6.86	1.44	1.52
1	A	83	ALA	CA-C	-6.86	1.44	1.52
1	B	207	GLU	C-N	6.86	1.42	1.33
3	M	163	LYS	CA-CB	6.86	1.61	1.53
1	C	130	ARG	NE-CZ	6.86	1.40	1.33
2	4	77	TYR	N-CA	-6.86	1.38	1.46
1	b	64	ILE	CA-CB	-6.85	1.46	1.54
1	C	28	ARG	CD-NE	6.85	1.55	1.46
3	H	312	PRO	N-CA	-6.85	1.40	1.46
1	E	133	GLY	N-CA	-6.85	1.35	1.45
2	6	68	ARG	N-CA	-6.85	1.38	1.46
2	h	148	TYR	N-CA	-6.84	1.38	1.46
1	a	122	GLN	CA-C	-6.84	1.43	1.52
1	C	139	ALA	CA-C	-6.84	1.44	1.52
3	K	109	ASN	C-N	6.83	1.44	1.33
3	L	17	GLU	C-N	6.83	1.42	1.33
2	2	88	ARG	CZ-NH1	6.83	1.42	1.32
2	h	115	ILE	CA-C	-6.83	1.44	1.52
3	H	190	LEU	N-CA	-6.83	1.38	1.46
3	I	364	ARG	CD-NE	6.82	1.55	1.46
3	K	282	LYS	C-N	6.82	1.42	1.33
1	E	206	PRO	N-CA	6.81	1.54	1.47
1	A	28	ARG	CZ-NH1	6.81	1.42	1.32
2	h	35	ASN	CA-C	6.81	1.61	1.52
3	I	175	PRO	C-N	6.81	1.42	1.33
2	5	135	LYS	N-CA	-6.80	1.38	1.46
2	2	98	LEU	C-N	6.80	1.42	1.33
2	7	145	LEU	CA-C	-6.79	1.44	1.52
2	2	151	LEU	CA-C	-6.79	1.44	1.52
3	K	49	ARG	CZ-NH2	6.79	1.42	1.33
3	L	24	ARG	NE-CZ	6.79	1.40	1.33
1	c	210	GLU	CA-C	-6.79	1.44	1.52
3	L	308	GLU	CA-C	-6.79	1.44	1.52
1	A	98	ILE	C-N	6.78	1.42	1.33
1	a	64	ILE	N-CA	-6.78	1.38	1.46
2	3	151	LEU	CA-CB	6.78	1.64	1.53
3	H	167	PHE	CA-CB	6.78	1.63	1.53
2	j	196	PHE	CA-C	-6.78	1.44	1.53
3	K	383	LEU	CA-CB	6.78	1.63	1.53
1	C	156	LEU	N-CA	-6.77	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	NE-CZ	6.77	1.40	1.33
2	m	178	ARG	NE-CZ	6.77	1.40	1.33
1	b	122	GLN	C-N	6.77	1.43	1.33
2	5	122	ILE	CA-CB	6.76	1.63	1.54
3	M	289	ARG	C-N	6.76	1.42	1.34
1	f	204	LEU	CA-C	-6.76	1.44	1.52
1	a	181	ASP	CA-C	-6.76	1.42	1.52
1	E	45	GLY	C-N	6.75	1.41	1.33
1	b	13	THR	CA-C	-6.75	1.44	1.52
3	K	86	LYS	C-N	6.75	1.42	1.33
1	C	39	GLY	CA-C	-6.75	1.45	1.51
1	E	121	GLN	CA-C	-6.75	1.43	1.52
2	2	102	ARG	NE-CZ	6.75	1.40	1.33
1	c	23	GLN	C-N	6.74	1.42	1.33
2	1	30	ARG	NE-CZ	6.74	1.40	1.33
2	7	43	LYS	N-CA	-6.74	1.37	1.46
2	m	188	VAL	CA-C	-6.74	1.44	1.52
2	n	76	LEU	N-CA	-6.74	1.38	1.46
3	J	76	ARG	NE-CZ	6.74	1.40	1.33
3	J	270	ALA	CA-C	6.74	1.61	1.52
1	B	10	ARG	CD-NE	6.74	1.55	1.46
1	b	171	VAL	N-CA	-6.73	1.37	1.46
1	e	11	ALA	N-CA	-6.73	1.37	1.46
2	k	146	THR	CA-C	-6.73	1.44	1.52
1	g	239	ARG	NE-CZ	6.73	1.40	1.33
1	a	10	ARG	CZ-NH1	6.72	1.42	1.32
2	2	154	ARG	CD-NE	6.72	1.55	1.46
2	i	93	LEU	N-CA	-6.72	1.38	1.46
3	H	374	ASP	CA-C	-6.72	1.44	1.52
3	K	289	ARG	CA-C	-6.72	1.44	1.52
1	C	210	GLU	N-CA	-6.72	1.37	1.46
2	3	44	LYS	CA-CB	6.72	1.64	1.54
1	A	226	PRO	N-CA	-6.71	1.38	1.47
1	d	45	GLY	CA-C	-6.71	1.45	1.52
1	F	53	ARG	CD-NE	6.71	1.55	1.46
2	5	113	GLY	N-CA	-6.71	1.38	1.45
3	H	28	ARG	CZ-NH2	6.71	1.42	1.33
3	J	224	ARG	CD-NE	6.71	1.55	1.46
1	D	53	ARG	NE-CZ	6.71	1.40	1.33
3	L	293	LEU	CA-C	-6.71	1.43	1.52
3	I	41	ARG	C-N	6.71	1.42	1.33
1	e	162	THR	C-N	6.70	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	305	ARG	NE-CZ	6.70	1.40	1.33
3	J	24	ARG	CD-NE	6.70	1.55	1.46
3	M	180	LEU	CA-C	-6.70	1.44	1.52
1	b	19	GLY	C-N	6.69	1.44	1.33
1	d	126	TYR	CA-CB	6.69	1.64	1.53
3	H	196	ALA	CA-C	-6.69	1.44	1.52
3	J	115	ILE	CA-C	-6.69	1.45	1.52
1	F	113	ALA	CA-C	-6.68	1.44	1.52
2	k	56	THR	CA-C	-6.68	1.44	1.52
2	2	83	ARG	CD-NE	6.68	1.55	1.46
1	A	69	LYS	N-CA	-6.68	1.37	1.46
1	E	144	VAL	CA-C	-6.68	1.45	1.52
1	E	199	SER	C-N	6.68	1.42	1.33
3	J	154	ARG	NE-CZ	6.67	1.40	1.33
3	M	57	ARG	NE-CZ	6.67	1.40	1.33
1	E	69	LYS	CA-CB	-6.67	1.43	1.53
2	3	81	ARG	CD-NE	6.67	1.55	1.46
1	g	136	LEU	CA-C	-6.66	1.44	1.52
3	I	61	PRO	CA-CB	6.66	1.60	1.53
2	3	39	SER	C-N	6.66	1.42	1.33
3	H	54	GLU	CA-C	-6.66	1.43	1.52
2	i	51	ARG	CZ-NH2	6.66	1.42	1.33
2	j	154	ARG	NE-CZ	6.66	1.40	1.33
3	H	107	ALA	CA-C	-6.66	1.44	1.52
2	6	116	ASP	CA-C	-6.65	1.44	1.52
3	K	341	ARG	NE-CZ	6.65	1.40	1.33
1	c	28	ARG	NE-CZ	6.65	1.40	1.33
1	E	67	ILE	CA-CB	-6.65	1.45	1.54
2	n	94	THR	CA-C	-6.65	1.44	1.52
2	4	83	ARG	CZ-NH1	6.65	1.42	1.32
3	H	96	ASN	CA-C	-6.65	1.44	1.52
1	d	91	ARG	CZ-NH1	6.65	1.42	1.32
1	C	75	CYS	CA-C	-6.64	1.44	1.52
2	2	87	VAL	CA-C	-6.64	1.44	1.52
3	J	19	ASP	CA-CB	6.64	1.63	1.53
3	J	59	ARG	CA-C	-6.64	1.43	1.52
1	d	85	ALA	CA-C	-6.64	1.44	1.52
1	A	85	ALA	N-CA	-6.64	1.38	1.46
1	A	219	ARG	CA-CB	6.64	1.63	1.53
1	b	20	ARG	CA-C	-6.64	1.44	1.52
2	i	176	MET	CA-C	-6.64	1.43	1.52
2	1	106	TYR	N-CA	-6.64	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	134	GLU	CA-C	6.63	1.61	1.52
3	J	361	PHE	C-N	6.63	1.42	1.33
1	G	103	TYR	N-CA	-6.63	1.37	1.46
2	5	40	LYS	N-CA	-6.63	1.38	1.46
1	b	73	HIS	CE1-NE2	-6.63	1.25	1.32
2	i	56	THR	N-CA	-6.63	1.38	1.46
3	L	364	ARG	C-N	6.63	1.43	1.34
1	a	65	GLU	CA-C	-6.63	1.44	1.52
1	c	156	LEU	CA-C	-6.63	1.44	1.52
1	d	195	ALA	N-CA	-6.63	1.38	1.46
1	F	171	VAL	C-N	6.63	1.42	1.33
3	M	210	GLU	CA-C	-6.62	1.44	1.52
1	B	15	PHE	N-CA	-6.62	1.38	1.46
2	j	32	THR	N-CA	-6.62	1.37	1.45
3	H	360	MET	CA-C	-6.62	1.43	1.52
1	g	212	GLY	CA-C	-6.62	1.45	1.51
2	7	168	ALA	N-CA	6.62	1.54	1.46
2	3	80	ARG	NE-CZ	6.61	1.40	1.33
1	G	203	GLU	CA-C	6.61	1.61	1.52
1	A	167	GLY	C-N	6.61	1.42	1.33
1	b	165	GLY	CA-C	-6.61	1.44	1.52
1	e	180	ARG	CA-C	-6.60	1.44	1.52
3	K	57	ARG	NE-CZ	6.60	1.40	1.33
3	I	117	ASN	C-N	6.60	1.41	1.33
3	K	217	GLY	N-CA	-6.60	1.34	1.45
1	B	89	ILE	C-N	6.59	1.42	1.33
2	6	28	GLU	CA-C	-6.59	1.44	1.52
1	D	28	ARG	CZ-NH2	6.59	1.42	1.33
2	7	57	ALA	C-N	6.59	1.41	1.32
3	K	224	ARG	NE-CZ	6.59	1.40	1.33
3	I	224	ARG	NE-CZ	6.58	1.40	1.33
1	a	208	ASN	N-CA	6.58	1.54	1.46
1	D	72	GLU	N-CA	-6.58	1.37	1.46
1	E	68	TYR	CA-C	-6.58	1.44	1.52
1	g	90	ASP	N-CA	-6.58	1.38	1.46
2	4	158	GLU	CA-CB	6.58	1.62	1.53
2	k	75	ASN	N-CA	-6.58	1.38	1.46
3	L	127	VAL	C-N	6.58	1.43	1.33
1	c	89	ILE	CA-C	-6.58	1.43	1.52
2	7	154	ARG	CD-NE	6.58	1.55	1.46
2	6	122	ILE	C-O	-6.58	1.17	1.24
3	K	268	LEU	N-CA	-6.57	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	378	ALA	N-CA	-6.57	1.38	1.46
1	a	141	VAL	CA-C	-6.57	1.44	1.52
1	g	55	GLY	CA-C	-6.57	1.42	1.52
2	l	89	ALA	CA-C	-6.57	1.44	1.52
2	6	109	GLN	CA-C	-6.57	1.45	1.52
1	d	136	LEU	CA-C	-6.57	1.44	1.52
3	K	277	PRO	N-CA	-6.57	1.39	1.47
2	m	178	ARG	C-N	6.56	1.42	1.33
2	n	121	SER	CA-C	-6.56	1.44	1.52
2	6	46	TYR	N-CA	-6.56	1.37	1.45
2	h	18	VAL	CA-CB	6.56	1.62	1.54
2	2	76	LEU	CB-CG	6.56	1.66	1.53
3	K	385	LYS	N-CA	-6.56	1.37	1.46
2	6	23	VAL	N-CA	-6.55	1.38	1.46
2	4	181	ALA	CA-C	-6.55	1.44	1.52
2	7	68	ARG	NE-CZ	6.55	1.40	1.33
3	M	76	ARG	CZ-NH1	6.55	1.42	1.32
1	D	28	ARG	CD-NE	6.54	1.55	1.46
3	M	52	ARG	CD-NE	6.54	1.55	1.46
3	L	86	LYS	CA-C	-6.54	1.45	1.52
1	g	15	PHE	CG-CD2	6.53	1.52	1.38
3	K	204	ILE	CA-C	-6.53	1.44	1.52
3	J	372	MET	CA-C	-6.53	1.44	1.52
1	e	10	ARG	NE-CZ	6.52	1.40	1.33
1	e	130	ARG	CD-NE	6.52	1.55	1.46
1	e	176	GLU	C-N	6.52	1.42	1.33
1	g	61	ALA	CA-C	-6.52	1.47	1.52
2	j	170	ARG	CZ-NH1	6.52	1.41	1.32
1	c	213	TYR	N-CA	-6.52	1.38	1.46
3	L	235	PRO	C-N	6.52	1.41	1.33
2	1	68	ARG	CA-CB	6.52	1.63	1.53
2	7	83	ARG	CD-NE	6.52	1.55	1.46
3	L	95	ILE	CA-C	-6.52	1.45	1.52
3	H	52	ARG	NE-CZ	6.51	1.40	1.33
3	J	38	GLU	N-CA	6.51	1.54	1.46
1	G	77	ALA	CA-C	-6.51	1.44	1.52
1	B	215	LYS	C-N	6.51	1.41	1.33
1	C	73	HIS	CE1-NE2	-6.51	1.26	1.32
1	d	80	GLY	CA-C	-6.51	1.44	1.52
2	i	22	GLY	N-CA	-6.51	1.35	1.45
2	7	84	LYS	CA-C	-6.51	1.46	1.53
1	b	71	ASP	CA-CB	6.50	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	VAL	C-N	6.50	1.42	1.33
3	L	115	ILE	C-N	6.50	1.42	1.33
1	A	175	PHE	N-CA	-6.50	1.37	1.46
1	a	33	ARG	CD-NE	6.50	1.55	1.46
1	d	12	ILE	C-N	6.50	1.43	1.33
3	H	12	LYS	C-N	6.50	1.42	1.33
2	7	158	GLU	CA-C	-6.49	1.43	1.52
3	L	66	GLY	N-CA	-6.49	1.38	1.45
2	i	65	PHE	C-O	-6.49	1.16	1.24
1	C	195	ALA	CA-C	-6.49	1.44	1.52
2	k	80	ARG	NE-CZ	6.49	1.40	1.33
1	a	103	TYR	C-N	6.48	1.42	1.33
3	L	288	ASN	C-N	6.48	1.42	1.33
3	H	115	ILE	CA-CB	-6.47	1.46	1.54
1	F	10	ARG	CZ-NH2	6.47	1.41	1.33
3	J	249	ARG	CA-C	-6.47	1.44	1.53
1	a	219	ARG	CD-NE	6.47	1.55	1.46
1	E	223	GLU	C-O	-6.47	1.16	1.24
3	M	221	ARG	CD-NE	6.47	1.55	1.46
3	I	53	SER	CA-C	-6.47	1.44	1.52
1	a	68	TYR	CA-C	-6.47	1.45	1.52
2	2	14	THR	N-CA	-6.47	1.37	1.45
2	j	115	ILE	CA-C	-6.47	1.44	1.52
3	H	229	LEU	C-O	-6.46	1.16	1.24
1	a	94	ILE	N-CA	6.46	1.54	1.46
1	a	187	ASP	CA-C	-6.46	1.44	1.52
1	C	180	ARG	NE-CZ	6.46	1.40	1.33
3	M	77	VAL	N-CA	-6.46	1.38	1.46
2	h	136	ASP	C-N	6.46	1.42	1.33
3	I	72	LEU	C-O	6.46	1.31	1.23
3	J	305	ARG	NE-CZ	6.46	1.40	1.33
1	B	99	ASN	N-CA	-6.46	1.38	1.46
1	D	101	LEU	CA-C	-6.45	1.44	1.52
2	2	113	GLY	CA-C	-6.45	1.46	1.52
2	2	134	GLU	CA-C	-6.45	1.44	1.52
2	4	172	ILE	N-CA	-6.45	1.38	1.46
1	A	180	ARG	NE-CZ	6.45	1.40	1.33
1	B	168	ARG	N-CA	-6.45	1.38	1.46
1	c	150	THR	C-N	6.45	1.41	1.32
2	5	80	ARG	NE-CZ	6.45	1.40	1.33
2	6	112	ILE	N-CA	-6.45	1.38	1.46
2	4	130	GLY	CA-C	-6.44	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	116	ILE	N-CA	-6.44	1.37	1.46
1	A	174	PHE	N-CA	-6.44	1.38	1.46
1	b	12	ILE	CA-CB	-6.44	1.47	1.54
2	7	85	PRO	CA-C	-6.44	1.44	1.52
3	I	230	ALA	CA-C	-6.44	1.44	1.52
3	I	278	ARG	CA-C	-6.44	1.44	1.52
1	g	76	ALA	C-N	6.44	1.42	1.33
1	e	173	GLU	CA-CB	6.43	1.63	1.53
1	G	216	VAL	CA-CB	6.43	1.62	1.54
3	L	41	ARG	N-CA	6.43	1.54	1.46
1	g	197	GLY	C-N	6.43	1.42	1.33
1	D	187	ASP	CA-C	-6.43	1.44	1.52
1	f	180	ARG	CD-NE	6.43	1.55	1.46
2	1	77	TYR	CA-CB	6.43	1.63	1.53
2	6	165	VAL	CA-C	-6.43	1.44	1.52
1	g	100	ARG	CA-C	6.42	1.61	1.52
2	3	68	ARG	NE-CZ	6.42	1.40	1.33
2	m	50	ASP	CA-C	-6.42	1.44	1.52
1	d	91	ARG	CD-NE	6.42	1.55	1.46
3	I	200	ARG	CZ-NH2	6.42	1.41	1.33
3	L	345	GLY	C-N	6.41	1.42	1.33
1	C	179	TYR	CA-CB	6.41	1.63	1.53
2	3	81	ARG	NE-CZ	6.41	1.40	1.33
2	j	185	GLY	C-N	6.41	1.41	1.33
3	K	222	LEU	CA-C	6.41	1.61	1.52
3	L	28	ARG	CD-NE	6.41	1.55	1.46
1	f	144	VAL	CA-CB	6.41	1.62	1.54
2	h	98	LEU	C-N	6.41	1.42	1.34
1	d	44	GLU	CA-CB	6.41	1.63	1.53
2	7	40	LYS	N-CA	-6.41	1.38	1.46
1	B	54	VAL	CA-C	-6.40	1.44	1.52
2	3	98	LEU	N-CA	-6.40	1.38	1.46
2	7	179	ASP	CA-CB	6.40	1.64	1.53
3	I	205	ARG	NE-CZ	6.40	1.40	1.33
1	F	214	VAL	C-N	6.40	1.42	1.33
2	1	154	ARG	NE-CZ	6.39	1.40	1.33
2	i	88	ARG	CA-C	-6.39	1.44	1.52
3	I	247	ALA	C-N	6.39	1.42	1.33
3	J	203	PHE	CA-C	-6.39	1.44	1.52
3	I	70	ASP	CA-CB	6.39	1.64	1.53
2	l	51	ARG	CZ-NH1	6.39	1.41	1.32
2	7	51	ARG	CD-NE	6.39	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	63	ALA	CA-CB	6.39	1.63	1.53
3	K	127	VAL	CA-C	6.39	1.61	1.52
1	b	83	ALA	N-CA	6.39	1.54	1.46
1	f	105	GLU	CA-C	6.39	1.59	1.52
3	H	180	LEU	CA-C	-6.39	1.45	1.52
3	K	126	MET	CA-C	-6.39	1.43	1.52
1	f	224	VAL	C-N	6.38	1.42	1.33
2	n	77	TYR	C-N	6.38	1.42	1.33
3	M	269	LEU	CA-C	-6.38	1.44	1.52
1	f	127	GLY	CA-C	-6.38	1.42	1.51
2	n	83	ARG	C-N	6.38	1.42	1.33
3	H	27	TYR	C-N	6.38	1.42	1.34
3	H	153	ILE	C-N	6.38	1.42	1.33
3	H	300	PRO	CA-C	6.38	1.61	1.52
3	H	317	ARG	CA-C	6.38	1.60	1.52
1	g	150	THR	N-CA	-6.37	1.38	1.46
1	a	168	ARG	N-CA	-6.37	1.38	1.46
2	2	59	SER	CA-C	6.37	1.61	1.52
1	c	168	ARG	CA-C	-6.37	1.44	1.52
2	n	67	ALA	C-N	6.37	1.42	1.33
3	M	82	SER	C-N	6.37	1.43	1.33
1	e	28	ARG	CA-C	6.36	1.61	1.52
1	G	123	TYR	CA-C	-6.36	1.44	1.52
2	k	97	LEU	CA-CB	6.36	1.63	1.53
2	m	104	PHE	C-O	-6.36	1.17	1.24
3	L	221	ARG	CD-NE	6.36	1.55	1.46
1	D	158	GLU	CA-C	-6.36	1.44	1.52
2	l	124	SER	C-N	6.36	1.42	1.33
1	F	58	LEU	N-CA	-6.36	1.37	1.46
1	B	13	THR	C-N	6.36	1.42	1.33
1	G	105	GLU	CA-CB	6.36	1.61	1.53
2	k	68	ARG	CZ-NH2	6.35	1.41	1.33
2	m	65	PHE	CA-C	-6.35	1.44	1.52
3	K	52	ARG	NE-CZ	6.35	1.40	1.33
1	C	12	ILE	C-N	6.35	1.42	1.33
2	6	203	GLU	C-N	6.35	1.41	1.33
3	L	330	LEU	C-N	6.35	1.41	1.33
3	M	184	PRO	CA-C	-6.35	1.46	1.52
1	F	191	LEU	N-CA	-6.35	1.38	1.46
1	a	137	LEU	CA-CB	6.34	1.62	1.53
2	l	14	THR	CA-C	-6.34	1.44	1.52
3	K	203	PHE	C-N	6.34	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	134	GLU	C-N	6.34	1.41	1.33
3	J	23	LEU	N-CA	-6.34	1.38	1.46
1	D	21	LEU	CA-C	-6.34	1.44	1.53
1	G	133	GLY	C-N	6.34	1.41	1.33
2	3	81	ARG	N-CA	-6.34	1.38	1.46
2	6	174	SER	CA-CB	6.34	1.63	1.53
1	f	64	ILE	C-N	6.34	1.41	1.33
1	g	16	SER	N-CA	-6.34	1.40	1.45
3	H	82	SER	CA-CB	6.33	1.64	1.53
2	n	168	ALA	N-CA	-6.33	1.38	1.46
3	L	141	GLU	C-N	6.33	1.44	1.33
1	f	180	ARG	CA-C	-6.33	1.44	1.52
2	l	132	ILE	C-O	-6.33	1.17	1.24
2	i	74	ALA	C-N	6.32	1.42	1.33
1	e	200	ILE	N-CA	-6.32	1.38	1.46
2	3	154	ARG	CD-NE	6.31	1.55	1.46
1	C	232	TYR	CA-C	-6.31	1.44	1.52
1	B	109	VAL	CA-CB	-6.31	1.46	1.54
2	2	159	ILE	C-N	6.31	1.42	1.33
3	H	307	ILE	CA-C	-6.31	1.44	1.52
3	M	154	ARG	CD-NE	6.31	1.55	1.46
1	B	18	ASP	N-CA	-6.31	1.37	1.46
2	i	97	LEU	CA-CB	6.31	1.63	1.53
1	E	144	VAL	C-N	6.30	1.42	1.33
2	6	187	ASP	N-CA	6.30	1.53	1.46
3	M	326	ARG	CD-NE	6.30	1.55	1.46
1	C	219	ARG	CD-NE	6.30	1.55	1.46
2	k	115	ILE	N-CA	-6.30	1.38	1.46
2	7	21	ASP	N-CA	6.29	1.55	1.46
1	f	162	THR	CA-C	-6.29	1.45	1.52
1	G	47	ILE	N-CA	-6.29	1.38	1.46
3	K	115	ILE	C-N	6.29	1.40	1.33
1	c	124	THR	N-CA	-6.29	1.38	1.46
2	h	81	ARG	NE-CZ	6.29	1.40	1.33
2	n	163	GLU	CA-C	-6.29	1.44	1.52
3	H	274	GLY	N-CA	-6.29	1.36	1.45
3	L	210	GLU	CA-CB	6.29	1.64	1.53
1	E	28	ARG	NE-CZ	6.28	1.40	1.33
2	l	24	VAL	CA-CB	-6.28	1.46	1.54
3	K	322	LYS	C-N	6.28	1.41	1.33
1	B	50	ALA	CA-C	-6.28	1.44	1.52
1	c	58	LEU	N-CA	-6.28	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	114	LYS	CA-C	-6.28	1.44	1.52
3	K	254	ASP	CA-C	-6.28	1.44	1.52
3	J	157	VAL	C-N	6.28	1.42	1.33
2	3	48	ILE	CA-CB	-6.28	1.48	1.55
2	4	202	GLU	CA-C	-6.28	1.44	1.52
2	3	76	LEU	CA-CB	6.28	1.63	1.53
2	n	114	GLY	N-CA	-6.28	1.37	1.45
3	K	115	ILE	CA-C	-6.28	1.45	1.52
3	L	76	ARG	CD-NE	6.28	1.55	1.46
3	J	198	GLN	N-CA	-6.28	1.38	1.46
3	K	201	ALA	C-N	6.27	1.42	1.33
2	4	67	ALA	CA-C	-6.27	1.44	1.52
3	H	52	ARG	CD-NE	6.27	1.55	1.46
3	L	154	ARG	CA-C	-6.27	1.44	1.52
2	m	127	PRO	CA-C	6.26	1.61	1.52
2	m	154	ARG	CD-NE	6.26	1.55	1.46
3	L	364	ARG	CA-C	-6.26	1.44	1.52
3	L	391	ASP	CA-C	6.26	1.61	1.52
2	3	30	ARG	CZ-NH2	6.26	1.41	1.33
1	E	204	LEU	C-N	6.26	1.40	1.33
1	g	90	ASP	C-N	6.26	1.42	1.33
3	K	24	ARG	CD-NE	6.26	1.55	1.46
3	K	43	ARG	CZ-NH2	6.26	1.41	1.33
1	f	143	GLU	C-N	6.26	1.40	1.33
1	G	77	ALA	C-N	6.26	1.41	1.33
1	G	106	PRO	C-N	6.25	1.41	1.33
2	3	76	LEU	CA-C	-6.25	1.44	1.52
2	n	57	ALA	N-CA	-6.25	1.38	1.46
1	A	143	GLU	C-N	6.25	1.38	1.33
1	F	97	GLN	C-N	6.25	1.41	1.33
2	3	125	ILE	CA-CB	-6.25	1.46	1.54
2	k	154	ARG	CD-NE	6.25	1.54	1.46
2	n	183	GLY	C-N	6.25	1.42	1.33
1	A	76	ALA	CA-C	-6.24	1.44	1.52
1	b	33	ARG	C-N	6.24	1.40	1.33
1	b	131	PRO	N-CA	-6.24	1.40	1.46
1	d	187	ASP	C-N	6.24	1.42	1.33
1	B	44	GLU	C-N	6.24	1.39	1.32
1	f	24	VAL	CA-CB	-6.24	1.46	1.54
1	b	145	PRO	CA-C	-6.24	1.44	1.52
1	g	117	CYS	CA-C	-6.24	1.44	1.52
1	f	90	ASP	CA-C	-6.23	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	190	LYS	CA-C	-6.23	1.45	1.52
3	K	78	VAL	C-N	6.23	1.41	1.33
3	J	54	GLU	C-N	6.23	1.41	1.33
1	B	18	ASP	CA-C	-6.23	1.44	1.52
3	L	250	ARG	NE-CZ	6.23	1.40	1.33
2	6	212	ARG	CD-NE	6.23	1.54	1.46
1	B	133	GLY	N-CA	-6.22	1.37	1.45
2	2	79	ILE	CA-CB	-6.22	1.46	1.54
2	i	44	LYS	N-CA	-6.22	1.39	1.46
2	6	29	LYS	C-N	6.22	1.42	1.33
1	f	20	ARG	CA-C	-6.22	1.44	1.52
2	6	60	VAL	C-N	6.22	1.41	1.33
1	c	14	VAL	C-N	6.22	1.42	1.33
3	L	71	ILE	C-N	6.22	1.42	1.33
3	M	339	LEU	CA-C	-6.22	1.44	1.52
1	a	33	ARG	NE-CZ	6.21	1.39	1.33
3	H	205	ARG	CD-NE	6.21	1.54	1.46
1	d	136	LEU	N-CA	-6.21	1.37	1.45
2	k	102	ARG	CZ-NH2	6.21	1.41	1.33
1	a	173	GLU	N-CA	-6.21	1.38	1.46
2	i	14	THR	N-CA	-6.21	1.38	1.45
2	j	36	PHE	CA-CB	6.21	1.63	1.53
3	H	222	LEU	N-CA	-6.21	1.38	1.46
3	L	176	LYS	CA-C	-6.21	1.44	1.52
1	D	126	TYR	CA-CB	6.20	1.63	1.53
1	F	98	ILE	C-N	6.20	1.42	1.33
3	K	74	ASP	C-N	6.20	1.41	1.33
3	M	11	GLU	N-CA	6.20	1.53	1.46
2	3	111	LEU	CA-C	-6.20	1.45	1.52
2	7	80	ARG	NE-CZ	6.20	1.39	1.33
2	7	140	THR	CA-C	-6.20	1.45	1.52
1	C	189	MET	CA-C	-6.20	1.44	1.52
1	E	83	ALA	C-N	6.20	1.42	1.33
1	E	103	TYR	CA-C	-6.19	1.44	1.52
2	1	126	ASP	C-N	-6.19	1.28	1.34
1	a	100	ARG	CZ-NH1	6.19	1.41	1.32
1	d	11	ALA	C-N	6.19	1.42	1.33
1	a	156	LEU	C-N	6.19	1.41	1.33
2	l	198	GLN	C-O	-6.18	1.17	1.24
1	B	149	GLU	CA-C	-6.18	1.44	1.52
2	6	36	PHE	C-N	6.18	1.41	1.33
3	I	129	GLY	C-N	6.18	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	148	TYR	CA-C	6.18	1.60	1.52
2	j	136	ASP	C-N	6.18	1.41	1.33
2	7	90	ILE	CA-C	-6.18	1.44	1.52
1	c	164	ILE	CA-C	-6.18	1.45	1.52
2	i	196	PHE	N-CA	-6.18	1.39	1.46
2	l	107	LEU	CA-C	-6.17	1.46	1.53
3	I	280	ASP	CA-CB	6.17	1.57	1.53
3	K	134	GLU	N-CA	6.17	1.54	1.46
2	7	103	TYR	N-CA	-6.17	1.38	1.46
1	d	59	LEU	CA-C	-6.17	1.44	1.52
1	g	46	VAL	CA-C	-6.17	1.45	1.52
2	n	37	ILE	CA-C	-6.17	1.46	1.52
1	E	235	ARG	C-N	6.17	1.42	1.33
2	2	205	GLU	N-CA	-6.16	1.38	1.46
2	3	33	MET	CA-CB	6.16	1.63	1.53
1	D	100	ARG	N-CA	-6.16	1.39	1.46
1	A	178	GLU	CA-C	-6.16	1.45	1.52
1	B	42	CYS	CA-C	-6.16	1.44	1.53
2	n	53	ALA	CA-C	-6.16	1.45	1.52
1	e	81	LEU	CA-C	-6.16	1.44	1.52
3	K	224	ARG	C-N	6.16	1.41	1.33
3	M	24	ARG	CZ-NH2	6.16	1.41	1.33
2	7	118	GLU	N-CA	-6.15	1.38	1.46
1	F	174	PHE	CA-CB	6.15	1.62	1.53
1	f	164	ILE	N-CA	-6.15	1.39	1.46
2	i	100	SER	N-CA	6.15	1.53	1.46
3	I	244	ASP	CA-C	-6.15	1.44	1.52
2	5	16	GLY	CA-C	-6.15	1.45	1.51
3	J	273	ASP	N-CA	6.15	1.54	1.46
1	f	77	ALA	CA-C	-6.15	1.45	1.52
2	4	79	ILE	N-CA	-6.15	1.39	1.46
1	A	100	ARG	NE-CZ	6.15	1.39	1.33
1	D	41	LYS	C-N	6.15	1.40	1.33
1	f	217	ASP	C-N	6.15	1.42	1.33
1	F	95	GLU	CA-CB	6.14	1.62	1.53
1	G	49	ILE	C-O	-6.14	1.17	1.24
2	1	94	THR	CA-C	6.14	1.60	1.52
2	7	164	ALA	CA-C	-6.14	1.44	1.52
3	H	13	LEU	C-N	6.14	1.42	1.33
3	H	254	ASP	C-N	6.14	1.42	1.33
3	H	338	GLU	C-O	-6.14	1.17	1.24
1	c	233	VAL	C-O	-6.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	42	ALA	CA-C	-6.14	1.45	1.52
3	L	389	ILE	C-N	6.14	1.41	1.33
3	L	142	ASP	CA-CB	6.14	1.63	1.54
1	A	203	GLU	N-CA	-6.14	1.37	1.45
1	e	98	ILE	C-N	6.14	1.42	1.33
2	2	198	GLN	N-CA	-6.14	1.39	1.46
1	g	236	ALA	C-N	6.13	1.42	1.34
1	E	66	LYS	CA-CB	6.13	1.62	1.54
1	A	20	ARG	NE-CZ	6.13	1.39	1.33
1	C	240	ILE	CA-C	-6.13	1.45	1.52
1	e	25	GLU	CA-CB	6.13	1.63	1.53
1	e	28	ARG	NE-CZ	6.13	1.39	1.33
2	1	178	ARG	CZ-NH1	6.13	1.41	1.32
3	J	259	ARG	NE-CZ	6.13	1.39	1.33
3	H	364	ARG	NE-CZ	6.13	1.39	1.33
1	d	22	PHE	CA-C	-6.13	1.44	1.52
2	i	23	VAL	CA-CB	-6.13	1.46	1.54
3	L	305	ARG	CA-C	-6.13	1.45	1.53
1	B	92	ALA	CA-C	-6.12	1.44	1.52
1	A	191	LEU	CA-CB	6.12	1.63	1.53
2	3	45	ILE	CA-C	-6.12	1.45	1.52
2	4	116	ASP	N-CA	-6.12	1.38	1.46
3	K	117	ASN	CA-C	-6.12	1.45	1.52
1	c	208	ASN	CA-C	-6.12	1.45	1.53
3	H	308	GLU	N-CA	-6.12	1.38	1.46
2	2	20	LYS	N-CA	-6.12	1.38	1.46
2	6	173	TYR	CA-CB	6.12	1.63	1.53
1	F	119	PHE	CA-C	-6.12	1.44	1.52
2	i	194	ASP	N-CA	-6.12	1.39	1.46
2	j	132	ILE	C-O	-6.12	1.17	1.24
3	I	105	ARG	CD-NE	6.12	1.54	1.46
3	K	27	TYR	N-CA	-6.12	1.38	1.46
3	M	367	ARG	CD-NE	6.12	1.54	1.46
1	E	81	LEU	C-N	6.11	1.41	1.33
2	1	170	ARG	CD-NE	6.11	1.54	1.46
3	L	87	PHE	C-N	6.11	1.41	1.33
2	j	104	PHE	CA-C	6.11	1.59	1.52
1	d	10	ARG	NE-CZ	6.11	1.39	1.33
1	e	208	ASN	CA-C	-6.11	1.44	1.52
2	3	30	ARG	CA-C	-6.11	1.44	1.52
2	4	162	ASP	CA-CB	6.10	1.62	1.53
3	L	197	ASN	CA-C	6.10	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	319	GLN	C-N	6.10	1.41	1.33
1	e	65	GLU	CA-C	-6.10	1.44	1.52
2	4	88	ARG	CD-NE	6.10	1.54	1.46
2	h	64	GLN	CA-C	-6.10	1.45	1.52
3	I	249	ARG	CZ-NH1	6.10	1.41	1.32
1	B	125	GLN	N-CA	-6.10	1.38	1.46
2	3	170	ARG	CD-NE	6.10	1.54	1.46
2	5	124	SER	N-CA	-6.10	1.38	1.46
3	H	144	GLY	C-N	6.10	1.42	1.33
3	J	59	ARG	CZ-NH1	6.10	1.41	1.32
3	I	172	ILE	CA-C	6.10	1.58	1.52
3	H	178	VAL	CA-C	-6.09	1.45	1.52
1	B	150	THR	CA-C	-6.09	1.45	1.52
1	D	157	LEU	C-N	6.09	1.42	1.33
1	c	22	PHE	C-N	6.09	1.42	1.33
3	M	34	LYS	C-N	6.09	1.42	1.34
1	E	29	GLU	CA-CB	6.08	1.63	1.53
2	1	21	ASP	CA-CB	6.08	1.64	1.54
1	B	103	TYR	CA-CB	6.08	1.63	1.53
1	C	108	THR	N-CA	-6.08	1.38	1.46
1	F	233	VAL	N-CA	-6.08	1.39	1.46
1	f	105	GLU	C-N	6.08	1.40	1.33
2	2	64	GLN	C-O	-6.08	1.16	1.24
2	n	114	GLY	CA-C	-6.08	1.44	1.52
2	l	92	THR	C-N	6.08	1.42	1.33
3	J	52	ARG	NE-CZ	6.08	1.39	1.33
1	b	182	ASP	CA-C	-6.08	1.45	1.52
3	K	250	ARG	CD-NE	6.08	1.54	1.46
2	7	40	LYS	CA-CB	6.08	1.62	1.53
3	I	149	GLN	C-N	6.08	1.41	1.33
1	B	64	ILE	C-N	6.07	1.41	1.33
1	f	48	LEU	CA-C	-6.07	1.45	1.52
3	K	272	LEU	N-CA	-6.07	1.38	1.46
3	J	39	SER	CA-C	6.07	1.60	1.52
1	d	109	VAL	CA-C	-6.07	1.45	1.52
1	f	10	ARG	CD-NE	6.07	1.54	1.46
2	i	27	THR	CA-C	-6.07	1.45	1.52
1	a	59	LEU	CA-C	-6.07	1.45	1.52
3	H	244	ASP	CA-C	-6.07	1.45	1.53
1	a	28	ARG	CZ-NH1	6.07	1.41	1.32
1	D	22	PHE	CA-C	-6.06	1.44	1.52
1	f	239	ARG	N-CA	-6.06	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	89	ALA	N-CA	-6.06	1.38	1.46
3	H	320	ILE	N-CA	-6.06	1.39	1.46
2	m	170	ARG	NE-CZ	6.06	1.39	1.33
1	c	239	ARG	NE-CZ	6.06	1.39	1.33
2	n	110	LEU	CA-C	-6.06	1.45	1.52
3	M	57	ARG	CZ-NH1	6.06	1.41	1.32
1	c	162	THR	CA-C	-6.06	1.45	1.52
2	n	169	VAL	C-N	6.06	1.41	1.33
2	l	58	GLY	CA-C	-6.06	1.43	1.51
3	J	216	ILE	CA-C	-6.06	1.45	1.52
3	H	10	LEU	CA-C	-6.05	1.45	1.52
3	I	126	MET	CA-C	-6.05	1.45	1.52
2	n	195	GLU	CA-CB	6.05	1.63	1.53
1	A	10	ARG	CD-NE	6.05	1.54	1.46
1	F	177	LYS	CA-C	-6.05	1.45	1.52
2	i	166	GLU	CA-C	-6.05	1.45	1.52
1	b	86	ARG	CD-NE	6.05	1.54	1.46
2	6	99	ASN	C-N	6.05	1.41	1.33
1	C	16	SER	CA-C	-6.05	1.44	1.52
3	H	216	ILE	C-O	-6.04	1.17	1.24
3	I	109	ASN	CA-C	-6.04	1.44	1.52
2	j	34	GLY	C-N	6.04	1.42	1.33
1	B	100	ARG	CD-NE	6.04	1.54	1.46
1	E	216	VAL	CA-CB	-6.04	1.47	1.54
1	e	209	ILE	CA-CB	-6.04	1.44	1.55
1	g	20	ARG	CA-C	-6.04	1.44	1.53
1	b	100	ARG	CD-NE	6.04	1.54	1.46
1	D	184	SER	N-CA	-6.04	1.37	1.45
1	d	63	THR	C-N	6.04	1.40	1.33
2	1	107	LEU	C-N	6.04	1.42	1.33
2	4	30	ARG	CA-C	-6.04	1.44	1.52
2	n	172	ILE	N-CA	-6.04	1.38	1.46
1	C	192	GLY	CA-C	-6.04	1.45	1.52
1	e	81	LEU	C-N	6.04	1.40	1.33
2	5	45	ILE	C-N	6.04	1.42	1.33
3	H	305	ARG	NE-CZ	6.04	1.39	1.33
3	M	264	THR	CA-CB	6.04	1.62	1.53
1	C	73	HIS	CB-CG	6.03	1.58	1.50
1	E	31	VAL	CA-C	-6.03	1.45	1.52
2	4	105	PRO	N-CA	6.03	1.55	1.47
2	l	172	ILE	CA-CB	-6.03	1.46	1.54
3	M	43	ARG	CZ-NH1	6.03	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	177	LYS	C-N	6.03	1.42	1.33
1	b	62	ASP	C-O	-6.03	1.17	1.24
3	L	129	GLY	C-O	-6.03	1.17	1.24
1	a	127	GLY	N-CA	-6.03	1.36	1.45
1	b	60	GLU	C-O	-6.03	1.16	1.23
1	g	71	ASP	CA-C	-6.03	1.45	1.52
1	e	97	GLN	N-CA	-6.02	1.39	1.46
1	a	28	ARG	CD-NE	6.02	1.54	1.46
1	E	98	ILE	CA-C	6.02	1.60	1.52
3	H	76	ARG	CZ-NH1	6.02	1.41	1.32
3	J	328	MET	N-CA	-6.02	1.39	1.46
1	e	26	TYR	N-CA	-6.02	1.38	1.46
3	I	216	ILE	N-CA	-6.02	1.38	1.46
2	6	75	ASN	C-N	-6.02	1.26	1.33
2	2	209	ALA	N-CA	-6.01	1.38	1.46
2	4	81	ARG	CZ-NH1	6.01	1.41	1.32
2	n	109	GLN	C-N	6.01	1.41	1.33
3	H	276	ASP	N-CA	-6.01	1.39	1.46
3	I	376	THR	CB-OG1	-6.01	1.34	1.43
3	M	255	THR	C-N	6.01	1.41	1.33
3	J	220	ALA	CA-C	6.01	1.60	1.52
1	d	92	ALA	CA-C	6.01	1.60	1.52
3	M	392	LEU	N-CA	-6.01	1.39	1.46
1	B	86	ARG	CD-NE	6.01	1.54	1.46
2	j	114	GLY	CA-C	-6.01	1.44	1.52
3	I	199	THR	C-N	6.00	1.41	1.33
3	J	49	ARG	CZ-NH2	6.00	1.41	1.33
1	a	116	ILE	CA-C	-6.00	1.45	1.52
2	1	132	ILE	CA-C	-6.00	1.45	1.52
2	7	46	TYR	CZ-OH	6.00	1.50	1.38
3	H	320	ILE	C-N	6.00	1.41	1.33
1	d	137	LEU	CA-C	6.00	1.59	1.52
1	d	10	ARG	CD-NE	6.00	1.54	1.46
1	G	143	GLU	N-CA	-6.00	1.38	1.46
3	K	81	SER	CA-C	-5.99	1.45	1.52
2	1	122	ILE	N-CA	-5.99	1.39	1.46
3	H	57	ARG	NE-CZ	5.99	1.39	1.33
3	J	47	GLU	CA-CB	5.99	1.62	1.53
2	k	163	GLU	CA-C	-5.99	1.44	1.52
3	I	339	LEU	CA-C	-5.99	1.45	1.52
1	g	201	GLU	N-CA	5.99	1.55	1.46
1	A	79	SER	N-CA	-5.99	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	230	ALA	CA-C	-5.99	1.45	1.52
1	B	229	LEU	CA-C	-5.98	1.45	1.52
2	k	151	LEU	CA-C	5.98	1.60	1.52
3	K	374	ASP	N-CA	-5.98	1.39	1.46
1	a	159	TYR	CA-C	-5.98	1.45	1.52
1	f	224	VAL	N-CA	-5.98	1.38	1.46
2	n	175	ALA	CA-CB	5.98	1.62	1.53
3	I	28	ARG	CA-CB	5.98	1.62	1.53
3	I	375	PHE	CA-CB	5.98	1.62	1.53
3	K	274	GLY	CA-C	-5.98	1.43	1.51
3	I	201	ALA	N-CA	-5.98	1.41	1.46
1	c	10	ARG	CD-NE	5.98	1.54	1.46
1	c	112	LEU	C-N	5.98	1.41	1.33
3	L	397	PHE	CA-C	-5.98	1.44	1.52
3	M	164	PRO	C-N	5.98	1.42	1.34
1	D	36	THR	N-CA	-5.98	1.38	1.46
1	C	91	ARG	NE-CZ	5.97	1.39	1.33
2	3	59	SER	N-CA	5.97	1.53	1.45
1	C	239	ARG	CA-C	-5.97	1.45	1.52
1	d	211	VAL	C-N	5.97	1.40	1.34
3	I	340	ALA	CA-C	-5.97	1.45	1.52
3	M	11	GLU	C-O	-5.97	1.17	1.24
1	B	107	ILE	N-CA	-5.97	1.38	1.46
2	l	71	LYS	N-CA	-5.97	1.39	1.46
2	6	86	THR	N-CA	-5.97	1.38	1.45
1	f	216	VAL	C-N	5.96	1.42	1.33
2	i	83	ARG	C-N	5.96	1.42	1.33
3	K	47	GLU	C-N	5.96	1.41	1.33
1	B	182	ASP	CA-CB	5.96	1.62	1.53
2	l	109	GLN	N-CA	-5.96	1.38	1.46
1	C	80	GLY	CA-C	-5.96	1.43	1.51
2	l	52	MET	N-CA	-5.96	1.38	1.46
3	M	163	LYS	C-N	5.96	1.39	1.33
2	i	104	PHE	CA-CB	5.96	1.61	1.53
1	C	28	ARG	N-CA	-5.96	1.38	1.46
2	h	15	VAL	N-CA	-5.96	1.39	1.46
1	G	138	ILE	C-O	-5.96	1.17	1.24
3	H	363	ILE	N-CA	-5.95	1.39	1.46
3	L	270	ALA	C-O	-5.95	1.17	1.24
3	J	358	ALA	C-N	5.95	1.41	1.33
1	B	67	ILE	N-CA	-5.95	1.39	1.46
1	E	60	GLU	N-CA	-5.95	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	235	ARG	NE-CZ	5.95	1.39	1.33
2	2	94	THR	CA-C	-5.95	1.45	1.52
1	B	130	ARG	CZ-NH1	5.95	1.41	1.32
2	n	154	ARG	CD-NE	5.95	1.54	1.46
3	K	190	LEU	CA-C	-5.95	1.45	1.52
3	J	360	MET	N-CA	-5.95	1.39	1.46
1	B	94	ILE	C-O	-5.95	1.17	1.24
1	D	212	GLY	CA-C	-5.95	1.46	1.52
1	F	100	ARG	CZ-NH1	5.95	1.41	1.32
3	K	305	ARG	C-N	5.94	1.41	1.33
1	G	140	GLY	N-CA	5.94	1.51	1.45
1	g	143	GLU	C-N	5.94	1.38	1.32
2	m	119	GLY	CA-C	-5.94	1.43	1.51
1	b	52	LYS	CA-C	-5.94	1.44	1.52
1	A	239	ARG	CZ-NH1	5.93	1.41	1.32
1	e	32	LYS	CA-CB	5.93	1.62	1.53
1	c	239	ARG	N-CA	-5.93	1.38	1.46
2	3	118	GLU	N-CA	5.93	1.53	1.46
2	6	195	GLU	N-CA	-5.93	1.38	1.46
3	H	295	PRO	CA-C	-5.93	1.45	1.52
3	M	183	PRO	CA-C	5.93	1.57	1.52
1	g	158	GLU	N-CA	-5.93	1.38	1.46
2	6	105	PRO	C-O	5.93	1.30	1.23
2	7	33	MET	C-N	-5.93	1.24	1.33
2	6	159	ILE	CA-C	-5.93	1.45	1.52
1	D	24	VAL	CA-C	-5.92	1.45	1.52
2	j	21	ASP	CA-C	-5.92	1.45	1.52
1	b	118	ASP	CA-CB	5.92	1.62	1.53
2	6	112	ILE	CA-C	-5.92	1.45	1.52
1	d	15	PHE	CA-CB	5.92	1.62	1.53
1	B	93	ARG	CD-NE	5.92	1.54	1.46
1	a	145	PRO	CA-CB	-5.92	1.45	1.53
1	B	140	GLY	C-O	-5.92	1.16	1.24
1	D	64	ILE	C-N	5.92	1.41	1.33
2	l	35	ASN	N-CA	-5.92	1.38	1.46
3	J	265	MET	C-N	5.92	1.42	1.34
1	E	137	LEU	N-CA	-5.92	1.39	1.46
3	H	46	ARG	N-CA	-5.92	1.39	1.46
1	A	109	VAL	CA-CB	-5.91	1.47	1.54
1	a	174	PHE	CA-C	-5.91	1.45	1.52
3	H	287	THR	CA-C	-5.91	1.45	1.52
3	M	247	ALA	CA-C	-5.91	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	200	SER	CA-CB	5.91	1.62	1.53
1	b	207	GLU	CA-C	-5.91	1.44	1.52
1	e	211	VAL	CA-CB	-5.91	1.46	1.54
2	j	172	ILE	CB-CG1	5.91	1.65	1.53
3	L	179	LEU	C-N	5.91	1.41	1.33
1	A	190	VAL	C-N	5.91	1.41	1.34
2	h	186	ILE	CA-C	-5.91	1.45	1.52
3	L	86	LYS	N-CA	-5.91	1.38	1.46
3	J	76	ARG	CZ-NH2	5.91	1.41	1.33
2	4	87	VAL	C-N	5.90	1.41	1.33
2	n	182	SER	CA-CB	-5.90	1.45	1.54
1	c	100	ARG	CZ-NH2	5.90	1.41	1.33
3	I	79	VAL	N-CA	-5.90	1.39	1.46
3	J	189	THR	CA-CB	-5.90	1.44	1.53
3	J	324	HIS	CA-CB	5.90	1.62	1.53
3	M	35	LYS	CA-CB	5.90	1.63	1.53
2	3	211	PHE	C-N	5.90	1.42	1.33
2	j	24	VAL	CA-C	-5.90	1.45	1.52
3	K	341	ARG	CZ-NH1	5.90	1.41	1.32
3	H	275	PHE	CA-C	-5.89	1.44	1.52
1	E	122	GLN	N-CA	-5.89	1.38	1.46
2	2	180	SER	CA-C	-5.89	1.45	1.52
2	5	103	TYR	CA-C	5.89	1.61	1.52
1	G	71	ASP	N-CA	-5.89	1.40	1.46
1	G	86	ARG	CZ-NH1	5.89	1.41	1.32
2	n	134	GLU	N-CA	-5.89	1.38	1.46
3	H	368	ALA	CA-C	-5.89	1.45	1.52
1	c	80	GLY	C-N	5.89	1.41	1.33
1	c	218	ASP	CA-C	-5.89	1.45	1.53
3	I	227	PHE	CA-C	-5.89	1.45	1.52
3	H	32	ASP	C-O	-5.89	1.17	1.24
3	M	358	ALA	CA-CB	-5.89	1.43	1.53
3	H	154	ARG	CZ-NH2	5.88	1.41	1.33
2	j	204	VAL	CA-CB	-5.88	1.47	1.54
3	I	177	GLY	CA-C	-5.88	1.43	1.51
3	H	43	ARG	CA-C	-5.88	1.45	1.52
1	B	85	ALA	N-CA	-5.88	1.39	1.46
2	m	67	ALA	N-CA	-5.88	1.39	1.46
1	B	39	GLY	N-CA	-5.88	1.39	1.45
1	E	143	GLU	C-N	5.88	1.40	1.33
1	e	191	LEU	N-CA	-5.88	1.39	1.46
1	B	136	LEU	CA-C	-5.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	121	SER	CA-C	-5.87	1.45	1.52
3	I	29	ARG	CZ-NH2	5.87	1.41	1.33
3	I	181	TYR	CA-CB	5.87	1.64	1.53
3	L	313	THR	CA-C	-5.87	1.45	1.53
3	M	314	PHE	CA-CB	5.87	1.62	1.53
3	J	237	ILE	N-CA	5.87	1.53	1.46
3	H	174	PRO	CA-C	5.87	1.57	1.52
1	f	28	ARG	CZ-NH1	5.86	1.41	1.32
2	1	73	GLU	N-CA	-5.86	1.39	1.46
1	A	217	ASP	C-N	5.86	1.41	1.33
1	D	60	GLU	CA-C	-5.86	1.45	1.52
2	n	164	ALA	C-N	5.86	1.41	1.33
3	H	175	PRO	N-CD	-5.86	1.39	1.47
3	H	178	VAL	N-CA	5.86	1.53	1.46
1	d	120	LYS	CA-C	-5.86	1.45	1.52
2	k	81	ARG	CZ-NH2	5.86	1.41	1.33
2	k	88	ARG	C-N	5.86	1.41	1.33
3	J	59	ARG	CZ-NH2	5.86	1.41	1.33
2	6	207	ILE	CA-CB	-5.85	1.46	1.54
2	j	178	ARG	CA-C	-5.85	1.45	1.52
2	5	28	GLU	CA-C	-5.85	1.45	1.52
3	I	299	ARG	NE-CZ	5.85	1.39	1.33
3	K	194	ALA	C-N	5.85	1.41	1.33
2	3	212	ARG	NE-CZ	5.85	1.39	1.33
1	e	66	LYS	CA-CB	5.85	1.62	1.54
2	6	182	SER	CA-C	-5.85	1.45	1.52
3	M	306	ILE	C-O	-5.85	1.17	1.23
3	J	179	LEU	CA-C	-5.85	1.45	1.52
1	b	18	ASP	N-CA	-5.84	1.38	1.46
3	I	80	LYS	CA-CB	5.84	1.60	1.53
3	J	221	ARG	NE-CZ	5.84	1.39	1.33
3	H	47	GLU	CA-CB	5.84	1.62	1.53
2	5	203	GLU	C-N	5.84	1.41	1.33
1	D	58	LEU	CA-C	-5.84	1.45	1.52
1	D	162	THR	C-O	-5.84	1.17	1.23
2	6	163	GLU	CA-C	-5.84	1.44	1.52
3	M	165	GLU	CA-C	-5.84	1.44	1.52
3	M	249	ARG	NE-CZ	5.84	1.39	1.33
3	K	50	ARG	NE-CZ	5.83	1.39	1.33
3	J	104	ALA	CA-CB	5.83	1.61	1.53
2	j	26	ALA	CA-C	-5.83	1.45	1.52
2	7	110	LEU	CA-C	-5.83	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	79	VAL	CA-CB	-5.83	1.47	1.54
3	M	100	LEU	N-CA	-5.83	1.38	1.46
3	K	283	VAL	C-N	5.83	1.41	1.33
1	B	121	GLN	C-N	5.83	1.41	1.33
1	c	70	ILE	CA-C	-5.83	1.47	1.52
1	F	192	GLY	C-N	5.83	1.41	1.33
3	I	19	ASP	CA-CB	5.83	1.62	1.53
2	4	138	VAL	CA-C	5.83	1.59	1.52
1	b	138	ILE	C-N	5.83	1.41	1.33
1	d	110	LYS	CA-CB	5.82	1.62	1.53
1	F	63	THR	N-CA	-5.82	1.39	1.46
1	f	69	LYS	C-O	-5.82	1.17	1.24
3	H	354	ILE	C-N	5.82	1.41	1.33
1	a	99	ASN	CA-C	-5.82	1.45	1.52
1	B	123	TYR	CA-C	-5.82	1.44	1.52
1	G	113	ALA	N-CA	-5.82	1.39	1.46
3	H	242	GLU	C-O	-5.82	1.16	1.24
1	a	110	LYS	C-N	5.82	1.41	1.33
1	C	111	GLU	N-CA	-5.82	1.38	1.46
1	D	53	ARG	CA-CB	5.82	1.61	1.53
1	f	212	GLY	N-CA	-5.82	1.39	1.45
3	H	281	VAL	CA-C	5.82	1.60	1.52
3	K	253	SER	CA-C	-5.82	1.45	1.52
1	D	38	ILE	N-CA	-5.81	1.39	1.46
3	M	196	ALA	CA-CB	5.81	1.62	1.53
1	a	186	ASP	CA-CB	5.81	1.62	1.53
1	G	237	ASN	CA-CB	5.81	1.62	1.53
1	B	16	SER	CA-CB	5.81	1.60	1.53
2	2	98	LEU	CA-CB	5.81	1.62	1.53
3	H	359	GLY	CA-C	-5.81	1.44	1.51
2	n	84	LYS	CA-CB	5.80	1.62	1.53
1	d	214	VAL	N-CA	-5.80	1.39	1.46
3	J	250	ARG	CD-NE	5.80	1.54	1.46
1	B	5	GLN	C-N	5.80	1.41	1.33
1	e	27	ALA	CA-C	-5.80	1.44	1.52
3	I	44	TYR	C-N	5.80	1.41	1.33
1	F	142	ASP	N-CA	-5.80	1.39	1.46
1	E	46	VAL	N-CA	-5.80	1.39	1.46
1	F	179	TYR	C-O	-5.80	1.17	1.23
2	1	24	VAL	C-N	5.79	1.41	1.33
3	L	367	ARG	CD-NE	5.79	1.54	1.46
3	J	229	LEU	CA-CB	5.79	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	70	ILE	CA-CB	5.79	1.62	1.54
1	D	47	ILE	CA-CB	-5.79	1.47	1.54
3	J	396	MET	CA-C	-5.79	1.45	1.52
1	C	193	LEU	CA-C	5.79	1.60	1.52
3	H	263	ARG	C-N	-5.79	1.25	1.34
2	4	150	VAL	N-CA	-5.79	1.38	1.46
1	G	112	LEU	C-N	5.78	1.41	1.33
3	H	299	ARG	CZ-NH1	5.78	1.40	1.32
2	6	132	ILE	C-O	5.78	1.30	1.23
3	H	367	ARG	NE-CZ	5.78	1.39	1.33
1	F	119	PHE	C-N	5.77	1.42	1.34
2	5	156	THR	C-O	-5.77	1.19	1.24
1	c	20	ARG	CZ-NH1	5.77	1.40	1.32
2	k	30	ARG	CD-NE	5.77	1.54	1.46
1	E	114	LYS	N-CA	-5.77	1.39	1.46
2	6	175	ALA	CA-C	-5.77	1.44	1.52
3	K	308	GLU	C-N	5.77	1.39	1.33
3	I	11	GLU	CA-CB	5.77	1.62	1.53
3	M	248	ALA	C-N	5.77	1.41	1.33
3	J	395	VAL	C-N	5.77	1.41	1.33
1	g	100	ARG	CZ-NH1	5.77	1.40	1.32
2	6	135	LYS	N-CA	-5.77	1.39	1.46
2	n	33	MET	CA-CB	5.77	1.62	1.54
3	I	226	VAL	CA-CB	-5.77	1.46	1.54
1	F	82	VAL	CA-CB	5.77	1.61	1.54
3	M	94	TYR	CA-C	-5.76	1.45	1.53
1	a	162	THR	CA-C	-5.76	1.45	1.52
3	M	274	GLY	C-N	5.76	1.41	1.33
2	2	77	TYR	C-N	5.76	1.41	1.33
2	5	166	GLU	CA-C	-5.76	1.45	1.52
1	E	86	ARG	CZ-NH2	5.76	1.41	1.33
1	F	38	ILE	CA-C	-5.76	1.45	1.52
1	e	139	ALA	N-CA	-5.76	1.39	1.46
2	l	48	ILE	CA-C	-5.76	1.45	1.53
2	n	18	VAL	N-CA	-5.76	1.39	1.46
3	H	177	GLY	C-O	5.76	1.29	1.23
3	H	45	GLU	CA-CB	5.75	1.62	1.53
3	M	285	GLY	N-CA	-5.75	1.38	1.45
1	b	112	LEU	N-CA	-5.75	1.39	1.46
1	e	40	ILE	CA-C	-5.75	1.45	1.52
1	F	16	SER	N-CA	-5.75	1.42	1.46
2	h	128	ILE	C-O	-5.75	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	62	ASP	CA-CB	5.75	1.62	1.53
3	I	11	GLU	CA-C	-5.75	1.45	1.52
3	H	310	PRO	CA-CB	5.75	1.61	1.53
3	K	31	GLU	CA-CB	5.75	1.62	1.53
1	A	240	ILE	C-N	5.75	1.41	1.33
2	2	63	ALA	CA-C	-5.75	1.45	1.52
2	5	54	MET	N-CA	-5.75	1.38	1.46
2	m	179	ASP	CA-C	-5.75	1.45	1.52
1	E	90	ASP	CA-CB	5.75	1.62	1.53
3	H	367	ARG	N-CA	-5.75	1.38	1.45
1	a	44	GLU	N-CA	-5.75	1.39	1.46
1	d	224	VAL	N-CA	-5.75	1.40	1.46
3	I	76	ARG	CZ-NH1	5.75	1.40	1.32
1	D	241	ARG	CZ-NH2	5.74	1.41	1.33
1	f	33	ARG	NE-CZ	5.74	1.39	1.33
1	f	214	VAL	N-CA	-5.74	1.39	1.46
3	I	114	ALA	N-CA	-5.74	1.38	1.46
1	b	45	GLY	C-N	5.74	1.40	1.33
2	5	76	LEU	C-O	-5.74	1.17	1.24
2	m	76	LEU	CA-C	5.74	1.60	1.52
2	7	124	SER	N-CA	-5.74	1.39	1.46
2	i	139	ALA	C-N	5.74	1.41	1.33
2	3	70	ILE	N-CA	-5.74	1.39	1.46
3	I	192	ALA	N-CA	-5.74	1.39	1.46
1	E	120	LYS	C-N	5.74	1.41	1.34
1	F	80	GLY	C-O	-5.74	1.20	1.24
3	L	249	ARG	CA-C	-5.74	1.45	1.52
2	7	146	THR	CA-C	-5.73	1.45	1.52
1	F	239	ARG	CZ-NH1	5.73	1.40	1.32
2	6	83	ARG	CZ-NH1	5.73	1.40	1.32
2	n	184	ASP	C-N	5.73	1.41	1.33
1	e	241	ARG	NE-CZ	5.73	1.39	1.33
2	2	83	ARG	N-CA	-5.73	1.39	1.46
2	6	31	ALA	N-CA	-5.73	1.39	1.46
2	n	19	CYS	CA-CB	5.73	1.62	1.53
3	H	112	THR	C-N	5.73	1.41	1.33
3	M	293	LEU	N-CA	-5.73	1.38	1.45
3	J	102	PRO	CA-C	-5.73	1.45	1.52
1	g	209	ILE	CA-C	5.73	1.59	1.52
3	H	195	VAL	N-CA	-5.73	1.39	1.46
3	L	125	PRO	C-N	5.73	1.41	1.34
2	i	99	ASN	CA-C	-5.72	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	106	TYR	N-CA	-5.72	1.39	1.45
1	D	241	ARG	CD-NE	5.72	1.54	1.46
1	e	239	ARG	CD-NE	5.72	1.54	1.46
1	D	17	PRO	C-N	5.72	1.41	1.33
1	f	222	LYS	N-CA	-5.72	1.38	1.45
1	f	21	LEU	CA-C	-5.72	1.45	1.52
2	2	92	THR	CA-C	5.72	1.60	1.52
1	b	154	GLY	CA-C	-5.72	1.44	1.51
3	L	79	VAL	N-CA	-5.72	1.39	1.46
1	E	10	ARG	C-N	5.72	1.40	1.33
2	2	149	GLY	C-N	5.72	1.41	1.33
3	J	133	GLU	CA-C	-5.72	1.45	1.52
1	c	241	ARG	CD-NE	5.71	1.54	1.46
1	A	29	GLU	N-CA	-5.71	1.38	1.46
1	g	187	ASP	N-CA	-5.71	1.39	1.46
3	M	371	THR	CA-C	-5.71	1.45	1.52
3	K	326	ARG	NE-CZ	5.71	1.39	1.33
1	b	28	ARG	CZ-NH2	5.71	1.40	1.33
2	3	107	LEU	CA-C	-5.71	1.46	1.53
2	k	84	LYS	CA-C	5.71	1.58	1.53
1	a	93	ARG	CZ-NH1	5.71	1.40	1.32
2	i	210	LYS	N-CA	-5.71	1.38	1.46
2	3	123	TYR	C-N	5.71	1.41	1.33
2	6	16	GLY	C-N	5.71	1.41	1.33
2	n	133	GLU	CA-C	-5.71	1.45	1.52
1	b	20	ARG	CZ-NH1	5.71	1.40	1.32
1	C	150	THR	CA-C	-5.70	1.45	1.52
2	2	84	LYS	CA-CB	5.70	1.61	1.53
2	m	146	THR	N-CA	-5.70	1.39	1.46
3	H	128	TYR	CZ-OH	5.70	1.50	1.38
3	H	173	GLU	CA-CB	5.70	1.62	1.52
1	g	72	GLU	C-N	5.70	1.41	1.33
1	c	80	GLY	CA-C	-5.70	1.45	1.52
1	c	144	VAL	CA-C	-5.70	1.47	1.52
3	M	272	LEU	CA-C	-5.70	1.45	1.52
1	c	61	ALA	CA-C	-5.70	1.45	1.52
2	k	118	GLU	CA-C	5.70	1.60	1.52
1	G	236	ALA	N-CA	-5.70	1.39	1.46
3	M	28	ARG	NE-CZ	5.70	1.39	1.33
3	J	139	SER	CA-C	-5.70	1.45	1.52
2	1	64	GLN	CA-C	-5.69	1.45	1.52
3	I	302	ARG	CZ-NH1	5.69	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	268	LEU	CA-C	-5.69	1.45	1.52
1	A	144	VAL	CA-C	-5.69	1.46	1.52
1	B	33	ARG	CD-NE	5.69	1.54	1.46
3	I	210	GLU	CA-CB	5.69	1.63	1.53
3	M	298	LEU	CA-CB	5.69	1.60	1.53
2	n	105	PRO	N-CD	-5.69	1.39	1.47
1	a	100	ARG	CD-NE	5.68	1.54	1.46
2	m	206	GLN	N-CA	-5.68	1.38	1.46
3	K	233	LYS	C-N	5.68	1.41	1.33
3	K	259	ARG	CZ-NH2	5.68	1.40	1.33
3	J	360	MET	C-N	5.68	1.41	1.34
1	c	145	PRO	CA-C	5.68	1.59	1.52
1	G	141	VAL	CA-C	-5.68	1.45	1.52
1	g	93	ARG	NE-CZ	5.68	1.39	1.33
2	l	13	THR	C-N	5.68	1.40	1.33
3	J	289	ARG	CD-NE	5.68	1.54	1.46
1	f	115	LYS	N-CA	-5.68	1.39	1.46
2	5	156	THR	C-N	-5.68	1.29	1.33
1	c	126	TYR	CA-C	5.68	1.60	1.52
1	D	165	GLY	C-O	-5.67	1.21	1.24
2	6	63	ALA	CA-C	-5.67	1.45	1.52
1	G	187	ASP	N-CA	-5.67	1.39	1.46
2	k	61	GLY	C-N	5.67	1.41	1.34
2	5	176	MET	N-CA	5.67	1.52	1.46
2	n	164	ALA	N-CA	-5.67	1.39	1.46
3	L	155	GLU	C-N	5.67	1.41	1.33
1	a	177	LYS	C-N	5.67	1.41	1.33
3	K	198	GLN	CA-C	-5.67	1.45	1.52
3	L	383	LEU	N-CA	-5.67	1.38	1.46
3	H	117	ASN	CA-C	-5.67	1.45	1.52
1	C	73	HIS	ND1-CE1	5.67	1.38	1.32
3	H	372	MET	CA-CB	5.67	1.62	1.53
2	j	133	GLU	CA-CB	5.67	1.60	1.53
2	m	27	THR	N-CA	-5.67	1.38	1.45
3	K	356	THR	C-O	-5.67	1.17	1.24
3	L	59	ARG	CZ-NH1	5.67	1.40	1.32
2	i	123	TYR	C-N	5.67	1.41	1.33
1	B	33	ARG	CZ-NH2	5.66	1.40	1.33
2	m	71	LYS	CA-C	-5.66	1.45	1.52
3	L	106	VAL	C-N	5.66	1.40	1.33
3	M	348	GLY	CA-C	-5.66	1.45	1.52
1	F	134	VAL	N-CA	-5.66	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	46	ARG	C-N	5.66	1.41	1.33
1	b	241	ARG	CD-NE	5.66	1.54	1.46
2	1	138	VAL	CA-CB	-5.66	1.49	1.55
2	h	189	VAL	CA-CB	-5.66	1.47	1.54
2	6	204	VAL	C-N	5.66	1.41	1.34
3	H	123	LYS	CA-C	-5.66	1.45	1.52
1	D	223	GLU	CA-C	-5.66	1.45	1.52
1	F	105	GLU	CA-C	-5.66	1.46	1.52
2	i	158	GLU	CA-CB	-5.66	1.45	1.53
3	J	364	ARG	CD-NE	5.66	1.54	1.46
1	B	24	VAL	C-N	5.66	1.42	1.33
1	c	136	LEU	CA-CB	5.66	1.64	1.53
1	D	245	LYS	C-N	5.66	1.41	1.33
2	1	46	TYR	N-CA	-5.65	1.39	1.46
2	h	124	SER	C-O	-5.65	1.17	1.24
3	M	331	ALA	CA-C	-5.65	1.46	1.52
1	B	53	ARG	CD-NE	5.65	1.54	1.46
1	C	191	LEU	CA-CB	5.65	1.62	1.53
1	C	232	TYR	C-N	5.65	1.40	1.33
1	b	196	MET	CA-C	-5.65	1.45	1.52
1	C	137	LEU	CA-C	-5.65	1.45	1.52
1	d	93	ARG	CA-C	-5.65	1.45	1.52
1	f	244	LEU	CA-C	-5.65	1.44	1.52
2	i	205	GLU	C-N	5.65	1.41	1.33
2	i	125	ILE	C-N	5.64	1.41	1.33
3	M	78	VAL	CA-CB	-5.64	1.47	1.54
1	D	33	ARG	NE-CZ	5.64	1.39	1.33
2	6	145	LEU	N-CA	-5.64	1.39	1.46
1	c	224	VAL	CA-CB	-5.64	1.47	1.54
1	E	104	ASP	C-N	5.64	1.41	1.33
1	a	168	ARG	CD-NE	5.64	1.54	1.46
2	4	85	PRO	CA-C	-5.64	1.46	1.52
3	H	221	ARG	CD-NE	5.64	1.54	1.46
3	L	264	THR	N-CA	-5.64	1.39	1.46
1	B	76	ALA	N-CA	-5.64	1.39	1.46
1	E	70	ILE	C-N	5.64	1.39	1.33
3	M	200	ARG	CZ-NH2	5.64	1.40	1.33
2	l	204	VAL	CA-CB	-5.63	1.46	1.54
1	C	155	ALA	C-N	5.63	1.42	1.33
2	4	151	LEU	N-CA	-5.63	1.39	1.46
2	n	30	ARG	NE-CZ	5.63	1.39	1.33
1	C	93	ARG	CZ-NH2	5.63	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	VAL	N-CA	-5.63	1.39	1.46
2	i	62	ASP	CA-CB	5.63	1.62	1.53
2	6	141	GLY	CA-C	-5.63	1.45	1.52
2	5	112	ILE	C-O	-5.63	1.18	1.24
1	A	132	PHE	CA-CB	5.63	1.62	1.53
1	g	111	GLU	CA-CB	5.63	1.62	1.53
2	4	82	GLU	CA-CB	5.63	1.61	1.53
2	6	81	ARG	NE-CZ	5.63	1.39	1.33
3	L	150	ILE	N-CA	-5.63	1.39	1.46
1	d	33	ARG	NE-CZ	5.62	1.39	1.33
3	L	387	THR	CA-C	-5.62	1.47	1.52
1	b	185	PHE	C-N	5.62	1.41	1.33
1	C	205	VAL	N-CA	-5.62	1.41	1.46
1	e	117	CYS	C-N	5.62	1.41	1.33
2	k	51	ARG	NE-CZ	5.62	1.39	1.33
1	A	67	ILE	CA-C	-5.62	1.45	1.52
1	B	5	GLN	CA-CB	5.62	1.64	1.53
1	g	86	ARG	NE-CZ	5.62	1.39	1.33
1	a	118	ASP	CA-C	-5.62	1.45	1.52
2	h	62	ASP	N-CA	-5.62	1.39	1.46
2	k	79	ILE	N-CA	-5.62	1.39	1.46
3	M	194	ALA	N-CA	-5.62	1.39	1.46
1	b	80	GLY	N-CA	-5.62	1.37	1.45
1	f	76	ALA	CA-C	-5.62	1.45	1.52
1	G	20	ARG	CD-NE	5.62	1.54	1.46
3	L	140	TYR	C-N	5.62	1.41	1.33
1	a	179	TYR	CA-CB	5.62	1.61	1.53
1	f	160	LYS	N-CA	-5.61	1.39	1.46
2	7	32	THR	N-CA	-5.61	1.39	1.46
3	H	224	ARG	CZ-NH1	5.61	1.40	1.32
1	E	215	LYS	N-CA	-5.61	1.39	1.46
2	7	154	ARG	C-N	5.61	1.41	1.33
3	L	200	ARG	CZ-NH1	5.61	1.40	1.32
1	E	93	ARG	CZ-NH2	5.61	1.40	1.33
1	c	111	GLU	C-N	5.61	1.41	1.33
1	d	119	PHE	CA-CB	5.61	1.62	1.53
2	4	191	ILE	CA-CB	-5.61	1.46	1.53
3	I	12	LYS	N-CA	-5.61	1.39	1.46
3	J	51	LEU	C-N	5.60	1.41	1.33
3	J	234	ALA	CA-C	-5.60	1.47	1.53
3	K	74	ASP	N-CA	-5.60	1.38	1.46
1	A	187	ASP	N-CA	-5.60	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	LEU	CA-C	-5.60	1.45	1.52
3	L	214	LYS	CA-CB	5.60	1.60	1.53
1	D	140	GLY	C-N	5.59	1.40	1.33
1	d	116	ILE	CA-C	-5.59	1.44	1.52
1	e	122	GLN	CA-C	-5.59	1.44	1.52
2	3	101	TYR	CA-C	-5.59	1.47	1.53
2	6	154	ARG	N-CA	-5.59	1.39	1.46
2	n	178	ARG	NE-CZ	5.59	1.39	1.33
2	m	47	GLN	N-CA	-5.59	1.39	1.46
3	H	302	ARG	CD-NE	5.59	1.54	1.46
2	l	29	LYS	CA-C	-5.59	1.45	1.52
2	n	103	TYR	CA-C	-5.59	1.45	1.52
3	K	126	MET	C-N	5.59	1.40	1.34
1	g	156	LEU	N-CA	-5.58	1.39	1.46
3	M	198	GLN	N-CA	-5.58	1.39	1.46
2	1	45	ILE	N-CA	-5.58	1.39	1.46
2	m	177	LYS	CA-CB	5.58	1.63	1.53
2	7	86	THR	N-CA	-5.58	1.38	1.45
3	L	263	ARG	CZ-NH1	5.58	1.40	1.32
1	a	130	ARG	NE-CZ	5.58	1.39	1.33
1	D	8	TYR	C-N	5.58	1.41	1.33
1	G	108	THR	N-CA	-5.58	1.39	1.45
2	4	16	GLY	CA-C	-5.58	1.44	1.51
2	6	42	ALA	CA-C	-5.58	1.46	1.52
1	B	47	ILE	N-CA	-5.58	1.39	1.46
2	j	178	ARG	NE-CZ	5.58	1.39	1.33
3	I	231	LYS	C-N	5.58	1.42	1.33
3	K	80	LYS	CA-C	-5.58	1.46	1.52
3	K	331	ALA	N-CA	-5.58	1.39	1.45
2	h	23	VAL	N-CA	-5.57	1.39	1.46
3	K	181	TYR	CA-C	-5.57	1.45	1.52
1	d	232	TYR	CA-C	-5.57	1.45	1.52
2	3	66	LEU	N-CA	-5.57	1.39	1.46
2	7	153	ASP	C-N	5.57	1.40	1.33
3	J	148	VAL	CA-CB	-5.57	1.47	1.54
2	k	137	ILE	C-N	5.57	1.40	1.33
3	J	48	VAL	CA-CB	-5.57	1.47	1.54
1	C	169	ASN	C-O	5.57	1.30	1.24
3	L	193	LYS	N-CA	-5.57	1.39	1.46
3	I	57	ARG	CD-NE	5.56	1.54	1.46
3	I	142	ASP	C-N	5.56	1.41	1.33
3	J	317	ARG	CD-NE	5.56	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	39	GLY	C-N	5.56	1.40	1.33
1	C	31	VAL	CA-CB	-5.56	1.47	1.54
1	G	21	LEU	CA-CB	5.56	1.60	1.53
2	j	58	GLY	C-O	-5.56	1.20	1.24
2	4	29	LYS	CA-C	-5.56	1.45	1.52
2	6	109	GLN	CA-CB	5.56	1.61	1.53
2	7	51	ARG	NE-CZ	5.56	1.39	1.33
2	7	64	GLN	CA-CB	5.56	1.62	1.53
3	L	259	ARG	CZ-NH2	5.56	1.40	1.33
3	J	116	VAL	CA-CB	-5.56	1.49	1.55
3	K	90	ASN	CG-ND2	5.56	1.45	1.33
1	E	180	ARG	CD-NE	5.56	1.54	1.46
2	4	182	SER	CA-C	-5.56	1.45	1.52
1	C	219	ARG	NE-CZ	5.56	1.39	1.33
1	F	70	ILE	CA-C	-5.56	1.45	1.52
3	J	205	ARG	CZ-NH1	5.56	1.40	1.32
1	f	207	GLU	N-CA	-5.55	1.38	1.46
2	7	83	ARG	CZ-NH1	5.55	1.40	1.32
3	M	78	VAL	CA-C	-5.55	1.46	1.52
3	J	41	ARG	CD-NE	5.55	1.54	1.46
3	K	326	ARG	CD-NE	5.55	1.54	1.46
1	D	201	GLU	CA-CB	5.55	1.62	1.53
1	e	24	VAL	C-N	5.55	1.41	1.33
1	f	168	ARG	CD-NE	5.55	1.54	1.46
2	6	144	SER	CA-CB	5.55	1.62	1.53
2	7	93	LEU	C-N	5.55	1.41	1.33
3	J	17	GLU	N-CA	-5.55	1.39	1.46
1	C	125	GLN	CA-C	-5.55	1.44	1.52
1	d	156	LEU	CA-C	-5.55	1.45	1.52
1	F	35	ALA	CA-C	-5.55	1.45	1.53
3	H	97	GLU	C-N	5.55	1.41	1.33
3	L	41	ARG	CD-NE	5.55	1.54	1.46
3	J	341	ARG	NE-CZ	5.55	1.39	1.33
1	E	153	SER	N-CA	-5.55	1.39	1.46
2	5	81	ARG	NE-CZ	5.55	1.39	1.33
2	n	78	GLU	N-CA	-5.55	1.39	1.46
1	E	53	ARG	CA-CB	5.55	1.62	1.53
2	7	88	ARG	CA-C	-5.55	1.45	1.52
2	1	161	VAL	CA-C	-5.54	1.45	1.52
2	2	212	ARG	CZ-NH2	5.54	1.40	1.33
2	5	171	ALA	CA-C	-5.54	1.45	1.52
1	e	49	ILE	CA-C	-5.54	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	218	ASP	N-CA	-5.54	1.39	1.46
2	3	94	THR	N-CA	-5.54	1.39	1.46
3	K	57	ARG	CZ-NH1	5.54	1.40	1.32
3	M	194	ALA	C-O	-5.54	1.17	1.24
1	a	76	ALA	C-N	5.54	1.41	1.33
1	F	176	GLU	N-CA	-5.54	1.39	1.46
2	h	134	GLU	CA-C	-5.54	1.45	1.52
3	L	76	ARG	CZ-NH1	5.54	1.40	1.32
3	J	24	ARG	CA-C	-5.54	1.45	1.52
1	b	180	ARG	NE-CZ	5.54	1.39	1.33
1	e	152	PRO	C-N	5.54	1.41	1.33
2	4	135	LYS	CA-CB	5.54	1.62	1.53
2	l	80	ARG	N-CA	-5.54	1.39	1.46
1	g	23	GLN	C-N	5.53	1.40	1.33
2	2	24	VAL	N-CA	5.53	1.52	1.46
2	4	188	VAL	C-N	5.53	1.40	1.33
1	B	222	LYS	N-CA	-5.53	1.39	1.45
1	f	110	LYS	N-CA	-5.53	1.39	1.46
3	H	263	ARG	CZ-NH2	5.53	1.40	1.33
3	H	338	GLU	CA-CB	5.53	1.62	1.53
1	D	232	TYR	CZ-OH	5.53	1.49	1.38
2	i	188	VAL	CA-C	-5.53	1.46	1.52
2	1	123	TYR	CA-C	-5.53	1.46	1.52
1	b	223	GLU	N-CA	5.53	1.52	1.46
1	f	74	ILE	C-N	5.53	1.41	1.33
1	b	26	TYR	C-N	5.53	1.41	1.33
1	D	237	ASN	CA-C	-5.52	1.45	1.52
3	K	275	PHE	CA-C	-5.52	1.45	1.52
1	B	240	ILE	N-CA	5.52	1.53	1.46
1	c	180	ARG	CD-NE	5.52	1.53	1.46
1	d	198	LEU	CA-CB	5.52	1.61	1.53
1	c	183	LEU	CA-C	-5.52	1.45	1.52
1	B	140	GLY	C-N	5.52	1.40	1.33
2	l	71	LYS	C-N	-5.52	1.26	1.33
1	F	33	ARG	CZ-NH2	5.52	1.40	1.33
2	i	25	MET	C-N	5.52	1.40	1.33
3	H	351	ILE	C-N	5.52	1.40	1.33
3	J	99	GLU	CA-C	-5.52	1.44	1.52
2	k	174	SER	C-O	-5.52	1.17	1.24
2	5	162	ASP	CA-C	5.52	1.60	1.52
3	K	112	THR	N-CA	5.52	1.52	1.46
1	c	75	CYS	CA-CB	5.51	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	159	TYR	C-N	5.51	1.41	1.33
2	n	179	ASP	N-CA	-5.51	1.39	1.46
1	B	111	GLU	N-CA	-5.51	1.39	1.46
1	e	73	HIS	ND1-CE1	5.51	1.38	1.32
2	5	137	ILE	CA-C	5.51	1.59	1.52
3	L	246	ILE	C-N	5.51	1.40	1.33
1	d	241	ARG	CA-CB	5.51	1.61	1.53
1	f	184	SER	C-N	5.51	1.41	1.33
1	B	113	ALA	C-O	-5.51	1.17	1.24
1	e	235	ARG	CA-CB	5.51	1.62	1.53
1	f	134	VAL	N-CA	-5.51	1.39	1.46
2	j	36	PHE	C-N	5.51	1.40	1.33
2	4	47	GLN	CA-CB	5.51	1.59	1.52
3	J	236	SER	N-CA	-5.51	1.39	1.45
3	M	326	ARG	NE-CZ	5.50	1.39	1.33
1	b	65	GLU	N-CA	5.50	1.53	1.45
3	I	317	ARG	CZ-NH1	5.50	1.40	1.32
1	A	139	ALA	C-O	-5.50	1.17	1.24
1	b	91	ARG	CA-C	-5.50	1.45	1.52
3	J	87	PHE	CA-C	-5.50	1.46	1.52
1	e	208	ASN	N-CA	-5.50	1.40	1.46
1	f	73	HIS	CA-C	-5.50	1.46	1.52
2	2	98	LEU	CA-C	-5.50	1.45	1.52
2	3	212	ARG	CD-NE	5.50	1.53	1.46
2	k	31	ALA	CA-C	-5.50	1.46	1.52
2	7	55	THR	CA-CB	-5.50	1.45	1.53
3	H	124	ASP	C-N	-5.50	1.26	1.33
3	H	327	LYS	C-N	5.50	1.40	1.33
3	H	389	ILE	C-N	5.50	1.40	1.33
3	J	367	ARG	NE-CZ	5.50	1.39	1.33
2	3	51	ARG	CZ-NH2	5.50	1.40	1.33
2	3	116	ASP	CA-C	-5.50	1.45	1.52
2	1	109	GLN	N-CA	-5.49	1.39	1.46
3	H	109	ASN	C-N	5.49	1.40	1.33
3	I	47	GLU	CA-C	-5.49	1.45	1.52
3	K	69	SER	C-N	5.49	1.40	1.33
2	7	210	LYS	CA-C	-5.49	1.45	1.52
1	C	93	ARG	NE-CZ	5.49	1.39	1.33
1	f	28	ARG	NE-CZ	5.49	1.39	1.33
2	1	30	ARG	C-O	-5.49	1.17	1.23
1	b	217	ASP	N-CA	-5.49	1.39	1.46
1	D	111	GLU	N-CA	-5.49	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	ARG	NE-CZ	5.49	1.39	1.33
1	g	162	THR	N-CA	-5.49	1.39	1.46
2	2	81	ARG	NE-CZ	5.49	1.39	1.33
1	D	87	VAL	N-CA	-5.49	1.39	1.46
1	A	175	PHE	CA-C	-5.48	1.45	1.52
1	d	240	ILE	CA-C	-5.48	1.45	1.52
2	2	178	ARG	NE-CZ	5.48	1.39	1.33
2	m	94	THR	C-N	5.48	1.41	1.34
3	L	31	GLU	C-N	5.48	1.41	1.33
1	d	192	GLY	C-N	5.48	1.41	1.33
2	4	90	ILE	CA-CB	-5.48	1.47	1.54
2	7	81	ARG	C-N	5.48	1.41	1.33
1	A	210	GLU	CA-C	-5.48	1.46	1.52
1	b	121	GLN	C-N	5.48	1.41	1.33
3	J	363	ILE	C-N	5.48	1.42	1.33
2	2	83	ARG	NE-CZ	5.48	1.39	1.33
2	i	109	GLN	CA-C	-5.48	1.46	1.52
1	B	93	ARG	CA-CB	5.48	1.61	1.53
3	H	283	VAL	N-CA	-5.48	1.39	1.46
3	I	163	LYS	C-N	5.48	1.40	1.34
1	D	239	ARG	CA-CB	5.47	1.61	1.53
2	6	168	ALA	CA-CB	5.47	1.61	1.53
2	7	39	SER	C-N	5.47	1.41	1.33
3	M	323	ILE	CA-C	-5.47	1.45	1.52
1	C	66	LYS	CA-CB	5.47	1.62	1.53
1	c	176	GLU	CA-C	-5.47	1.45	1.52
2	l	46	TYR	CA-C	-5.47	1.46	1.52
1	a	189	MET	CA-CB	5.47	1.61	1.53
2	k	150	VAL	CA-CB	-5.47	1.47	1.54
2	j	98	LEU	CA-C	-5.47	1.45	1.52
3	M	368	ALA	CA-C	-5.47	1.45	1.52
3	J	305	ARG	CA-C	-5.47	1.46	1.53
2	3	101	TYR	C-N	5.47	1.40	1.33
2	1	89	ALA	CA-C	-5.47	1.45	1.52
2	n	67	ALA	N-CA	5.47	1.53	1.46
3	L	57	ARG	CZ-NH2	5.47	1.40	1.33
1	B	148	TYR	CA-CB	5.46	1.63	1.54
1	F	25	GLU	CA-C	-5.46	1.45	1.52
2	3	131	ALA	CA-C	-5.46	1.46	1.52
2	4	178	ARG	CZ-NH2	5.46	1.40	1.33
2	5	178	ARG	N-CA	-5.46	1.40	1.46
2	l	139	ALA	CA-CB	5.46	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	112	LEU	C-O	-5.46	1.17	1.24
3	M	150	ILE	N-CA	-5.46	1.40	1.46
3	H	32	ASP	CA-CB	5.46	1.61	1.53
3	K	226	VAL	C-O	-5.46	1.18	1.24
2	6	186	ILE	N-CA	-5.46	1.39	1.46
3	K	199	THR	N-CA	-5.46	1.38	1.45
1	e	18	ASP	C-O	-5.45	1.17	1.23
3	H	205	ARG	NE-CZ	5.45	1.39	1.33
3	K	223	VAL	CA-CB	5.45	1.60	1.54
3	J	51	LEU	CA-C	-5.45	1.45	1.52
3	J	76	ARG	N-CA	-5.45	1.39	1.45
3	I	57	ARG	NE-CZ	5.45	1.39	1.33
3	L	294	ASP	CA-CB	5.45	1.61	1.53
1	E	239	ARG	CD-NE	5.45	1.53	1.46
1	a	151	ASP	CA-C	5.45	1.57	1.52
1	E	125	GLN	N-CA	-5.45	1.39	1.46
1	B	20	ARG	CA-C	-5.45	1.46	1.52
1	c	186	ASP	N-CA	5.45	1.53	1.46
1	F	38	ILE	C-N	5.45	1.39	1.33
1	f	168	ARG	CZ-NH2	5.45	1.40	1.33
1	G	201	GLU	CA-C	-5.45	1.46	1.53
1	g	205	VAL	C-N	-5.45	1.27	1.34
2	6	29	LYS	CA-CB	5.45	1.63	1.53
3	I	386	THR	CA-C	5.45	1.59	1.52
1	F	51	ASP	CA-CB	5.44	1.61	1.53
1	g	64	ILE	N-CA	5.44	1.52	1.46
3	K	251	THR	N-CA	-5.44	1.40	1.46
3	L	172	ILE	N-CA	-5.44	1.39	1.46
1	C	137	LEU	CA-CB	5.44	1.60	1.53
1	c	30	ALA	N-CA	5.44	1.53	1.46
1	d	95	GLU	C-N	5.44	1.41	1.33
1	E	92	ALA	N-CA	-5.44	1.39	1.46
2	h	70	ILE	N-CA	-5.44	1.39	1.46
3	L	299	ARG	N-CA	-5.44	1.38	1.45
1	A	35	ALA	C-N	5.44	1.41	1.33
2	k	167	LEU	CA-CB	5.44	1.61	1.53
2	5	84	LYS	N-CA	-5.44	1.38	1.45
3	I	84	GLY	C-N	5.44	1.40	1.33
3	L	52	ARG	CD-NE	5.44	1.53	1.46
3	L	249	ARG	C-N	5.44	1.41	1.33
3	J	43	ARG	CZ-NH1	5.44	1.40	1.32
3	I	115	ILE	N-CA	-5.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	140	THR	CA-CB	-5.44	1.44	1.53
2	6	178	ARG	CD-NE	5.44	1.53	1.46
3	I	128	TYR	CE1-CZ	5.44	1.51	1.38
3	L	323	ILE	CA-C	-5.44	1.46	1.52
3	J	267	GLN	C-N	5.44	1.41	1.33
1	a	196	MET	CA-C	-5.43	1.45	1.52
1	F	11	ALA	CA-C	-5.43	1.46	1.52
1	G	162	THR	C-O	5.43	1.30	1.23
1	G	242	GLU	CA-CB	5.43	1.61	1.53
3	M	265	MET	N-CA	5.43	1.53	1.46
1	d	208	ASN	C-N	5.43	1.41	1.33
2	n	36	PHE	N-CA	-5.43	1.39	1.45
3	L	317	ARG	NE-CZ	5.43	1.39	1.33
1	B	140	GLY	CA-C	-5.43	1.44	1.51
1	C	202	SER	CA-C	-5.43	1.46	1.52
1	C	212	GLY	N-CA	-5.43	1.39	1.45
2	4	152	GLU	C-N	5.43	1.41	1.33
3	H	115	ILE	C-N	5.43	1.38	1.33
1	G	86	ARG	NE-CZ	5.42	1.39	1.33
2	i	65	PHE	CA-C	-5.42	1.46	1.52
2	l	88	ARG	CD-NE	5.42	1.53	1.46
3	L	262	GLN	CD-NE2	5.42	1.44	1.33
1	E	156	LEU	C-N	5.42	1.41	1.33
2	3	210	LYS	CA-CB	5.42	1.61	1.53
3	I	249	ARG	CA-CB	5.42	1.62	1.53
1	b	168	ARG	CD-NE	5.42	1.53	1.46
1	e	101	LEU	CA-C	-5.42	1.46	1.52
3	J	196	ALA	CA-C	-5.42	1.45	1.52
1	C	130	ARG	N-CA	-5.42	1.37	1.46
3	J	183	PRO	C-O	5.42	1.30	1.24
2	7	44	LYS	C-O	-5.42	1.18	1.24
3	I	286	ALA	CA-C	-5.42	1.46	1.52
1	C	239	ARG	NE-CZ	5.41	1.39	1.33
1	d	40	ILE	C-N	5.41	1.41	1.33
2	h	184	ASP	CA-CB	5.41	1.61	1.53
2	h	210	LYS	N-CA	-5.41	1.40	1.46
2	2	184	ASP	C-N	5.41	1.41	1.33
1	f	180	ARG	NE-CZ	5.41	1.39	1.33
1	e	182	ASP	C-N	5.41	1.41	1.33
2	n	153	ASP	CA-CB	5.41	1.61	1.53
2	j	80	ARG	CZ-NH2	5.41	1.40	1.33
2	6	39	SER	CA-CB	5.41	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	130	GLY	C-N	5.41	1.40	1.33
1	e	236	ALA	CA-C	-5.41	1.46	1.52
2	m	169	VAL	N-CA	-5.41	1.39	1.46
2	n	116	ASP	C-N	5.41	1.41	1.34
1	E	91	ARG	CA-CB	5.40	1.61	1.53
3	K	231	LYS	CA-CB	5.40	1.61	1.53
1	d	133	GLY	CA-C	-5.40	1.44	1.51
1	g	239	ARG	CZ-NH1	5.40	1.40	1.32
2	h	116	ASP	C-N	5.40	1.41	1.33
3	M	52	ARG	NE-CZ	5.40	1.39	1.33
1	c	235	ARG	NE-CZ	5.40	1.39	1.33
2	3	72	ILE	N-CA	-5.40	1.40	1.46
2	n	101	TYR	C-O	-5.40	1.16	1.23
1	c	28	ARG	CD-NE	5.40	1.53	1.46
2	6	77	TYR	C-N	5.40	1.41	1.33
2	n	143	GLY	C-O	-5.40	1.18	1.24
1	E	129	VAL	CA-C	-5.40	1.45	1.52
2	j	73	GLU	N-CA	-5.40	1.39	1.46
1	E	28	ARG	CD-NE	5.39	1.53	1.46
2	4	111	LEU	CA-C	-5.39	1.46	1.52
3	M	302	ARG	C-N	5.39	1.43	1.33
1	c	121	GLN	C-N	5.39	1.41	1.33
1	f	219	ARG	CA-C	-5.39	1.46	1.53
2	j	195	GLU	CA-C	-5.39	1.46	1.52
2	4	41	ALA	CA-C	-5.39	1.46	1.52
2	2	121	SER	CA-C	-5.39	1.46	1.52
2	6	182	SER	C-N	5.39	1.41	1.33
3	M	295	PRO	CA-CB	-5.39	1.46	1.53
1	B	86	ARG	NE-CZ	5.39	1.39	1.33
1	F	219	ARG	NE-CZ	5.39	1.39	1.33
3	M	272	LEU	C-N	5.39	1.41	1.33
3	J	20	TYR	CA-CB	5.39	1.61	1.53
1	c	116	ILE	N-CA	-5.38	1.39	1.46
1	E	73	HIS	CB-CG	5.38	1.57	1.50
1	e	29	GLU	CA-CB	5.38	1.62	1.53
2	5	78	GLU	N-CA	-5.38	1.39	1.46
2	i	179	ASP	C-N	5.38	1.40	1.33
2	j	197	TYR	N-CA	-5.38	1.39	1.46
1	D	208	ASN	CA-CB	5.38	1.60	1.53
1	E	7	GLY	CA-C	-5.38	1.44	1.51
1	f	235	ARG	CA-C	-5.38	1.45	1.52
2	2	43	LYS	CA-C	-5.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	136	ASP	N-CA	-5.38	1.39	1.46
1	e	166	MET	N-CA	-5.38	1.39	1.46
2	m	99	ASN	CA-C	-5.38	1.46	1.52
1	F	143	GLU	C-N	5.37	1.39	1.33
2	l	126	ASP	CA-CB	5.37	1.61	1.53
2	l	106	TYR	CA-C	-5.37	1.46	1.52
3	K	150	ILE	N-CA	-5.37	1.40	1.46
2	h	30	ARG	NE-CZ	5.37	1.39	1.33
2	n	199	TYR	CA-C	-5.37	1.45	1.52
3	M	156	ALA	CA-C	5.37	1.59	1.52
1	B	228	GLU	N-CA	-5.37	1.39	1.46
1	E	191	LEU	CA-CB	5.37	1.62	1.53
2	6	160	GLY	CA-C	-5.37	1.46	1.52
3	L	396	MET	CA-CB	5.37	1.62	1.53
1	B	185	PHE	CA-CB	5.37	1.61	1.53
1	d	40	ILE	CA-C	-5.37	1.46	1.52
1	F	66	LYS	C-N	5.37	1.38	1.33
2	i	141	GLY	CA-C	-5.37	1.46	1.52
3	M	87	PHE	C-N	5.37	1.40	1.33
3	H	38	GLU	C-N	5.36	1.41	1.33
1	f	177	LYS	C-N	5.36	1.40	1.33
3	M	14	LYS	C-N	5.36	1.40	1.33
1	F	53	ARG	CZ-NH1	5.36	1.40	1.32
1	G	33	ARG	NE-CZ	5.36	1.39	1.33
2	m	103	TYR	N-CA	5.36	1.53	1.46
2	7	13	THR	CA-C	-5.36	1.46	1.52
1	a	73	HIS	ND1-CE1	5.36	1.38	1.32
1	G	71	ASP	CA-C	-5.36	1.48	1.53
2	1	68	ARG	CZ-NH1	5.36	1.40	1.32
2	2	145	LEU	CA-C	-5.36	1.45	1.52
2	m	154	ARG	NE-CZ	5.36	1.39	1.33
1	a	205	VAL	CA-C	-5.36	1.48	1.52
2	j	205	GLU	CA-C	-5.36	1.45	1.52
2	4	106	TYR	C-N	5.36	1.41	1.33
2	m	141	GLY	CA-C	-5.36	1.45	1.51
2	7	158	GLU	CA-CB	5.36	1.60	1.53
2	n	18	VAL	CA-C	-5.36	1.45	1.52
1	d	198	LEU	N-CA	-5.35	1.40	1.46
1	E	101	LEU	N-CA	-5.35	1.40	1.46
1	G	64	ILE	C-O	-5.35	1.18	1.24
1	e	188	ALA	CA-C	-5.35	1.45	1.52
2	j	191	ILE	CA-CB	5.35	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	40	LYS	CA-CB	5.35	1.61	1.54
2	j	168	ALA	N-CA	-5.35	1.40	1.46
2	5	193	GLU	CA-C	-5.35	1.45	1.52
3	J	23	LEU	CA-C	-5.35	1.45	1.52
1	a	76	ALA	CA-C	-5.35	1.46	1.52
2	4	97	LEU	C-N	5.35	1.40	1.33
3	I	28	ARG	CZ-NH2	5.35	1.40	1.33
3	M	19	ASP	CA-CB	5.35	1.62	1.53
1	E	181	ASP	CA-C	-5.34	1.45	1.52
3	H	316	GLY	N-CA	-5.34	1.39	1.45
1	f	54	VAL	N-CA	-5.34	1.38	1.46
2	l	76	LEU	CA-C	-5.34	1.45	1.52
2	n	212	ARG	NE-CZ	5.34	1.39	1.33
3	L	47	GLU	CA-C	-5.34	1.46	1.52
3	J	266	MET	CA-CB	5.34	1.62	1.53
2	7	172	ILE	CA-CB	-5.34	1.47	1.54
1	E	91	ARG	NE-CZ	5.34	1.39	1.33
3	K	317	ARG	CA-C	-5.34	1.45	1.52
1	E	9	ASP	CA-C	-5.33	1.45	1.52
1	F	198	LEU	CA-C	5.33	1.59	1.52
1	E	214	VAL	CA-C	-5.33	1.45	1.52
2	m	45	ILE	C-O	-5.33	1.18	1.24
3	M	80	LYS	N-CA	-5.33	1.39	1.46
3	M	341	ARG	NE-CZ	5.33	1.39	1.33
1	A	18	ASP	CA-C	-5.33	1.46	1.52
1	C	219	ARG	CZ-NH1	5.33	1.40	1.32
1	e	169	ASN	CA-CB	5.33	1.61	1.53
2	h	188	VAL	CA-CB	-5.33	1.46	1.55
2	4	191	ILE	N-CA	5.33	1.53	1.46
2	5	40	LYS	C-N	5.33	1.41	1.33
2	7	201	PRO	C-N	5.33	1.40	1.33
2	n	48	ILE	N-CA	-5.33	1.40	1.46
3	L	143	ILE	N-CA	-5.33	1.40	1.46
1	B	231	PRO	N-CD	-5.33	1.40	1.47
1	b	78	THR	CA-C	-5.33	1.46	1.52
1	C	155	ALA	CA-C	-5.33	1.46	1.52
1	D	67	ILE	CA-CB	5.33	1.59	1.53
2	5	178	ARG	CZ-NH2	5.33	1.40	1.33
2	m	187	ASP	CA-C	-5.33	1.46	1.52
3	H	279	GLY	C-N	5.33	1.41	1.33
3	L	309	VAL	N-CA	-5.33	1.42	1.46
3	J	102	PRO	N-CD	-5.33	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	191	LEU	CA-C	-5.33	1.45	1.52
3	J	318	ILE	C-O	-5.33	1.17	1.24
1	B	235	ARG	CA-C	-5.33	1.46	1.52
2	4	102	ARG	NE-CZ	5.33	1.39	1.33
3	K	152	GLU	C-N	5.33	1.40	1.33
1	D	44	GLU	N-CA	-5.32	1.39	1.46
1	F	53	ARG	N-CA	-5.32	1.39	1.46
3	J	80	LYS	CA-C	-5.32	1.46	1.52
1	g	10	ARG	CZ-NH2	5.32	1.40	1.33
3	I	342	ILE	C-O	-5.32	1.18	1.24
1	a	56	SER	N-CA	-5.32	1.38	1.45
1	g	145	PRO	N-CA	-5.32	1.40	1.47
2	i	38	ALA	CA-C	-5.32	1.46	1.52
2	3	195	GLU	CA-C	-5.32	1.45	1.52
2	j	102	ARG	NE-CZ	5.32	1.38	1.33
2	6	13	THR	N-CA	-5.32	1.39	1.46
1	G	92	ALA	CA-C	5.32	1.59	1.52
2	5	176	MET	C-N	5.32	1.41	1.33
2	l	199	TYR	CA-C	-5.32	1.45	1.52
2	n	80	ARG	CZ-NH2	5.32	1.40	1.33
1	F	209	ILE	CA-CB	-5.31	1.47	1.55
2	m	100	SER	CA-C	-5.31	1.45	1.52
2	n	54	MET	CA-C	-5.31	1.46	1.52
3	L	218	GLU	C-N	5.31	1.41	1.33
3	J	116	VAL	C-N	5.31	1.40	1.33
2	k	77	TYR	CZ-OH	5.31	1.49	1.38
3	K	21	TYR	N-CA	-5.31	1.39	1.46
1	A	69	LYS	C-O	-5.31	1.17	1.24
2	7	129	GLY	C-O	-5.31	1.18	1.24
2	1	95	SER	CA-CB	5.31	1.61	1.53
2	h	55	THR	N-CA	5.31	1.52	1.46
3	J	368	ALA	N-CA	-5.31	1.40	1.46
2	j	41	ALA	N-CA	-5.31	1.39	1.46
3	I	212	VAL	C-N	5.31	1.40	1.33
3	L	135	LYS	C-N	-5.31	1.26	1.33
2	4	95	SER	CA-C	-5.31	1.46	1.52
1	F	47	ILE	CB-CG1	5.30	1.64	1.53
2	i	140	THR	C-N	5.30	1.40	1.32
3	I	256	SER	CA-C	-5.30	1.45	1.52
3	L	360	MET	CA-C	-5.30	1.45	1.52
1	E	71	ASP	CA-C	-5.30	1.46	1.52
2	k	57	ALA	CA-C	-5.30	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	27	ALA	CA-C	-5.30	1.45	1.52
1	d	12	ILE	CA-CB	-5.30	1.47	1.54
3	I	41	ARG	CZ-NH2	5.30	1.40	1.33
1	f	245	LYS	C-N	5.30	1.40	1.33
1	G	183	LEU	CA-C	-5.30	1.46	1.52
2	3	180	SER	N-CA	-5.30	1.39	1.46
2	n	47	GLN	C-O	-5.30	1.17	1.24
1	a	227	GLU	C-N	5.30	1.41	1.33
1	C	204	LEU	C-N	5.30	1.38	1.33
1	c	244	LEU	CA-CB	5.30	1.60	1.52
1	E	218	ASP	CA-C	-5.30	1.45	1.52
2	l	87	VAL	C-N	5.30	1.41	1.33
3	M	305	ARG	CZ-NH2	5.30	1.40	1.33
2	3	104	PHE	N-CA	-5.29	1.41	1.46
2	1	51	ARG	CD-NE	5.29	1.53	1.46
2	5	115	ILE	C-N	5.29	1.39	1.33
1	F	107	ILE	C-N	5.29	1.40	1.33
2	n	162	ASP	CA-C	-5.29	1.45	1.52
1	D	86	ARG	CZ-NH1	5.29	1.40	1.32
2	3	79	ILE	C-N	5.29	1.41	1.33
3	K	168	ALA	CA-C	-5.29	1.46	1.52
3	K	184	PRO	N-CA	-5.29	1.40	1.47
3	L	194	ALA	C-N	5.29	1.40	1.33
3	M	114	ALA	CA-C	-5.29	1.46	1.52
3	H	241	ASP	C-O	-5.29	1.17	1.24
3	M	102	PRO	CA-CB	-5.29	1.46	1.53
1	C	30	ALA	N-CA	-5.29	1.39	1.46
2	1	113	GLY	N-CA	-5.29	1.39	1.45
2	i	124	SER	N-CA	-5.29	1.39	1.46
3	J	278	ARG	CD-NE	5.29	1.53	1.46
1	b	81	LEU	N-CA	-5.28	1.39	1.46
1	f	94	ILE	N-CA	-5.28	1.40	1.46
2	i	154	ARG	CZ-NH1	5.28	1.40	1.32
2	5	51	ARG	CZ-NH1	5.28	1.40	1.32
3	L	353	ALA	CA-C	-5.28	1.46	1.52
2	h	30	ARG	CD-NE	5.28	1.53	1.46
1	G	73	HIS	CB-CG	5.28	1.57	1.50
3	H	141	GLU	C-N	5.28	1.40	1.33
1	d	185	PHE	CA-CB	5.28	1.61	1.53
1	E	128	GLY	CA-C	5.28	1.58	1.51
2	1	21	ASP	C-N	5.28	1.41	1.33
3	K	371	THR	CA-CB	5.28	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	178	GLU	N-CA	-5.28	1.39	1.46
1	g	28	ARG	CZ-NH1	5.28	1.40	1.32
2	j	176	MET	N-CA	5.28	1.52	1.46
3	K	43	ARG	CZ-NH1	5.28	1.40	1.32
3	J	268	LEU	CA-CB	5.28	1.61	1.53
1	A	76	ALA	N-CA	-5.28	1.39	1.45
1	C	203	GLU	CA-CB	5.28	1.61	1.53
1	c	30	ALA	CA-C	-5.28	1.44	1.52
1	e	218	ASP	CA-CB	5.28	1.62	1.53
1	g	25	GLU	N-CA	5.28	1.52	1.46
2	k	107	LEU	CA-CB	5.28	1.60	1.53
2	7	45	ILE	C-N	5.28	1.41	1.33
3	L	281	VAL	CA-CB	5.28	1.60	1.54
3	M	246	ILE	N-CA	-5.28	1.39	1.46
3	M	311	LEU	CA-CB	5.28	1.61	1.53
1	f	14	VAL	C-N	5.27	1.40	1.33
3	H	379	ILE	CA-C	-5.27	1.46	1.52
3	K	173	GLU	C-N	-5.27	1.27	1.33
1	B	147	LEU	CA-C	-5.27	1.46	1.52
3	I	12	LYS	CA-CB	5.27	1.61	1.53
1	c	193	LEU	C-N	5.27	1.40	1.33
2	6	112	ILE	CA-CB	-5.27	1.47	1.54
3	L	352	LYS	CA-C	-5.27	1.46	1.52
1	E	230	LYS	N-CA	-5.27	1.41	1.46
1	f	50	ALA	C-N	5.27	1.41	1.33
3	M	354	ILE	C-O	-5.27	1.17	1.24
3	M	187	GLY	CA-C	-5.27	1.44	1.51
1	a	241	ARG	CZ-NH2	5.26	1.40	1.33
2	i	73	GLU	C-N	5.26	1.40	1.33
2	h	138	VAL	CA-C	-5.26	1.46	1.52
2	h	17	LEU	CA-CB	5.26	1.63	1.53
3	H	201	ALA	C-N	5.26	1.41	1.33
3	J	32	ASP	N-CA	5.26	1.52	1.46
1	e	37	ALA	C-N	5.26	1.40	1.33
2	2	124	SER	CA-CB	5.26	1.61	1.53
2	3	136	ASP	N-CA	-5.26	1.39	1.46
2	j	88	ARG	CZ-NH1	5.26	1.40	1.32
2	4	118	GLU	CA-CB	5.26	1.61	1.54
2	4	161	VAL	N-CA	-5.26	1.39	1.46
1	b	160	LYS	CA-CB	5.26	1.62	1.53
2	h	65	PHE	CG-CD2	5.26	1.49	1.38
2	k	85	PRO	C-O	-5.26	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	43	ARG	CD-NE	5.26	1.53	1.46
3	K	278	ARG	CZ-NH1	5.26	1.40	1.32
1	G	21	LEU	N-CA	-5.25	1.40	1.46
2	1	162	ASP	CA-C	-5.25	1.46	1.52
2	h	95	SER	CA-C	-5.25	1.46	1.52
3	I	344	GLU	C-N	5.25	1.40	1.33
2	j	66	LEU	C-O	5.25	1.30	1.24
2	5	85	PRO	N-CD	-5.25	1.40	1.47
2	5	161	VAL	C-N	5.25	1.41	1.34
2	7	144	SER	CA-CB	5.25	1.61	1.53
3	H	318	ILE	N-CA	-5.25	1.40	1.46
2	4	128	ILE	C-N	5.25	1.41	1.33
1	D	199	SER	C-N	5.25	1.41	1.34
3	K	293	LEU	CA-C	-5.25	1.46	1.52
3	K	359	GLY	C-N	5.25	1.41	1.34
2	l	146	THR	N-CA	-5.25	1.40	1.46
3	H	105	ARG	N-CA	-5.25	1.39	1.46
3	L	364	ARG	CD-NE	5.25	1.53	1.46
1	A	137	LEU	N-CA	-5.24	1.39	1.46
1	E	11	ALA	C-N	5.24	1.39	1.33
2	k	50	ASP	C-N	5.24	1.41	1.33
2	6	186	ILE	C-N	5.24	1.40	1.33
3	I	242	GLU	N-CA	-5.24	1.39	1.46
1	C	41	LYS	N-CA	-5.24	1.39	1.46
3	M	115	ILE	C-N	5.24	1.40	1.33
1	a	164	ILE	N-CA	-5.24	1.40	1.46
1	C	144	VAL	N-CA	-5.24	1.40	1.46
2	4	80	ARG	N-CA	-5.24	1.40	1.46
3	I	236	SER	CA-C	-5.24	1.46	1.52
1	B	157	LEU	C-N	5.24	1.40	1.33
1	C	226	PRO	N-CA	-5.24	1.40	1.47
2	l	127	PRO	N-CA	5.24	1.51	1.47
2	7	194	ASP	CA-C	-5.24	1.46	1.52
3	K	24	ARG	CZ-NH1	5.24	1.40	1.32
3	L	60	SER	CA-C	5.24	1.58	1.52
1	A	9	ASP	C-O	-5.24	1.17	1.23
1	E	219	ARG	CA-CB	5.24	1.61	1.53
1	e	92	ALA	CA-CB	5.24	1.61	1.53
1	e	141	VAL	CA-C	-5.24	1.46	1.52
1	b	53	ARG	CD-NE	5.23	1.53	1.46
1	e	93	ARG	NE-CZ	5.23	1.38	1.33
2	j	126	ASP	N-CA	5.23	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	69	LYS	C-N	5.23	1.40	1.33
2	5	132	ILE	C-N	5.23	1.41	1.33
3	M	392	LEU	CA-CB	5.23	1.62	1.53
1	A	17	PRO	N-CA	-5.23	1.40	1.47
1	a	230	LYS	N-CA	-5.23	1.41	1.46
1	C	37	ALA	CA-C	-5.23	1.46	1.52
1	c	53	ARG	CZ-NH2	5.23	1.40	1.33
1	c	170	ALA	N-CA	-5.23	1.40	1.46
1	d	228	GLU	N-CA	-5.23	1.39	1.46
2	h	186	ILE	C-N	5.23	1.40	1.33
3	H	258	ASP	CA-C	-5.23	1.46	1.52
3	M	12	LYS	C-O	-5.23	1.18	1.24
1	C	240	ILE	N-CA	-5.23	1.40	1.46
1	e	32	LYS	N-CA	-5.23	1.40	1.46
2	1	179	ASP	CA-C	-5.23	1.46	1.52
1	A	33	ARG	CD-NE	5.23	1.53	1.46
1	d	33	ARG	N-CA	-5.23	1.39	1.46
1	c	193	LEU	N-CA	-5.23	1.40	1.46
1	c	83	ALA	CA-C	-5.22	1.46	1.52
1	F	172	THR	N-CA	-5.22	1.40	1.46
3	H	326	ARG	NE-CZ	5.22	1.38	1.33
1	b	22	PHE	CA-C	-5.22	1.45	1.52
1	c	93	ARG	CA-CB	5.22	1.61	1.53
1	g	82	VAL	C-N	5.22	1.41	1.33
2	6	102	ARG	CA-C	-5.22	1.45	1.52
3	L	41	ARG	NE-CZ	5.22	1.38	1.33
1	G	245	LYS	CA-C	-5.22	1.46	1.52
2	m	182	SER	CA-C	-5.22	1.46	1.52
2	7	87	VAL	N-CA	-5.22	1.40	1.46
3	L	76	ARG	C-O	-5.22	1.17	1.23
1	a	123	TYR	CA-C	-5.22	1.45	1.52
2	4	75	ASN	C-N	5.22	1.41	1.34
2	m	38	ALA	CA-C	-5.22	1.46	1.52
3	L	270	ALA	CA-C	-5.22	1.46	1.52
1	b	147	LEU	N-CA	-5.21	1.39	1.46
1	E	50	ALA	N-CA	-5.21	1.39	1.46
2	h	68	ARG	NE-CZ	5.21	1.38	1.33
2	i	41	ALA	C-N	5.21	1.40	1.33
3	H	250	ARG	NE-CZ	5.21	1.38	1.33
3	H	289	ARG	CZ-NH1	5.21	1.40	1.32
3	K	258	ASP	N-CA	5.21	1.52	1.46
3	L	104	ALA	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	123	LYS	CA-C	-5.21	1.45	1.52
1	a	236	ALA	N-CA	-5.21	1.40	1.46
1	B	23	GLN	N-CA	-5.21	1.40	1.46
3	I	389	ILE	N-CA	-5.21	1.40	1.46
3	L	265	MET	N-CA	-5.21	1.40	1.46
3	L	291	ASP	CA-C	-5.21	1.45	1.52
3	J	158	GLU	C-N	5.21	1.41	1.33
1	B	90	ASP	CA-C	-5.21	1.46	1.52
3	K	215	TYR	N-CA	-5.21	1.39	1.45
3	L	43	ARG	CZ-NH1	5.21	1.40	1.32
2	i	181	ALA	CA-C	-5.21	1.45	1.52
3	I	41	ARG	N-CA	5.21	1.52	1.46
2	2	135	LYS	CA-C	-5.21	1.46	1.52
2	4	23	VAL	C-N	5.21	1.39	1.33
2	l	25	MET	CA-C	-5.21	1.46	1.52
2	k	181	ALA	CA-C	-5.21	1.45	1.52
3	H	364	ARG	CD-NE	5.21	1.53	1.46
1	D	149	GLU	CA-C	-5.20	1.46	1.52
1	G	170	ALA	CA-C	-5.20	1.46	1.52
1	g	107	ILE	C-N	5.20	1.40	1.33
2	7	53	ALA	N-CA	5.20	1.52	1.45
3	L	152	GLU	CA-C	-5.20	1.46	1.52
3	J	343	THR	C-N	5.20	1.41	1.33
1	b	50	ALA	CA-C	-5.20	1.46	1.52
1	e	33	ARG	NE-CZ	5.20	1.38	1.33
2	j	212	ARG	NE-CZ	5.20	1.38	1.33
1	A	158	GLU	N-CA	-5.20	1.39	1.46
1	E	205	VAL	CA-CB	-5.20	1.47	1.54
2	1	45	ILE	CA-CB	-5.20	1.48	1.54
2	2	81	ARG	CZ-NH2	5.20	1.40	1.33
2	3	102	ARG	NE-CZ	5.20	1.38	1.33
2	6	159	ILE	C-N	5.20	1.39	1.33
3	M	47	GLU	N-CA	-5.20	1.40	1.46
1	a	47	ILE	CA-CB	5.20	1.61	1.54
2	l	44	LYS	CA-CB	5.20	1.60	1.53
3	K	138	VAL	CA-C	-5.20	1.46	1.52
1	C	148	TYR	N-CA	-5.20	1.39	1.45
1	g	201	GLU	CA-C	-5.20	1.46	1.52
2	k	144	SER	CA-C	-5.20	1.46	1.52
1	F	222	LYS	C-N	5.19	1.40	1.33
1	G	24	VAL	C-N	5.19	1.41	1.33
2	j	85	PRO	N-CA	-5.19	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	90	ILE	CA-C	-5.19	1.46	1.52
3	J	239	PHE	CA-CB	5.19	1.59	1.53
1	A	5	GLN	C-N	5.19	1.40	1.33
2	5	155	PHE	C-N	5.19	1.38	1.33
2	l	71	LYS	CA-C	-5.19	1.46	1.52
2	7	166	GLU	CA-C	-5.19	1.45	1.52
3	L	279	GLY	C-N	5.19	1.40	1.33
1	C	98	ILE	CA-CB	-5.19	1.47	1.54
1	d	239	ARG	CA-CB	5.19	1.61	1.53
1	e	140	GLY	CA-C	-5.19	1.46	1.51
2	h	35	ASN	N-CA	-5.19	1.39	1.46
2	6	14	THR	C-N	5.19	1.40	1.33
3	L	59	ARG	CD-NE	5.19	1.53	1.46
2	3	169	VAL	C-N	5.19	1.40	1.33
3	H	212	VAL	C-N	5.19	1.40	1.33
3	M	13	LEU	C-O	-5.19	1.18	1.24
3	J	317	ARG	NE-CZ	5.19	1.38	1.33
1	e	127	GLY	CA-C	5.18	1.59	1.51
2	3	30	ARG	CZ-NH1	5.18	1.40	1.32
2	3	156	THR	CA-CB	5.18	1.60	1.53
3	L	105	ARG	NE-CZ	5.18	1.38	1.33
1	D	142	ASP	CA-CB	5.18	1.61	1.53
1	d	20	ARG	NE-CZ	5.18	1.38	1.33
2	3	25	MET	CA-C	-5.18	1.46	1.52
2	7	168	ALA	CA-C	-5.18	1.45	1.52
3	H	166	LEU	C-N	5.18	1.40	1.33
3	M	236	SER	C-N	5.18	1.39	1.33
1	a	150	THR	N-CA	-5.18	1.39	1.45
1	a	214	VAL	CA-CB	5.18	1.60	1.53
2	j	119	GLY	CA-C	-5.18	1.45	1.52
3	K	80	LYS	N-CA	-5.18	1.40	1.46
1	c	93	ARG	NE-CZ	5.18	1.38	1.33
1	d	102	THR	N-CA	-5.18	1.39	1.46
2	m	177	LYS	N-CA	-5.18	1.39	1.46
2	2	186	ILE	N-CA	-5.18	1.39	1.46
3	L	41	ARG	CZ-NH2	5.18	1.40	1.33
2	5	50	ASP	N-CA	-5.18	1.39	1.46
2	l	194	ASP	CA-CB	5.18	1.62	1.53
3	I	127	VAL	CA-CB	-5.18	1.48	1.54
3	K	29	ARG	N-CA	-5.18	1.40	1.46
1	d	74	ILE	N-CA	-5.17	1.39	1.46
3	L	153	ILE	CA-C	-5.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	278	ARG	N-CA	-5.17	1.40	1.46
3	M	105	ARG	CZ-NH1	5.17	1.40	1.32
1	E	103	TYR	CZ-OH	5.17	1.49	1.38
2	k	88	ARG	N-CA	-5.17	1.40	1.46
2	k	128	ILE	CA-CB	-5.17	1.47	1.54
2	4	96	ASN	C-N	5.17	1.40	1.33
3	K	209	SER	C-N	5.17	1.41	1.33
3	J	318	ILE	C-N	5.17	1.40	1.34
1	D	24	VAL	N-CA	-5.17	1.40	1.46
1	f	97	GLN	C-N	5.17	1.40	1.33
2	k	100	SER	C-N	5.17	1.40	1.33
1	C	74	ILE	N-CA	-5.17	1.40	1.46
1	D	74	ILE	C-N	5.17	1.40	1.33
2	7	49	ALA	N-CA	-5.17	1.40	1.46
3	I	158	GLU	CA-CB	5.17	1.61	1.53
3	J	161	LEU	N-CA	-5.17	1.40	1.46
2	1	198	GLN	CA-CB	5.17	1.61	1.53
2	k	184	ASP	C-N	5.17	1.40	1.32
3	L	118	VAL	C-O	-5.17	1.18	1.24
3	J	30	LEU	C-N	5.17	1.40	1.33
1	D	211	VAL	N-CA	-5.16	1.40	1.46
1	D	228	GLU	CA-C	-5.16	1.45	1.52
1	E	86	ARG	C-N	5.16	1.40	1.33
2	1	188	VAL	C-N	5.16	1.40	1.33
3	I	115	ILE	CA-C	-5.16	1.47	1.53
1	f	233	VAL	C-O	-5.16	1.18	1.24
2	h	178	ARG	CZ-NH1	5.16	1.40	1.32
2	5	103	TYR	C-N	-5.16	1.27	1.33
3	I	43	ARG	NE-CZ	5.16	1.38	1.33
1	a	171	VAL	N-CA	-5.16	1.40	1.46
1	c	53	ARG	CZ-NH1	5.16	1.40	1.32
2	5	113	GLY	CA-C	-5.16	1.47	1.52
3	L	196	ALA	C-N	5.16	1.40	1.33
1	B	63	THR	CA-C	5.16	1.59	1.52
3	I	294	ASP	CA-CB	5.16	1.61	1.53
3	L	265	MET	CA-CB	5.16	1.61	1.53
1	C	36	THR	N-CA	-5.15	1.39	1.46
1	D	235	ARG	CD-NE	5.15	1.53	1.46
2	3	208	LEU	CA-CB	5.15	1.62	1.53
2	n	197	TYR	CA-C	-5.15	1.46	1.52
3	H	249	ARG	NE-CZ	5.15	1.38	1.33
1	f	239	ARG	NE-CZ	5.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	43	LYS	N-CA	-5.15	1.39	1.46
2	l	35	ASN	CA-CB	5.15	1.62	1.53
3	K	223	VAL	C-N	5.15	1.40	1.33
2	i	18	VAL	CA-C	-5.15	1.46	1.52
3	M	108	LEU	CA-CB	5.15	1.62	1.53
2	3	177	LYS	C-N	5.15	1.41	1.33
2	j	26	ALA	C-O	-5.15	1.17	1.23
2	l	31	ALA	CA-C	-5.15	1.46	1.52
3	K	249	ARG	CZ-NH2	5.15	1.40	1.33
1	C	162	THR	N-CA	-5.14	1.40	1.46
1	g	212	GLY	C-N	5.14	1.40	1.33
2	2	81	ARG	CZ-NH1	5.14	1.40	1.32
2	6	161	VAL	C-O	-5.14	1.18	1.24
2	n	78	GLU	C-N	5.14	1.40	1.33
1	D	235	ARG	CZ-NH2	5.14	1.40	1.33
2	4	64	GLN	C-N	5.14	1.41	1.33
3	I	52	ARG	NE-CZ	5.14	1.38	1.33
1	G	79	SER	C-N	5.14	1.41	1.33
3	H	200	ARG	CZ-NH1	5.14	1.40	1.32
1	a	42	CYS	CA-CB	5.14	1.61	1.53
2	m	135	LYS	N-CA	5.14	1.51	1.46
3	M	317	ARG	N-CA	-5.14	1.40	1.46
3	J	92	SER	N-CA	-5.14	1.38	1.46
1	B	223	GLU	C-N	5.14	1.39	1.33
1	F	52	LYS	CA-C	-5.14	1.46	1.52
2	i	85	PRO	N-CA	-5.14	1.40	1.47
2	3	45	ILE	CA-CB	-5.14	1.47	1.53
2	5	61	GLY	CA-C	-5.14	1.46	1.51
3	H	104	ALA	CA-CB	5.14	1.60	1.53
3	K	157	VAL	CA-CB	-5.14	1.47	1.54
3	J	322	LYS	C-N	5.14	1.40	1.33
2	h	33	MET	N-CA	-5.13	1.39	1.45
2	k	212	ARG	CZ-NH1	5.13	1.40	1.32
2	h	196	PHE	CA-C	-5.13	1.46	1.53
2	3	50	ASP	N-CA	-5.13	1.40	1.46
2	4	146	THR	N-CA	-5.13	1.40	1.46
1	B	40	ILE	N-CA	-5.13	1.40	1.46
2	m	138	VAL	N-CA	-5.13	1.39	1.46
3	H	386	THR	C-N	5.13	1.40	1.33
1	f	103	TYR	CA-C	-5.13	1.46	1.52
2	2	102	ARG	CZ-NH1	5.13	1.40	1.32
2	l	44	LYS	C-N	5.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	48	LEU	C-N	5.13	1.40	1.33
1	D	223	GLU	C-N	5.13	1.40	1.33
2	l	107	LEU	CA-CB	5.13	1.62	1.53
2	k	170	ARG	CA-CB	5.13	1.61	1.53
2	n	148	TYR	CA-CB	5.13	1.61	1.53
3	M	52	ARG	CZ-NH1	5.13	1.40	1.32
1	A	46	VAL	CA-C	-5.13	1.46	1.52
2	i	183	GLY	CA-C	-5.13	1.46	1.52
3	M	52	ARG	C-O	-5.13	1.18	1.24
1	c	58	LEU	C-O	-5.12	1.17	1.24
1	E	192	GLY	C-N	5.12	1.41	1.33
2	l	178	ARG	CA-C	5.12	1.59	1.52
3	L	318	ILE	C-N	5.12	1.40	1.33
1	c	213	TYR	C-N	5.12	1.40	1.33
1	f	208	ASN	N-CA	-5.12	1.41	1.46
1	g	69	LYS	CA-C	-5.12	1.46	1.52
3	I	50	ARG	CD-NE	5.12	1.53	1.46
3	K	200	ARG	C-N	5.12	1.39	1.33
3	M	304	ASP	CA-C	-5.12	1.46	1.52
1	A	241	ARG	C-N	5.12	1.40	1.33
1	a	70	ILE	C-N	5.12	1.40	1.33
1	g	44	GLU	C-N	5.12	1.40	1.32
2	4	43	LYS	CA-C	-5.12	1.46	1.52
2	4	161	VAL	CA-C	-5.12	1.45	1.52
2	k	30	ARG	CZ-NH1	5.12	1.40	1.32
3	I	262	GLN	CA-C	-5.12	1.45	1.52
2	l	194	ASP	CA-C	5.12	1.59	1.52
3	I	67	VAL	CA-C	-5.12	1.46	1.52
3	J	224	ARG	CZ-NH1	5.12	1.40	1.32
1	e	33	ARG	CZ-NH1	5.12	1.40	1.32
3	I	61	PRO	CA-C	5.12	1.54	1.51
1	C	30	ALA	C-N	5.11	1.40	1.33
1	c	180	ARG	NE-CZ	5.11	1.38	1.33
1	D	123	TYR	C-N	5.11	1.40	1.33
1	e	181	ASP	N-CA	-5.11	1.39	1.46
1	a	240	ILE	N-CA	-5.11	1.40	1.46
1	f	149	GLU	C-N	5.11	1.40	1.33
2	h	83	ARG	CZ-NH2	5.11	1.40	1.33
2	h	139	ALA	CA-C	-5.11	1.46	1.52
2	n	178	ARG	N-CA	-5.11	1.40	1.46
1	B	83	ALA	CA-C	-5.11	1.46	1.52
1	d	93	ARG	CZ-NH1	5.11	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	192	THR	C-N	5.11	1.40	1.33
2	k	179	ASP	CA-C	-5.11	1.46	1.52
3	K	207	VAL	N-CA	-5.11	1.40	1.46
3	J	99	GLU	C-N	5.11	1.40	1.33
1	c	105	GLU	CA-C	-5.11	1.46	1.52
1	D	245	LYS	CA-C	-5.11	1.46	1.52
1	d	239	ARG	NE-CZ	5.11	1.38	1.33
2	6	67	ALA	CA-C	-5.11	1.46	1.52
3	K	167	PHE	CA-C	-5.11	1.46	1.52
1	e	200	ILE	CA-CB	5.10	1.61	1.54
2	4	196	PHE	CA-C	-5.10	1.46	1.53
1	D	110	LYS	CA-C	-5.10	1.46	1.52
2	1	60	VAL	CA-C	-5.10	1.46	1.52
2	5	53	ALA	N-CA	-5.10	1.39	1.45
3	L	18	GLU	CA-C	-5.10	1.46	1.52
1	B	56	SER	CA-CB	5.10	1.62	1.53
1	b	14	VAL	N-CA	5.10	1.52	1.46
1	D	93	ARG	CZ-NH2	5.10	1.40	1.33
1	g	234	GLU	CA-CB	5.10	1.61	1.53
2	k	47	GLN	CA-CB	5.10	1.59	1.53
2	k	139	ALA	C-N	5.10	1.40	1.33
3	J	41	ARG	NE-CZ	5.10	1.38	1.33
2	6	50	ASP	N-CA	-5.10	1.40	1.46
3	K	388	PRO	CA-CB	5.10	1.59	1.54
3	M	393	LYS	CA-C	-5.10	1.46	1.52
1	g	91	ARG	CD-NE	5.09	1.53	1.46
2	i	81	ARG	CD-NE	5.09	1.53	1.46
3	J	354	ILE	N-CA	-5.09	1.40	1.46
1	A	20	ARG	CD-NE	5.09	1.53	1.46
1	d	196	MET	C-O	5.09	1.30	1.24
1	a	86	ARG	CD-NE	5.09	1.53	1.46
1	e	216	VAL	C-O	-5.09	1.19	1.24
2	k	197	TYR	C-N	5.09	1.40	1.33
3	H	43	ARG	CD-NE	5.09	1.53	1.46
1	B	135	SER	CA-C	-5.09	1.46	1.52
1	c	28	ARG	N-CA	-5.09	1.40	1.46
1	G	78	THR	C-O	-5.09	1.17	1.23
3	J	17	GLU	CA-CB	5.09	1.61	1.53
1	g	137	LEU	CA-C	-5.09	1.46	1.52
3	K	29	ARG	NE-CZ	5.09	1.38	1.33
2	1	86	THR	CA-C	-5.09	1.46	1.52
1	e	99	ASN	N-CA	-5.08	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	212	ARG	CZ-NH2	5.08	1.40	1.33
3	J	193	LYS	CA-C	-5.08	1.46	1.52
1	e	228	GLU	N-CA	-5.08	1.39	1.46
1	F	147	LEU	CA-C	-5.08	1.46	1.52
1	F	226	PRO	N-CA	-5.08	1.40	1.47
3	L	94	TYR	CA-CB	-5.08	1.47	1.54
3	M	143	ILE	CA-C	-5.08	1.46	1.52
3	L	173	GLU	C-N	5.08	1.39	1.33
2	n	175	ALA	C-N	5.08	1.40	1.33
3	I	329	LYS	C-N	5.08	1.40	1.33
3	J	26	LEU	C-O	-5.08	1.18	1.24
3	H	22	LYS	C-O	-5.08	1.18	1.24
3	J	43	ARG	NE-CZ	5.08	1.38	1.33
1	C	91	ARG	C-N	5.08	1.40	1.33
1	C	180	ARG	CZ-NH2	5.08	1.40	1.33
1	G	12	ILE	C-O	-5.08	1.16	1.23
1	g	61	ALA	N-CA	-5.08	1.42	1.47
2	i	44	LYS	CA-C	-5.08	1.46	1.52
2	4	86	THR	C-N	5.08	1.40	1.33
2	4	170	ARG	CZ-NH2	5.08	1.40	1.33
3	H	311	LEU	CA-C	-5.08	1.48	1.53
3	M	307	ILE	N-CA	-5.08	1.39	1.46
3	J	57	ARG	CZ-NH2	5.08	1.40	1.33
1	B	93	ARG	C-O	-5.07	1.18	1.24
1	G	164	ILE	N-CA	-5.07	1.40	1.46
2	j	77	TYR	C-N	5.07	1.40	1.33
1	D	28	ARG	CZ-NH1	5.07	1.39	1.32
1	e	213	TYR	C-N	5.07	1.39	1.33
2	5	71	LYS	C-O	5.07	1.29	1.24
3	J	28	ARG	CZ-NH2	5.07	1.40	1.33
1	e	38	ILE	N-CA	-5.07	1.40	1.46
2	2	169	VAL	CA-CB	5.07	1.61	1.54
3	K	224	ARG	CD-NE	5.07	1.53	1.46
1	C	53	ARG	CZ-NH2	5.07	1.40	1.33
1	e	242	GLU	C-N	5.07	1.40	1.33
2	k	200	SER	CA-C	-5.07	1.46	1.52
2	7	81	ARG	NE-CZ	5.07	1.38	1.33
1	b	111	GLU	CA-C	-5.07	1.46	1.52
1	d	115	LYS	CA-C	5.07	1.59	1.52
1	g	174	PHE	CA-C	-5.07	1.46	1.52
1	F	89	ILE	N-CA	-5.06	1.39	1.46
1	G	43	LYS	C-O	-5.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	178	ARG	NE-CZ	5.06	1.38	1.33
1	a	194	VAL	CA-C	5.06	1.59	1.52
1	F	156	LEU	CA-CB	5.06	1.63	1.53
2	h	108	VAL	CA-C	-5.06	1.46	1.52
2	2	175	ALA	CA-C	5.06	1.59	1.52
2	j	140	THR	N-CA	5.06	1.51	1.46
2	7	55	THR	CA-C	-5.06	1.46	1.52
3	M	28	ARG	CZ-NH1	5.06	1.39	1.32
2	5	35	ASN	C-N	5.06	1.40	1.33
1	A	239	ARG	CZ-NH2	5.06	1.40	1.33
1	C	180	ARG	N-CA	-5.06	1.39	1.46
2	1	54	MET	CA-C	-5.06	1.46	1.52
2	j	95	SER	N-CA	-5.06	1.40	1.46
3	H	168	ALA	CA-C	-5.06	1.46	1.52
3	I	224	ARG	CD-NE	5.06	1.53	1.46
3	J	334	VAL	C-N	5.06	1.40	1.33
1	B	160	LYS	CA-C	-5.06	1.46	1.52
1	C	48	LEU	C-N	5.06	1.40	1.33
1	c	66	LYS	N-CA	-5.06	1.39	1.46
1	D	198	LEU	C-N	5.06	1.40	1.33
2	n	29	LYS	CA-C	-5.06	1.46	1.52
3	L	162	LEU	CA-C	-5.06	1.46	1.52
3	M	378	ALA	CA-C	-5.06	1.46	1.52
1	f	81	LEU	N-CA	-5.06	1.39	1.45
1	d	28	ARG	CA-CB	5.05	1.61	1.53
2	1	64	GLN	CA-CB	5.05	1.61	1.53
2	4	49	ALA	N-CA	-5.05	1.40	1.46
3	K	300	PRO	N-CA	-5.05	1.41	1.46
3	J	304	ASP	CA-C	5.05	1.59	1.52
1	e	179	TYR	C-N	5.05	1.40	1.33
1	f	88	LEU	CA-C	-5.05	1.46	1.52
1	f	125	GLN	C-N	5.05	1.40	1.33
3	H	341	ARG	NE-CZ	5.05	1.38	1.33
3	M	237	ILE	CA-C	-5.05	1.46	1.52
1	g	219	ARG	C-N	5.05	1.41	1.33
2	i	27	THR	C-N	5.05	1.40	1.33
3	K	240	ILE	N-CA	-5.05	1.40	1.46
1	C	156	LEU	CA-C	-5.05	1.46	1.52
1	c	180	ARG	CZ-NH2	5.05	1.40	1.33
1	F	178	GLU	C-N	5.05	1.40	1.33
2	h	151	LEU	C-N	5.05	1.41	1.33
3	H	55	VAL	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	139	ALA	C-N	5.04	1.40	1.33
3	H	81	SER	CA-CB	5.04	1.61	1.53
1	c	100	ARG	CA-C	5.04	1.59	1.52
1	c	169	ASN	CA-CB	5.04	1.61	1.53
1	e	140	GLY	N-CA	-5.04	1.39	1.45
1	g	130	ARG	CD-NE	5.04	1.53	1.46
1	g	177	LYS	N-CA	-5.04	1.39	1.46
2	2	139	ALA	N-CA	-5.04	1.39	1.46
1	b	17	PRO	CA-C	-5.04	1.45	1.52
1	c	78	THR	CA-C	-5.04	1.46	1.52
3	M	105	ARG	N-CA	-5.04	1.40	1.46
3	M	335	ASP	N-CA	-5.04	1.40	1.46
3	J	94	TYR	N-CA	5.04	1.52	1.46
3	J	347	SER	CA-CB	5.04	1.60	1.53
1	E	156	LEU	CA-CB	5.04	1.62	1.53
3	L	250	ARG	CZ-NH1	5.04	1.39	1.32
3	J	57	ARG	CZ-NH1	5.04	1.39	1.32
1	B	210	GLU	C-O	-5.04	1.17	1.24
1	e	139	ALA	CA-C	-5.04	1.46	1.52
1	C	6	MET	CA-C	-5.04	1.46	1.52
1	e	171	VAL	C-N	5.04	1.40	1.33
1	F	75	CYS	CA-C	-5.04	1.46	1.52
3	L	286	ALA	CA-C	-5.04	1.46	1.52
3	J	35	LYS	N-CA	5.04	1.52	1.46
1	A	79	SER	CA-C	-5.04	1.46	1.52
1	A	211	VAL	CA-C	-5.04	1.46	1.52
1	D	75	CYS	C-N	5.04	1.40	1.33
1	d	33	ARG	CD-NE	5.04	1.53	1.46
2	3	186	ILE	CA-CB	-5.04	1.48	1.54
2	4	155	PHE	CA-CB	5.04	1.61	1.53
2	m	57	ALA	N-CA	-5.04	1.39	1.45
1	d	109	VAL	CA-CB	-5.03	1.48	1.54
1	E	169	ASN	CA-CB	5.03	1.61	1.53
3	I	15	LYS	CA-C	-5.03	1.46	1.52
3	K	46	ARG	CZ-NH2	5.03	1.40	1.33
3	J	116	VAL	CA-C	-5.03	1.45	1.52
3	J	192	ALA	N-CA	5.03	1.52	1.46
1	A	135	SER	CA-C	-5.03	1.46	1.52
1	c	189	MET	C-N	5.03	1.40	1.33
1	e	186	ASP	CA-C	-5.03	1.46	1.52
2	i	181	ALA	C-N	5.03	1.40	1.33
3	H	105	ARG	NE-CZ	5.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	84	LYS	C-N	5.03	1.39	1.33
1	e	219	ARG	CD-NE	5.03	1.53	1.46
2	h	51	ARG	CA-C	-5.03	1.46	1.52
1	B	182	ASP	CA-C	-5.03	1.46	1.52
1	c	82	VAL	N-CA	-5.03	1.39	1.46
1	e	139	ALA	C-N	5.03	1.40	1.33
2	7	24	VAL	C-N	5.03	1.40	1.33
2	7	66	LEU	CA-C	-5.03	1.46	1.52
3	H	209	SER	C-N	5.03	1.40	1.33
3	J	162	LEU	C-N	5.03	1.40	1.33
1	B	175	PHE	C-O	-5.03	1.17	1.24
1	d	169	ASN	N-CA	-5.03	1.40	1.46
1	g	113	ALA	CA-C	-5.03	1.46	1.52
2	j	194	ASP	CA-C	-5.03	1.46	1.52
2	5	52	MET	CA-C	-5.03	1.46	1.52
1	f	35	ALA	C-N	5.02	1.40	1.33
1	D	67	ILE	CB-CG1	5.02	1.63	1.53
2	j	100	SER	C-N	5.02	1.39	1.33
2	5	125	ILE	C-N	5.02	1.40	1.33
2	m	19	CYS	CA-C	-5.02	1.46	1.52
3	I	238	ILE	C-O	-5.02	1.18	1.24
2	7	23	VAL	CA-C	-5.02	1.46	1.52
1	A	91	ARG	CD-NE	5.02	1.53	1.46
1	b	180	ARG	CZ-NH2	5.02	1.40	1.33
2	6	96	ASN	CA-C	-5.02	1.46	1.52
1	c	113	ALA	C-N	5.02	1.40	1.33
1	E	161	ALA	CA-C	-5.02	1.46	1.52
1	f	75	CYS	CA-C	-5.02	1.46	1.52
2	k	109	GLN	CA-C	-5.02	1.46	1.52
3	K	142	ASP	C-N	5.02	1.40	1.33
1	g	10	ARG	NE-CZ	5.02	1.38	1.33
2	5	68	ARG	CZ-NH2	5.02	1.40	1.33
1	G	53	ARG	CZ-NH1	5.01	1.39	1.32
3	I	119	LEU	CA-C	5.01	1.59	1.52
1	B	194	VAL	CA-CB	-5.01	1.48	1.54
1	C	54	VAL	C-N	5.01	1.39	1.33
1	d	77	ALA	C-N	5.01	1.40	1.33
1	D	185	PHE	CA-C	-5.01	1.46	1.52
1	f	40	ILE	C-N	-5.01	1.26	1.33
2	1	123	TYR	N-CA	-5.01	1.40	1.46
3	H	388	PRO	CA-C	-5.01	1.45	1.52
3	I	343	THR	C-N	5.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	214	LYS	C-N	5.01	1.40	1.33
1	D	219	ARG	NE-CZ	5.01	1.38	1.33
1	F	60	GLU	C-N	5.01	1.40	1.33
2	6	191	ILE	CA-C	-5.01	1.46	1.52
1	c	71	ASP	CA-C	-5.01	1.46	1.53
1	g	168	ARG	NE-CZ	5.01	1.38	1.33
2	3	27	THR	CA-C	-5.01	1.46	1.52
2	3	128	ILE	CA-C	-5.01	1.46	1.52
2	j	101	TYR	CA-C	-5.01	1.45	1.52
1	E	62	ASP	N-CA	-5.00	1.40	1.47
2	2	170	ARG	CA-C	-5.00	1.46	1.52
2	2	203	GLU	C-N	5.00	1.40	1.33
2	j	127	PRO	C-N	5.00	1.39	1.33
3	H	50	ARG	CD-NE	5.00	1.53	1.46
3	H	116	VAL	N-CA	-5.00	1.42	1.46
1	D	153	SER	N-CA	-5.00	1.40	1.46
1	G	220	THR	C-N	5.00	1.40	1.33
2	h	26	ALA	CA-C	5.00	1.58	1.52
3	M	181	TYR	CA-CB	5.00	1.61	1.54
1	c	185	PHE	C-N	5.00	1.40	1.33
1	g	53	ARG	N-CA	5.00	1.52	1.46
3	M	379	ILE	C-N	-5.00	1.27	1.33
3	J	23	LEU	CB-CG	5.00	1.63	1.53

All (4549) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	170	ARG	NE-CZ-NH2	-24.18	97.44	119.20
2	5	170	ARG	NE-CZ-NH2	-21.65	99.72	119.20
1	B	70	ILE	N-CA-C	-15.73	98.91	112.12
3	M	386	THR	N-CA-C	-14.25	98.38	114.62
1	B	217	ASP	CA-CB-CG	13.65	126.25	112.60
3	L	124	ASP	CA-C-O	-13.21	109.01	119.71
1	d	66	LYS	N-CA-C	-12.74	98.21	113.88
2	2	199	TYR	N-CA-C	12.65	124.81	111.14
3	I	261	VAL	N-CA-C	-12.31	100.00	111.45
2	6	156	THR	O-C-N	-12.30	113.84	121.71
2	6	65	PHE	CA-CB-CG	-12.22	101.58	113.80
3	H	211	PHE	CA-CB-CG	-11.96	101.84	113.80
2	4	104	PHE	CA-CB-CG	11.95	125.75	113.80
2	5	194	ASP	N-CA-C	-11.69	100.02	114.75
3	L	288	ASN	CA-CB-CG	-11.62	100.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	273	ASP	CA-C-N	11.43	132.83	120.03
3	I	273	ASP	C-N-CA	11.43	132.83	120.03
1	G	82	VAL	N-CA-C	-11.36	101.61	112.29
1	D	151	ASP	CA-CB-CG	-11.23	101.37	112.60
3	M	372	MET	N-CA-C	-11.05	99.92	113.41
2	4	118	GLU	N-CA-C	-10.88	98.99	114.12
1	a	142	ASP	N-CA-C	-10.87	102.22	114.62
1	D	144	VAL	CA-C-O	-10.83	114.31	119.94
1	b	12	ILE	CA-C-O	10.78	128.68	118.98
1	C	205	VAL	N-CA-C	-10.74	96.88	109.01
2	1	196	PHE	CA-CB-CG	-10.71	103.09	113.80
2	l	170	ARG	NH1-CZ-NH2	10.69	133.19	119.30
3	J	167	PHE	CA-CB-CG	-10.67	103.13	113.80
1	d	185	PHE	CA-CB-CG	-10.65	103.15	113.80
1	g	15	PHE	CA-CB-CG	-10.59	103.21	113.80
3	M	273	ASP	CA-C-N	10.58	133.36	120.14
3	M	273	ASP	C-N-CA	10.58	133.36	120.14
2	i	104	PHE	N-CA-CB	10.56	122.64	110.71
2	m	76	LEU	CA-C-N	10.49	134.34	120.28
2	m	76	LEU	C-N-CA	10.49	134.34	120.28
1	D	52	LYS	N-CA-C	-10.46	98.07	110.41
3	K	183	PRO	CA-C-O	-10.40	112.51	120.73
1	B	181	ASP	CA-CB-CG	-10.36	102.24	112.60
3	L	281	VAL	O-C-N	-10.35	112.08	123.26
2	l	198	GLN	N-CA-C	-10.34	91.38	108.34
2	i	200	SER	CA-C-N	10.29	132.70	119.84
2	i	200	SER	C-N-CA	10.29	132.70	119.84
2	h	136	ASP	CA-CB-CG	-10.26	102.34	112.60
1	c	205	VAL	N-CA-C	-10.24	95.43	107.61
3	I	324	HIS	CB-CG-CD2	-10.21	117.93	131.20
2	j	50	ASP	CA-CB-CG	-10.20	102.41	112.60
2	j	71	LYS	CA-C-N	10.16	133.36	120.56
2	j	71	LYS	C-N-CA	10.16	133.36	120.56
3	I	294	ASP	CA-CB-CG	-10.16	102.44	112.60
2	7	35	ASN	CA-C-N	10.06	134.99	120.71
2	7	35	ASN	C-N-CA	10.06	134.99	120.71
1	b	202	SER	N-CA-CB	10.04	126.92	111.46
3	L	314	PHE	CA-CB-CG	-10.00	103.80	113.80
2	5	137	ILE	N-CA-C	-9.96	94.14	108.48
1	F	143	GLU	N-CA-C	-9.94	102.22	114.75
3	L	124	ASP	CA-C-N	9.92	129.68	119.56
3	L	124	ASP	C-N-CA	9.92	129.68	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	170	ARG	NE-CZ-NH1	9.90	131.40	121.50
1	C	93	ARG	CA-C-N	9.88	134.44	120.42
1	C	93	ARG	C-N-CA	9.88	134.44	120.42
3	H	60	SER	CA-C-N	9.88	130.55	120.38
3	H	60	SER	C-N-CA	9.88	130.55	120.38
1	G	206	PRO	N-CA-CB	9.87	110.12	101.83
3	I	258	ASP	CA-CB-CG	-9.85	102.75	112.60
3	M	170	VAL	N-CA-C	-9.84	102.30	111.45
3	I	174	PRO	CA-C-N	9.82	129.90	119.78
3	I	174	PRO	C-N-CA	9.82	129.90	119.78
1	D	70	ILE	N-CA-C	-9.78	103.91	112.12
2	k	167	LEU	CA-C-N	9.69	133.62	120.44
2	k	167	LEU	C-N-CA	9.69	133.62	120.44
2	6	139	ALA	CA-C-N	9.69	139.15	121.70
2	6	139	ALA	C-N-CA	9.69	139.15	121.70
2	7	35	ASN	CA-CB-CG	9.64	122.24	112.60
1	b	141	VAL	N-CA-C	-9.62	93.70	107.75
1	A	144	VAL	O-C-N	-9.61	115.00	121.72
3	I	142	ASP	CA-C-O	9.60	128.97	119.08
1	A	212	GLY	O-C-N	-9.60	114.64	123.57
3	L	61	PRO	CA-C-O	-9.59	113.99	120.90
1	d	39	GLY	O-C-N	9.58	131.16	123.49
3	H	10	LEU	CA-C-N	9.58	132.89	120.44
3	H	10	LEU	C-N-CA	9.58	132.89	120.44
1	a	226	PRO	CA-C-N	9.58	132.89	120.44
1	a	226	PRO	C-N-CA	9.58	132.89	120.44
1	b	129	VAL	CA-C-O	-9.57	112.92	120.96
2	3	102	ARG	N-CA-C	-9.56	101.76	112.57
1	B	80	GLY	N-CA-C	-9.56	101.90	111.56
2	i	94	THR	CA-C-N	9.56	133.09	120.28
2	i	94	THR	C-N-CA	9.56	133.09	120.28
2	n	50	ASP	CA-CB-CG	-9.55	103.05	112.60
1	g	151	ASP	N-CA-C	-9.53	97.92	110.40
3	H	298	LEU	N-CA-C	-9.49	100.59	113.30
1	G	186	ASP	O-C-N	9.47	132.31	122.09
2	m	179	ASP	CA-CB-CG	9.47	122.07	112.60
1	A	92	ALA	CA-C-N	9.44	132.93	120.28
1	A	92	ALA	C-N-CA	9.44	132.93	120.28
3	I	66	GLY	N-CA-C	-9.42	96.67	111.18
2	h	199	TYR	CA-C-O	9.33	130.31	120.42
1	c	223	GLU	CA-C-N	9.32	134.52	121.66
1	c	223	GLU	C-N-CA	9.32	134.52	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	203	GLU	CA-C-N	9.31	132.48	120.56
2	i	203	GLU	C-N-CA	9.31	132.48	120.56
1	a	191	LEU	CA-C-O	-9.30	110.69	120.55
3	H	254	ASP	CA-CB-CG	9.30	121.91	112.60
1	d	33	ARG	N-CA-C	-9.29	102.07	113.50
1	F	185	PHE	O-C-N	9.28	131.96	122.12
2	h	194	ASP	N-CA-CB	9.25	126.13	110.49
1	f	241	ARG	NE-CZ-NH1	-9.24	112.26	121.50
2	2	108	VAL	N-CA-C	-9.23	96.17	108.35
1	C	160	LYS	N-CA-C	-9.23	102.84	114.56
3	L	210	GLU	N-CA-C	-9.21	101.81	113.23
2	l	211	PHE	CA-CB-CG	-9.21	104.59	113.80
2	n	48	ILE	N-CA-C	-9.20	101.90	110.82
1	F	114	LYS	N-CA-CB	9.20	123.64	110.12
2	i	122	ILE	CB-CA-C	9.19	123.75	110.33
1	C	13	THR	N-CA-C	-9.19	101.62	112.92
1	b	35	ALA	CA-C-N	9.18	134.61	120.75
1	b	35	ALA	C-N-CA	9.18	134.61	120.75
3	H	394	GLY	O-C-N	9.18	131.49	122.77
2	6	93	LEU	CA-C-N	9.16	132.56	120.28
2	6	93	LEU	C-N-CA	9.16	132.56	120.28
3	M	318	ILE	CA-C-O	-9.16	111.46	121.17
3	K	397	PHE	CA-CB-CG	-9.14	104.66	113.80
3	L	227	PHE	CA-CB-CG	-9.14	104.66	113.80
1	c	130	ARG	N-CA-CB	9.12	125.23	110.10
1	C	118	ASP	CA-C-N	9.11	132.28	120.44
1	C	118	ASP	C-N-CA	9.11	132.28	120.44
2	5	51	ARG	NE-CZ-NH2	9.05	127.35	119.20
2	i	104	PHE	CA-C-N	9.01	131.11	119.84
2	i	104	PHE	C-N-CA	9.01	131.11	119.84
1	G	224	VAL	N-CA-CB	8.99	120.80	110.82
1	E	143	GLU	N-CA-C	-8.99	101.62	114.12
3	M	124	ASP	CA-C-N	8.98	128.92	120.03
3	M	124	ASP	C-N-CA	8.98	128.92	120.03
1	d	58	LEU	N-CA-C	-8.96	101.46	111.14
2	7	196	PHE	CA-CB-CG	-8.94	104.86	113.80
2	6	122	ILE	O-C-N	-8.90	113.58	123.10
2	2	51	ARG	CA-C-O	8.90	131.84	121.34
3	K	263	ARG	NE-CZ-NH1	-8.90	112.60	121.50
1	A	186	ASP	CA-C-N	8.88	132.18	120.28
1	A	186	ASP	C-N-CA	8.88	132.18	120.28
1	c	92	ALA	CA-C-N	8.88	131.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	92	ALA	C-N-CA	8.88	131.98	120.44
2	n	23	VAL	N-CA-C	-8.87	94.44	108.81
1	e	185	PHE	CA-C-N	8.86	133.78	120.31
1	e	185	PHE	C-N-CA	8.86	133.78	120.31
1	g	237	ASN	CA-CB-CG	-8.86	103.74	112.60
1	e	205	VAL	CA-C-O	-8.86	114.02	119.51
3	K	382	VAL	N-CA-C	8.85	118.92	110.42
1	F	233	VAL	CA-C-N	8.84	131.93	120.44
1	F	233	VAL	C-N-CA	8.84	131.93	120.44
1	B	142	ASP	CA-CB-CG	8.83	121.43	112.60
2	4	137	ILE	CA-C-O	-8.80	110.84	120.43
1	c	84	ASP	CA-C-N	8.79	131.87	120.44
1	c	84	ASP	C-N-CA	8.79	131.87	120.44
1	D	211	VAL	CA-C-N	8.79	128.25	122.18
1	D	211	VAL	C-N-CA	8.79	128.25	122.18
1	g	174	PHE	CA-CB-CG	8.78	122.58	113.80
3	L	109	ASN	CA-CB-CG	-8.75	103.85	112.60
3	L	317	ARG	CA-C-N	8.75	131.59	120.56
3	L	317	ARG	C-N-CA	8.75	131.59	120.56
1	f	120	LYS	CA-C-N	8.75	133.61	120.31
1	f	120	LYS	C-N-CA	8.75	133.61	120.31
3	K	101	LYS	N-CA-CB	8.75	120.28	111.10
3	K	303	PHE	CA-C-N	8.73	131.97	120.28
3	K	303	PHE	C-N-CA	8.73	131.97	120.28
1	E	226	PRO	CA-C-N	8.71	131.94	120.28
1	E	226	PRO	C-N-CA	8.71	131.94	120.28
2	n	126	ASP	N-CA-C	-8.70	97.95	110.40
2	m	58	GLY	N-CA-C	-8.70	102.16	111.21
1	b	105	GLU	O-C-N	8.69	127.99	121.65
3	M	164	PRO	CA-C-N	8.68	132.77	120.28
3	M	164	PRO	C-N-CA	8.68	132.77	120.28
1	B	35	ALA	CA-C-N	8.67	133.02	120.71
1	B	35	ALA	C-N-CA	8.67	133.02	120.71
1	e	189	MET	CA-C-N	8.67	132.34	120.46
1	e	189	MET	C-N-CA	8.67	132.34	120.46
2	4	51	ARG	NE-CZ-NH2	8.67	127.00	119.20
1	g	33	ARG	CD-NE-CZ	-8.66	112.28	124.40
2	2	59	SER	CA-C-N	8.66	131.47	120.56
2	2	59	SER	C-N-CA	8.66	131.47	120.56
1	A	185	PHE	CA-CB-CG	-8.64	105.16	113.80
1	c	19	GLY	N-CA-C	-8.63	103.19	114.85
3	H	262	GLN	CA-C-N	8.63	131.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	262	GLN	C-N-CA	8.63	131.67	120.44
1	A	135	SER	N-CA-CB	8.62	125.30	110.81
2	h	155	PHE	CA-CB-CG	8.62	122.42	113.80
3	K	101	LYS	N-CA-C	-8.62	100.46	108.22
3	I	321	PHE	CA-C-N	8.61	131.82	120.28
3	I	321	PHE	C-N-CA	8.61	131.82	120.28
1	f	235	ARG	CA-C-N	8.61	131.63	120.44
1	f	235	ARG	C-N-CA	8.61	131.63	120.44
3	I	324	HIS	CB-CG-ND1	8.61	135.61	122.70
2	j	114	GLY	CA-C-O	8.61	131.09	121.02
1	E	151	ASP	CA-CB-CG	-8.60	104.00	112.60
3	M	146	LEU	N-CA-C	-8.60	100.26	110.41
1	f	109	VAL	CA-C-N	8.60	131.80	120.28
1	f	109	VAL	C-N-CA	8.60	131.80	120.28
2	l	147	ALA	CA-C-N	8.60	131.80	120.28
2	l	147	ALA	C-N-CA	8.60	131.80	120.28
3	K	18	GLU	CA-C-N	8.59	132.49	120.29
3	K	18	GLU	C-N-CA	8.59	132.49	120.29
3	I	335	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	183	LEU	N-CA-CB	8.59	122.53	110.17
1	D	210	GLU	CA-C-N	8.59	134.93	122.99
1	D	210	GLU	C-N-CA	8.59	134.93	122.99
3	L	183	PRO	CA-C-N	8.59	128.60	119.76
3	L	183	PRO	C-N-CA	8.59	128.60	119.76
1	F	12	ILE	CA-C-O	8.57	127.10	118.96
1	F	212	GLY	O-C-N	-8.56	115.63	123.42
3	M	168	ALA	N-CA-C	-8.55	102.65	113.43
3	I	282	LYS	N-CA-CB	8.54	125.03	110.50
3	H	227	PHE	CA-CB-CG	-8.53	105.27	113.80
3	K	335	ASP	CA-CB-CG	8.53	121.13	112.60
2	j	116	ASP	CA-CB-CG	8.52	121.12	112.60
2	h	153	ASP	CA-C-O	-8.50	112.07	121.00
3	L	283	VAL	CA-C-N	8.50	137.00	121.70
3	L	283	VAL	C-N-CA	8.50	137.00	121.70
1	B	112	LEU	CA-C-N	8.49	132.35	120.29
1	B	112	LEU	C-N-CA	8.49	132.35	120.29
3	I	101	LYS	CA-C-N	8.49	130.46	119.84
3	I	101	LYS	C-N-CA	8.49	130.46	119.84
1	a	191	LEU	O-C-N	8.49	131.12	122.12
3	K	146	LEU	N-CA-C	-8.49	99.84	111.56
1	F	30	ALA	CA-C-N	8.49	132.09	120.46
1	F	30	ALA	C-N-CA	8.49	132.09	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	68	TYR	CA-C-N	8.49	132.92	120.87
1	F	68	TYR	C-N-CA	8.49	132.92	120.87
2	6	126	ASP	CA-C-N	8.49	128.62	119.28
2	6	126	ASP	C-N-CA	8.49	128.62	119.28
1	B	23	GLN	CA-C-N	8.48	134.88	120.29
1	B	23	GLN	C-N-CA	8.48	134.88	120.29
3	K	361	PHE	N-CA-C	-8.48	102.12	111.36
1	c	240	ILE	CA-C-N	8.47	132.32	120.29
1	c	240	ILE	C-N-CA	8.47	132.32	120.29
1	d	220	THR	N-CA-C	-8.47	94.67	109.06
3	M	303	PHE	CA-CB-CG	-8.46	105.34	113.80
1	a	24	VAL	N-CA-C	8.45	119.24	110.62
2	1	211	PHE	N-CA-C	-8.45	102.52	113.17
3	L	294	ASP	CA-C-N	8.45	128.58	119.28
3	L	294	ASP	C-N-CA	8.45	128.58	119.28
3	K	138	VAL	CA-C-O	8.45	129.61	120.57
1	G	234	GLU	N-CA-C	8.45	121.42	111.71
3	H	369	LYS	N-CA-C	-8.45	95.99	109.59
1	E	230	LYS	CA-C-O	-8.44	110.86	118.63
2	7	37	ILE	N-CA-C	-8.44	96.33	108.48
1	G	195	ALA	CA-C-N	8.44	131.58	120.28
1	G	195	ALA	C-N-CA	8.44	131.58	120.28
1	b	61	ALA	N-CA-C	-8.43	100.46	113.02
2	4	78	GLU	CA-C-N	8.43	131.18	120.56
2	4	78	GLU	C-N-CA	8.43	131.18	120.56
2	6	74	ALA	CA-C-N	8.43	131.90	120.44
2	6	74	ALA	C-N-CA	8.43	131.90	120.44
3	J	326	ARG	CA-C-N	8.43	131.57	120.28
3	J	326	ARG	C-N-CA	8.43	131.57	120.28
1	e	115	LYS	O-C-N	-8.42	112.55	122.15
3	J	294	ASP	CA-C-O	-8.42	113.03	120.60
2	i	108	VAL	CA-C-O	-8.41	113.89	120.96
1	b	47	ILE	O-C-N	-8.41	114.18	123.26
2	3	108	VAL	O-C-N	-8.41	115.65	122.97
3	H	254	ASP	N-CA-C	-8.40	103.89	114.56
2	i	171	ALA	N-CA-C	8.39	120.51	111.36
3	H	124	ASP	N-CA-C	-8.39	98.52	108.25
2	7	135	LYS	N-CA-C	-8.38	100.48	111.71
3	L	374	ASP	CA-C-N	8.38	131.33	120.44
3	L	374	ASP	C-N-CA	8.38	131.33	120.44
1	G	205	VAL	O-C-N	-8.37	114.12	121.57
3	K	36	PHE	CA-C-N	8.37	133.69	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	36	PHE	C-N-CA	8.37	133.69	120.47
3	J	262	GLN	CA-C-N	8.36	133.02	120.31
3	J	262	GLN	C-N-CA	8.36	133.02	120.31
2	5	211	PHE	CA-CB-CG	-8.36	105.44	113.80
2	l	96	ASN	CA-CB-CG	-8.36	104.24	112.60
2	6	212	ARG	N-CA-C	-8.35	102.87	113.72
3	J	169	GLU	CA-C-N	8.35	131.24	120.56
3	J	169	GLU	C-N-CA	8.35	131.24	120.56
1	B	233	VAL	CB-CA-C	-8.34	101.29	111.97
2	5	102	ARG	N-CA-C	-8.33	103.63	113.88
2	n	31	ALA	O-C-N	8.33	133.06	123.31
2	3	75	ASN	CA-C-N	8.32	131.77	120.54
2	3	75	ASN	C-N-CA	8.32	131.77	120.54
3	H	189	THR	CA-C-N	8.30	132.08	120.29
3	H	189	THR	C-N-CA	8.30	132.08	120.29
1	G	208	ASN	CA-CB-CG	8.30	120.90	112.60
3	J	202	THR	CA-C-O	-8.30	112.28	121.58
1	d	129	VAL	N-CA-C	-8.29	96.44	107.88
3	J	124	ASP	O-C-N	-8.29	111.79	121.32
3	K	56	GLU	CA-C-N	8.28	132.21	120.28
3	K	56	GLU	C-N-CA	8.28	132.21	120.28
2	2	66	LEU	CA-C-N	8.28	131.37	120.28
2	2	66	LEU	C-N-CA	8.28	131.37	120.28
3	K	386	THR	N-CA-C	-8.27	103.00	113.43
1	c	124	THR	CA-C-O	8.27	129.55	119.79
2	3	79	ILE	CA-C-O	-8.27	112.08	120.85
1	e	152	PRO	N-CA-C	-8.26	103.87	114.03
1	B	144	VAL	CA-C-N	8.25	128.01	119.76
1	B	144	VAL	C-N-CA	8.25	128.01	119.76
2	l	44	LYS	N-CA-C	-8.25	101.69	112.41
2	3	108	VAL	CA-C-O	8.25	127.89	120.96
1	E	169	ASN	CA-C-N	8.24	131.32	120.28
1	E	169	ASN	C-N-CA	8.24	131.32	120.28
1	e	191	LEU	CA-C-N	8.24	129.12	119.98
1	e	191	LEU	C-N-CA	8.24	129.12	119.98
1	A	221	PHE	CA-CB-CG	-8.23	105.57	113.80
2	l	38	ALA	N-CA-C	-8.23	104.38	114.75
3	H	92	SER	N-CA-C	8.23	115.53	108.78
3	I	253	SER	CA-C-O	-8.23	111.48	121.36
1	D	205	VAL	N-CA-C	-8.23	97.82	107.61
3	K	97	GLU	CA-C-N	8.23	131.13	120.44
3	K	97	GLU	C-N-CA	8.23	131.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	136	ASP	CA-C-N	8.22	136.76	121.97
2	h	136	ASP	C-N-CA	8.22	136.76	121.97
2	4	80	ARG	CA-C-O	-8.21	112.24	120.70
3	K	12	LYS	N-CA-C	8.21	120.01	111.14
3	L	94	TYR	N-CA-C	-8.21	103.72	114.31
1	C	46	VAL	N-CA-C	-8.20	97.03	108.27
3	I	57	ARG	NE-CZ-NH1	8.19	129.69	121.50
1	D	65	GLU	N-CA-CB	8.19	124.43	110.50
3	J	395	VAL	CA-C-N	8.19	131.60	120.38
3	J	395	VAL	C-N-CA	8.19	131.60	120.38
1	g	20	ARG	N-CA-C	-8.19	98.72	110.59
1	E	241	ARG	NE-CZ-NH2	8.17	126.55	119.20
1	c	71	ASP	N-CA-C	-8.16	97.46	108.24
2	3	123	TYR	O-C-N	-8.16	113.65	123.19
1	f	104	ASP	CA-CB-CG	-8.14	104.46	112.60
2	i	88	ARG	CA-C-N	8.14	131.84	120.29
2	i	88	ARG	C-N-CA	8.14	131.84	120.29
2	m	46	TYR	N-CA-C	-8.14	95.23	109.06
1	C	230	LYS	CA-C-N	8.13	127.42	118.97
1	C	230	LYS	C-N-CA	8.13	127.42	118.97
2	1	130	GLY	CA-C-N	8.13	134.23	122.77
2	1	130	GLY	C-N-CA	8.13	134.23	122.77
2	5	126	ASP	CA-CB-CG	-8.12	104.48	112.60
1	g	169	ASN	N-CA-C	8.12	119.76	111.07
3	L	183	PRO	N-CA-C	8.12	120.61	110.70
1	d	63	THR	N-CA-C	-8.12	104.52	114.75
3	I	158	GLU	CA-C-O	8.12	129.15	120.55
2	m	177	LYS	N-CA-C	-8.11	103.41	113.38
2	3	65	PHE	CA-CB-CG	-8.10	105.70	113.80
2	3	73	GLU	CA-C-N	8.10	131.79	120.29
2	3	73	GLU	C-N-CA	8.10	131.79	120.29
1	D	25	GLU	N-CA-C	-8.10	103.12	113.16
1	e	25	GLU	CA-C-N	8.09	132.60	120.31
1	e	25	GLU	C-N-CA	8.09	132.60	120.31
1	f	182	ASP	CA-CB-CG	-8.09	104.51	112.60
1	D	186	ASP	CA-CB-CG	8.08	120.68	112.60
2	6	70	ILE	CA-C-O	-8.08	112.55	120.95
1	a	80	GLY	N-CA-C	-8.07	103.41	111.56
3	K	289	ARG	NE-CZ-NH2	-8.07	111.94	119.20
2	i	77	TYR	N-CA-C	-8.07	102.43	111.14
2	h	140	THR	N-CA-CB	8.07	124.12	110.49
1	G	216	VAL	CA-C-O	-8.06	112.10	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	53	ARG	N-CA-C	-8.06	103.02	113.17
2	n	111	LEU	N-CA-C	-8.05	95.16	108.76
1	A	218	ASP	CA-CB-CG	-8.04	104.56	112.60
1	D	196	MET	CA-C-N	8.04	128.86	119.94
1	D	196	MET	C-N-CA	8.04	128.86	119.94
2	h	167	LEU	CA-C-N	8.03	130.87	120.44
2	h	167	LEU	C-N-CA	8.03	130.87	120.44
3	M	336	PHE	CA-C-N	8.03	131.03	120.28
3	M	336	PHE	C-N-CA	8.03	131.03	120.28
3	I	60	SER	CA-C-N	8.02	125.52	119.66
3	I	60	SER	C-N-CA	8.02	125.52	119.66
1	a	123	TYR	CA-C-O	8.02	129.37	119.11
1	A	100	ARG	NE-CZ-NH1	-8.02	113.48	121.50
2	i	72	ILE	N-CA-C	8.01	118.79	110.62
2	5	31	ALA	N-CA-CB	8.00	121.91	109.83
3	I	377	LYS	CA-C-N	8.00	131.00	120.28
3	I	377	LYS	C-N-CA	8.00	131.00	120.28
1	E	90	ASP	N-CA-CB	7.99	121.84	109.94
1	e	129	VAL	N-CA-C	-7.98	93.37	107.18
1	e	95	GLU	CA-C-N	7.98	130.81	120.44
1	e	95	GLU	C-N-CA	7.98	130.81	120.44
2	4	75	ASN	N-CA-C	-7.98	102.66	111.36
2	6	148	TYR	N-CA-CB	7.98	121.58	110.01
3	L	168	ALA	N-CA-C	7.98	119.98	111.28
3	I	61	PRO	O-C-N	-7.97	117.64	121.31
3	L	157	VAL	CB-CA-C	-7.96	104.94	111.71
3	J	43	ARG	N-CA-C	7.96	119.59	111.07
1	E	113	ALA	N-CA-C	-7.96	102.69	111.36
2	j	122	ILE	N-CA-CB	7.96	122.39	111.41
2	j	155	PHE	CA-CB-CG	-7.95	105.85	113.80
2	k	31	ALA	O-C-N	7.95	132.76	123.30
1	f	42	CYS	N-CA-C	-7.94	97.31	109.14
2	h	156	THR	CA-C-N	7.93	127.57	119.56
2	h	156	THR	C-N-CA	7.93	127.57	119.56
2	2	210	LYS	N-CA-C	-7.93	103.82	113.97
1	a	198	LEU	CA-C-N	7.93	131.24	120.54
1	a	198	LEU	C-N-CA	7.93	131.24	120.54
1	f	231	PRO	CA-C-N	7.93	132.36	120.31
1	f	231	PRO	C-N-CA	7.93	132.36	120.31
3	M	14	LYS	CA-C-N	7.93	130.75	120.44
3	M	14	LYS	C-N-CA	7.93	130.75	120.44
3	H	42	ILE	O-C-N	-7.92	114.19	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	22	PHE	CA-C-N	7.92	131.53	120.29
1	b	22	PHE	C-N-CA	7.92	131.53	120.29
3	L	295	PRO	N-CA-CB	7.91	111.94	103.39
2	7	146	THR	CA-C-N	7.91	130.88	120.28
2	7	146	THR	C-N-CA	7.91	130.88	120.28
1	g	196	MET	CA-C-N	7.91	128.92	119.99
1	g	196	MET	C-N-CA	7.91	128.92	119.99
1	B	31	VAL	CA-C-N	7.91	133.92	120.72
1	B	31	VAL	C-N-CA	7.91	133.92	120.72
2	j	157	PRO	N-CA-C	-7.90	103.60	114.27
1	b	218	ASP	N-CA-C	-7.90	103.48	113.43
1	E	42	CYS	N-CA-C	-7.89	97.73	108.86
3	H	335	ASP	CA-C-N	7.89	132.31	120.31
3	H	335	ASP	C-N-CA	7.89	132.31	120.31
3	M	328	MET	N-CA-C	7.89	120.76	110.43
3	J	10	LEU	CA-C-N	7.88	130.84	120.28
3	J	10	LEU	C-N-CA	7.88	130.84	120.28
1	C	8	TYR	N-CA-C	-7.88	103.23	112.92
1	d	152	PRO	CA-C-N	7.87	131.47	120.29
1	d	152	PRO	C-N-CA	7.87	131.47	120.29
2	l	170	ARG	NE-CZ-NH1	7.87	129.37	121.50
2	h	67	ALA	N-CA-C	7.87	119.86	111.28
3	M	384	LYS	CA-C-O	7.87	129.10	120.92
1	c	132	PHE	CA-CB-CG	-7.87	105.94	113.80
1	D	64	ILE	CA-C-N	7.86	135.85	121.70
1	D	64	ILE	C-N-CA	7.86	135.85	121.70
2	j	147	ALA	N-CA-C	7.86	119.92	111.36
3	M	27	TYR	CA-C-N	7.86	130.66	120.44
3	M	27	TYR	C-N-CA	7.86	130.66	120.44
3	M	223	VAL	CA-C-N	7.86	130.81	120.28
3	M	223	VAL	C-N-CA	7.86	130.81	120.28
3	I	84	GLY	CA-C-N	7.85	127.91	119.90
3	I	84	GLY	C-N-CA	7.85	127.91	119.90
1	A	94	ILE	N-CA-C	-7.85	102.79	110.72
2	1	169	VAL	O-C-N	-7.85	114.26	121.87
1	A	151	ASP	CA-C-N	7.84	127.50	119.19
1	A	151	ASP	C-N-CA	7.84	127.50	119.19
1	A	194	VAL	O-C-N	7.84	129.60	121.91
1	g	144	VAL	O-C-N	-7.84	114.35	121.41
2	i	198	GLN	CA-C-N	7.84	131.42	120.29
2	i	198	GLN	C-N-CA	7.84	131.42	120.29
1	c	169	ASN	O-C-N	7.83	131.08	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	227	PHE	CA-CB-CG	-7.83	105.97	113.80
1	C	205	VAL	O-C-N	-7.83	116.24	121.72
2	2	45	ILE	N-CA-C	-7.83	96.32	107.75
3	J	41	ARG	NE-CZ-NH1	-7.83	113.67	121.50
2	3	49	ALA	N-CA-C	-7.82	98.43	109.69
2	3	170	ARG	CD-NE-CZ	-7.82	113.45	124.40
1	g	239	ARG	CA-C-N	7.82	130.41	120.56
1	g	239	ARG	C-N-CA	7.82	130.41	120.56
2	n	116	ASP	N-CA-C	-7.82	97.83	108.38
3	I	323	ILE	N-CA-C	-7.82	102.83	110.72
2	6	98	LEU	N-CA-C	7.81	120.70	111.71
3	L	212	VAL	N-CA-CB	7.81	124.12	111.23
3	L	386	THR	N-CA-C	-7.81	103.77	113.38
2	k	83	ARG	CA-C-N	7.81	131.24	120.39
2	k	83	ARG	C-N-CA	7.81	131.24	120.39
3	K	73	GLU	N-CA-C	-7.81	103.33	113.17
1	E	28	ARG	NE-CZ-NH2	-7.80	112.18	119.20
3	L	174	PRO	CA-C-N	7.80	128.27	119.92
3	L	174	PRO	C-N-CA	7.80	128.27	119.92
1	f	70	ILE	N-CA-C	-7.80	105.10	111.81
2	l	166	GLU	CA-C-N	7.79	131.35	120.29
2	l	166	GLU	C-N-CA	7.79	131.35	120.29
3	L	313	THR	CA-C-N	7.79	131.06	120.54
3	L	313	THR	C-N-CA	7.79	131.06	120.54
2	n	182	SER	N-CA-C	-7.79	103.60	113.72
3	J	281	VAL	CA-C-N	7.78	135.71	121.70
3	J	281	VAL	C-N-CA	7.78	135.71	121.70
3	L	323	ILE	CA-C-N	7.78	132.14	120.31
3	L	323	ILE	C-N-CA	7.78	132.14	120.31
1	f	234	GLU	CA-C-N	7.78	130.70	120.28
1	f	234	GLU	C-N-CA	7.78	130.70	120.28
2	1	78	GLU	O-C-N	-7.77	113.88	122.12
1	g	85	ALA	N-CA-CB	7.76	121.53	110.12
1	b	54	VAL	N-CA-C	-7.76	98.11	108.35
1	d	49	ILE	CB-CA-C	7.76	124.60	110.71
3	K	45	GLU	CA-C-N	7.76	130.68	120.28
3	K	45	GLU	C-N-CA	7.76	130.68	120.28
1	C	191	LEU	CA-C-N	7.76	128.53	120.00
1	C	191	LEU	C-N-CA	7.76	128.53	120.00
3	M	24	ARG	CA-C-N	7.76	130.68	120.28
3	M	24	ARG	C-N-CA	7.76	130.68	120.28
1	f	105	GLU	N-CA-C	-7.75	96.20	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	139	ALA	N-CA-C	-7.75	96.48	108.42
1	c	91	ARG	CA-C-N	7.75	130.52	120.44
1	c	91	ARG	C-N-CA	7.75	130.52	120.44
2	5	57	ALA	CA-C-O	-7.75	111.74	120.66
3	I	147	ASP	CA-C-N	7.75	131.08	120.46
3	I	147	ASP	C-N-CA	7.75	131.08	120.46
1	E	28	ARG	N-CA-C	-7.75	102.47	112.23
1	E	244	LEU	CA-C-N	7.75	133.94	122.08
1	E	244	LEU	C-N-CA	7.75	133.94	122.08
2	h	159	ILE	CA-C-O	-7.74	112.10	121.54
2	i	88	ARG	CB-CA-C	-7.73	97.95	110.79
1	d	226	PRO	CA-C-N	7.73	130.64	120.28
1	d	226	PRO	C-N-CA	7.73	130.64	120.28
3	H	96	ASN	CA-CB-CG	-7.73	104.87	112.60
3	M	134	GLU	CB-CG-CD	-7.72	99.47	112.60
3	K	337	LYS	CA-C-O	7.72	128.61	120.42
2	3	128	ILE	N-CA-C	-7.72	104.84	112.17
2	n	62	ASP	CA-CB-CG	-7.71	104.89	112.60
1	a	170	ALA	O-C-N	7.70	130.41	122.09
1	G	46	VAL	N-CA-C	-7.70	96.33	108.81
2	2	114	GLY	CA-C-O	-7.70	114.12	121.05
3	M	77	VAL	N-CA-C	-7.70	97.39	108.48
1	B	179	TYR	CB-CG-CD2	-7.70	109.25	120.80
2	2	116	ASP	CA-CB-CG	7.70	120.30	112.60
3	L	394	GLY	CA-C-N	7.70	135.56	121.70
3	L	394	GLY	C-N-CA	7.70	135.56	121.70
3	M	74	ASP	N-CA-C	-7.70	102.40	112.41
2	l	189	VAL	N-CA-C	-7.70	96.34	108.81
1	G	86	ARG	NE-CZ-NH2	7.70	126.12	119.20
3	I	23	LEU	CA-C-N	7.69	130.44	120.44
3	I	23	LEU	C-N-CA	7.69	130.44	120.44
1	c	22	PHE	N-CA-CB	7.69	121.43	110.12
2	j	140	THR	N-CA-C	-7.69	96.09	108.55
2	5	36	PHE	CA-CB-CG	-7.69	106.11	113.80
2	5	199	TYR	N-CA-C	7.68	119.65	111.28
1	d	39	GLY	CA-C-O	-7.68	114.95	120.94
1	G	196	MET	CA-C-N	7.68	128.67	119.99
1	G	196	MET	C-N-CA	7.68	128.67	119.99
1	a	28	ARG	N-CA-CB	7.68	121.52	110.16
2	1	59	SER	CA-C-N	7.67	130.08	120.72
2	1	59	SER	C-N-CA	7.67	130.08	120.72
1	d	194	VAL	CA-C-N	7.67	130.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	194	VAL	C-N-CA	7.67	130.56	120.28
1	g	185	PHE	N-CA-C	-7.66	102.87	111.14
2	6	105	PRO	CA-C-O	-7.66	112.29	121.48
2	h	146	THR	CA-C-N	7.66	130.54	120.28
2	h	146	THR	C-N-CA	7.66	130.54	120.28
2	6	107	LEU	N-CA-C	-7.66	96.79	108.96
3	I	128	TYR	N-CA-CB	7.65	121.53	110.06
1	B	87	VAL	CA-C-N	7.65	130.53	120.28
1	B	87	VAL	C-N-CA	7.65	130.53	120.28
2	6	147	ALA	CA-C-N	7.65	130.38	120.44
2	6	147	ALA	C-N-CA	7.65	130.38	120.44
3	M	120	PRO	CA-C-N	7.65	136.15	121.54
3	M	120	PRO	C-N-CA	7.65	136.15	121.54
1	b	81	LEU	CA-C-O	7.65	128.76	120.43
2	n	85	PRO	CB-CA-C	7.64	120.05	111.11
3	H	99	GLU	N-CA-C	-7.64	103.55	113.17
1	G	194	VAL	CA-C-N	7.63	131.12	120.29
1	G	194	VAL	C-N-CA	7.63	131.12	120.29
2	i	124	SER	N-CA-C	-7.62	96.47	108.90
3	I	256	SER	N-CA-C	7.62	119.59	111.28
1	b	200	ILE	CA-C-N	7.62	133.56	122.36
1	b	200	ILE	C-N-CA	7.62	133.56	122.36
2	4	144	SER	N-CA-C	7.61	120.46	111.71
2	k	139	ALA	CA-C-N	7.61	135.40	121.70
2	k	139	ALA	C-N-CA	7.61	135.40	121.70
2	6	17	LEU	CA-C-O	7.61	129.90	120.54
2	4	140	THR	N-CA-CB	7.60	123.34	110.49
1	A	180	ARG	NE-CZ-NH2	7.59	126.04	119.20
1	g	135	SER	N-CA-C	-7.59	97.50	109.50
3	J	119	LEU	CA-C-O	-7.59	111.32	120.05
3	J	195	VAL	CA-C-O	-7.59	113.05	120.95
2	j	114	GLY	N-CA-C	-7.58	100.67	110.38
2	7	174	SER	CA-C-O	7.58	128.59	120.55
1	F	63	THR	CA-C-N	7.58	135.61	121.97
1	F	63	THR	C-N-CA	7.58	135.61	121.97
3	I	117	ASN	CA-CB-CG	7.58	120.18	112.60
2	j	47	GLN	CA-C-N	7.57	130.25	120.56
2	j	47	GLN	C-N-CA	7.57	130.25	120.56
1	A	208	ASN	N-CA-C	-7.57	101.15	110.61
1	c	207	GLU	N-CA-CB	7.57	121.61	110.56
2	l	171	ALA	O-C-N	7.57	129.86	122.07
1	A	188	ALA	N-CA-C	7.56	119.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	294	ASP	CA-C-N	7.56	128.00	119.83
3	H	294	ASP	C-N-CA	7.56	128.00	119.83
2	i	150	VAL	CA-C-N	7.56	130.27	120.44
2	i	150	VAL	C-N-CA	7.56	130.27	120.44
2	i	66	LEU	O-C-N	7.56	130.13	122.12
3	M	217	GLY	CA-C-N	7.56	131.16	120.28
3	M	217	GLY	C-N-CA	7.56	131.16	120.28
1	D	207	GLU	CA-C-O	-7.55	110.14	119.28
1	d	57	LYS	CA-C-N	7.55	130.71	120.44
1	d	57	LYS	C-N-CA	7.55	130.71	120.44
3	L	302	ARG	N-CA-C	-7.55	104.97	114.56
3	L	357	GLU	CA-C-N	7.55	130.39	120.28
3	L	357	GLU	C-N-CA	7.55	130.39	120.28
2	4	157	PRO	CA-C-N	7.54	134.44	122.83
2	4	157	PRO	C-N-CA	7.54	134.44	122.83
1	d	147	LEU	N-CA-C	-7.54	95.34	108.69
1	D	122	GLN	N-CA-C	-7.54	103.00	111.07
2	i	156	THR	N-CA-C	-7.54	96.80	108.55
2	h	60	VAL	CA-C-N	7.53	128.15	119.94
2	h	60	VAL	C-N-CA	7.53	128.15	119.94
2	7	77	TYR	CA-C-O	-7.53	112.43	120.42
1	D	102	THR	CA-C-O	7.53	127.33	119.05
1	D	237	ASN	N-CA-C	7.53	119.49	111.28
3	K	264	THR	N-CA-C	-7.53	104.62	113.88
1	a	25	GLU	CA-C-N	7.53	130.36	120.28
1	a	25	GLU	C-N-CA	7.53	130.36	120.28
1	G	113	ALA	CA-C-N	7.52	131.74	120.31
1	G	113	ALA	C-N-CA	7.52	131.74	120.31
2	l	200	SER	CA-C-N	7.52	127.89	119.32
2	l	200	SER	C-N-CA	7.52	127.89	119.32
1	A	24	VAL	N-CA-C	-7.52	103.13	110.72
1	d	15	PHE	CA-CB-CG	-7.51	106.28	113.80
1	G	109	VAL	CA-C-N	7.51	130.35	120.28
1	G	109	VAL	C-N-CA	7.51	130.35	120.28
3	I	334	VAL	O-C-N	7.51	131.15	122.81
2	n	186	ILE	N-CA-C	-7.51	97.27	108.46
2	k	137	ILE	N-CA-C	-7.51	97.34	108.45
1	A	67	ILE	N-CA-CB	7.50	123.61	111.23
2	5	68	ARG	CA-C-O	-7.50	112.47	120.42
1	c	237	ASN	N-CA-C	7.50	119.45	111.28
2	i	104	PHE	CA-C-O	-7.49	114.30	121.34
3	I	300	PRO	N-CA-CB	7.49	110.31	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	170	VAL	O-C-N	-7.49	114.57	121.91
3	L	309	VAL	N-CA-C	-7.49	99.59	107.60
1	E	31	VAL	CA-C-O	-7.49	113.16	120.95
1	B	160	LYS	N-CA-C	-7.49	102.38	113.61
2	l	174	SER	CB-CA-C	-7.48	98.13	110.85
1	f	208	ASN	CA-CB-CG	7.48	120.08	112.60
2	n	211	PHE	CA-CB-CG	7.47	121.27	113.80
1	E	28	ARG	N-CA-CB	7.47	121.81	110.30
1	b	228	GLU	N-CA-C	-7.46	103.75	114.12
1	G	200	ILE	N-CA-C	-7.46	105.74	112.90
1	e	96	ALA	CA-C-N	7.46	130.27	120.28
1	e	96	ALA	C-N-CA	7.46	130.27	120.28
1	G	62	ASP	CA-C-N	7.45	131.32	120.82
1	G	62	ASP	C-N-CA	7.45	131.32	120.82
3	M	38	GLU	N-CA-C	7.45	119.04	111.07
2	n	139	ALA	CA-C-N	7.44	135.10	121.70
2	n	139	ALA	C-N-CA	7.44	135.10	121.70
2	h	146	THR	CA-CB-OG1	7.44	120.76	109.60
2	4	145	LEU	N-CA-C	-7.44	103.17	111.28
1	C	218	ASP	N-CA-C	-7.44	104.73	113.88
2	n	164	ALA	N-CA-C	7.44	119.47	111.36
1	a	200	ILE	O-C-N	-7.44	114.93	122.14
1	D	36	THR	N-CA-C	7.44	121.17	110.24
1	G	62	ASP	CA-CB-CG	-7.44	105.16	112.60
1	c	181	ASP	N-CA-C	-7.43	103.16	112.90
1	f	173	GLU	CA-C-N	7.43	130.23	120.28
1	f	173	GLU	C-N-CA	7.43	130.23	120.28
3	I	288	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	E	132	PHE	N-CA-CB	7.43	120.86	110.17
1	G	91	ARG	CA-C-N	7.42	130.23	120.28
1	G	91	ARG	C-N-CA	7.42	130.23	120.28
2	6	144	SER	N-CA-C	7.42	120.31	111.33
1	F	83	ALA	CA-C-N	7.42	130.22	120.28
1	F	83	ALA	C-N-CA	7.42	130.22	120.28
2	2	155	PHE	CA-CB-CG	7.42	121.22	113.80
1	b	132	PHE	CA-CB-CG	-7.42	106.38	113.80
1	d	100	ARG	N-CA-C	7.42	119.36	111.28
1	g	80	GLY	N-CA-C	-7.41	100.45	110.97
2	5	178	ARG	N-CA-C	-7.41	102.22	112.30
1	a	230	LYS	CA-C-O	-7.41	111.81	118.63
1	c	143	GLU	N-CA-C	-7.40	104.40	113.50
3	J	65	VAL	N-CA-CB	7.40	118.78	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	139	ALA	CA-C-N	7.39	135.01	121.70
2	3	139	ALA	C-N-CA	7.39	135.01	121.70
1	f	210	GLU	N-CA-C	-7.39	96.49	109.06
2	4	79	ILE	N-CA-C	7.39	117.52	110.42
1	a	151	ASP	CA-C-N	7.39	128.32	120.12
1	a	151	ASP	C-N-CA	7.39	128.32	120.12
1	a	205	VAL	N-CA-C	-7.38	99.60	108.45
3	L	333	ASP	CA-C-N	7.38	135.25	121.97
3	L	333	ASP	C-N-CA	7.38	135.25	121.97
3	K	365	GLU	CA-C-N	7.37	132.58	122.34
3	K	365	GLU	C-N-CA	7.37	132.58	122.34
3	M	281	VAL	CA-C-O	7.37	128.59	120.48
2	6	17	LEU	O-C-N	-7.37	114.79	123.41
3	J	257	GLY	CA-C-N	7.36	134.96	121.70
3	J	257	GLY	C-N-CA	7.36	134.96	121.70
2	5	170	ARG	NH1-CZ-NH2	7.36	128.87	119.30
3	J	288	ASN	CA-CB-CG	7.36	119.96	112.60
2	n	173	TYR	CA-C-N	7.36	130.14	120.28
2	n	173	TYR	C-N-CA	7.36	130.14	120.28
2	j	144	SER	N-CA-C	7.36	120.23	111.33
1	A	66	LYS	O-C-N	-7.36	114.24	122.55
3	H	205	ARG	NE-CZ-NH1	-7.35	114.15	121.50
3	K	74	ASP	CA-CB-CG	-7.35	105.25	112.60
2	6	148	TYR	N-CA-C	-7.35	103.21	111.07
1	f	108	THR	CA-C-O	-7.34	113.02	121.47
3	H	130	PHE	CA-CB-CG	-7.34	106.46	113.80
1	c	71	ASP	CA-CB-CG	7.34	119.94	112.60
1	b	199	SER	N-CA-CB	7.33	120.64	110.01
3	K	81	SER	N-CA-CB	7.33	121.44	110.29
1	A	80	GLY	N-CA-C	-7.33	101.26	112.84
3	J	119	LEU	CA-C-N	7.33	127.78	119.93
3	J	119	LEU	C-N-CA	7.33	127.78	119.93
1	e	192	GLY	CA-C-N	7.33	130.70	120.29
1	e	192	GLY	C-N-CA	7.33	130.70	120.29
1	E	93	ARG	NE-CZ-NH2	-7.33	112.61	119.20
3	K	149	GLN	CA-C-N	7.33	129.79	120.56
3	K	149	GLN	C-N-CA	7.33	129.79	120.56
3	H	230	ALA	CA-C-N	7.32	130.09	120.28
3	H	230	ALA	C-N-CA	7.32	130.09	120.28
1	a	217	ASP	CA-C-O	7.32	127.50	119.15
1	G	53	ARG	CA-C-N	7.32	130.59	120.49
1	G	53	ARG	C-N-CA	7.32	130.59	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	43	ARG	CA-C-N	7.31	130.08	120.28
3	J	43	ARG	C-N-CA	7.31	130.08	120.28
1	G	22	PHE	CA-CB-CG	-7.31	106.49	113.80
2	h	40	LYS	CB-CA-C	-7.31	97.73	109.13
2	i	63	ALA	CA-C-N	7.30	130.66	120.29
2	i	63	ALA	C-N-CA	7.30	130.66	120.29
3	K	222	LEU	CA-C-N	7.30	129.76	120.56
3	K	222	LEU	C-N-CA	7.30	129.76	120.56
1	C	214	VAL	O-C-N	-7.30	115.95	123.03
2	j	204	VAL	CA-C-N	7.30	131.03	120.38
2	j	204	VAL	C-N-CA	7.30	131.03	120.38
1	G	86	ARG	NE-CZ-NH1	-7.29	114.21	121.50
2	3	112	ILE	N-CA-C	-7.29	97.10	107.75
1	B	73	HIS	CE1-NE2-CD2	-7.29	101.71	109.00
1	C	109	VAL	CA-C-N	7.29	129.92	120.44
1	C	109	VAL	C-N-CA	7.29	129.92	120.44
1	G	212	GLY	N-CA-C	-7.29	100.50	111.14
2	j	143	GLY	CA-C-N	7.29	130.36	120.38
2	j	143	GLY	C-N-CA	7.29	130.36	120.38
1	a	245	LYS	N-CA-C	-7.28	104.92	113.88
2	3	32	THR	O-C-N	7.28	131.88	123.29
1	c	160	LYS	N-CA-C	-7.28	102.52	111.40
1	a	212	GLY	N-CA-C	-7.28	99.97	111.18
3	H	236	SER	CA-C-N	7.28	135.07	121.97
3	H	236	SER	C-N-CA	7.28	135.07	121.97
1	a	130	ARG	N-CA-C	-7.28	100.00	110.40
1	A	168	ARG	CA-C-O	-7.27	113.12	120.90
2	5	87	VAL	CA-C-N	7.27	130.03	120.28
2	5	87	VAL	C-N-CA	7.27	130.03	120.28
1	d	181	ASP	N-CA-C	-7.27	104.15	113.16
2	1	128	ILE	CA-C-O	7.26	126.97	119.35
2	5	153	ASP	CA-C-O	-7.26	112.73	120.42
2	k	76	LEU	CA-C-N	7.25	129.87	120.44
2	k	76	LEU	C-N-CA	7.25	129.87	120.44
2	l	69	ILE	CA-C-O	-7.25	113.41	120.95
1	D	169	ASN	OD1-CG-ND2	-7.25	115.35	122.60
2	6	45	ILE	N-CA-C	-7.25	98.78	108.35
3	L	292	ILE	N-CA-C	-7.25	105.65	112.83
1	a	21	LEU	CA-C-N	7.25	130.00	120.28
1	a	21	LEU	C-N-CA	7.25	130.00	120.28
3	M	142	ASP	CA-CB-CG	-7.25	105.35	112.60
2	5	25	MET	N-CA-CB	7.25	123.77	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	VAL	CA-C-O	-7.25	110.24	119.95
1	e	18	ASP	CA-CB-CG	7.25	119.85	112.60
1	G	15	PHE	CA-CB-CG	-7.25	106.55	113.80
2	i	165	VAL	CA-C-N	7.25	130.58	120.29
2	i	165	VAL	C-N-CA	7.25	130.58	120.29
3	J	234	ALA	O-C-N	-7.25	114.24	121.27
2	1	172	ILE	CA-C-N	7.24	130.58	120.29
2	1	172	ILE	C-N-CA	7.24	130.58	120.29
3	I	338	GLU	CA-C-N	7.24	129.86	120.44
3	I	338	GLU	C-N-CA	7.24	129.86	120.44
2	h	51	ARG	NE-CZ-NH2	7.24	125.72	119.20
3	M	347	SER	CA-C-N	7.24	129.19	120.14
3	M	347	SER	C-N-CA	7.24	129.19	120.14
1	E	19	GLY	N-CA-C	-7.24	104.74	114.95
1	G	94	ILE	N-CA-C	-7.24	103.41	110.72
2	5	184	ASP	CA-CB-CG	-7.24	105.36	112.60
3	L	288	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	4	108	VAL	CB-CA-C	7.23	121.85	111.80
2	5	112	ILE	N-CA-CB	7.22	121.03	111.64
2	4	128	ILE	N-CA-C	-7.22	104.23	111.88
2	1	160	GLY	CA-C-N	7.22	130.67	120.42
2	1	160	GLY	C-N-CA	7.22	130.67	120.42
2	7	143	GLY	CA-C-N	7.22	129.95	120.28
2	7	143	GLY	C-N-CA	7.22	129.95	120.28
1	e	90	ASP	N-CA-CB	7.21	120.72	110.12
3	J	301	GLY	CA-C-N	7.21	133.25	121.99
3	J	301	GLY	C-N-CA	7.21	133.25	121.99
1	A	97	GLN	CA-C-N	7.21	131.87	120.47
1	A	97	GLN	C-N-CA	7.21	131.87	120.47
2	4	102	ARG	NE-CZ-NH2	7.21	125.69	119.20
3	L	54	GLU	CA-C-N	7.21	130.33	120.46
3	L	54	GLU	C-N-CA	7.21	130.33	120.46
2	1	156	THR	CA-C-O	-7.20	112.32	120.46
1	b	125	GLN	CA-C-N	7.20	132.24	120.94
1	b	125	GLN	C-N-CA	7.20	132.24	120.94
2	5	142	SER	N-CA-C	-7.19	106.42	114.62
2	4	61	GLY	CA-C-N	7.19	129.79	120.44
2	4	61	GLY	C-N-CA	7.19	129.79	120.44
1	B	182	ASP	CA-C-N	7.19	131.70	121.42
1	B	182	ASP	C-N-CA	7.19	131.70	121.42
3	H	321	PHE	CA-C-N	7.19	130.24	120.54
3	H	321	PHE	C-N-CA	7.19	130.24	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	25	GLU	CB-CG-CD	-7.18	100.39	112.60
1	g	70	ILE	CB-CA-C	-7.18	104.74	111.06
3	J	295	PRO	N-CA-C	-7.18	104.88	113.86
2	1	41	ALA	N-CA-C	-7.18	102.96	114.09
3	I	27	TYR	CA-C-N	7.18	129.77	120.44
3	I	27	TYR	C-N-CA	7.18	129.77	120.44
3	I	358	ALA	CA-C-O	7.18	128.16	120.55
1	A	180	ARG	O-C-N	-7.18	115.07	123.25
2	6	60	VAL	N-CA-C	7.17	117.30	110.42
3	J	389	ILE	CA-C-N	7.17	127.78	120.04
3	J	389	ILE	C-N-CA	7.17	127.78	120.04
1	B	53	ARG	N-CA-C	-7.17	104.14	113.17
1	B	241	ARG	CA-C-N	7.17	129.88	120.28
1	B	241	ARG	C-N-CA	7.17	129.88	120.28
1	c	30	ALA	CA-C-N	7.17	132.59	121.34
1	c	30	ALA	C-N-CA	7.17	132.59	121.34
2	6	156	THR	CA-C-N	7.17	127.01	119.05
2	6	156	THR	C-N-CA	7.17	127.01	119.05
3	K	199	THR	CA-C-N	7.17	135.23	121.54
3	K	199	THR	C-N-CA	7.17	135.23	121.54
3	K	27	TYR	CA-C-N	7.16	129.75	120.44
3	K	27	TYR	C-N-CA	7.16	129.75	120.44
2	4	178	ARG	O-C-N	7.16	129.57	122.19
1	b	78	THR	CA-C-O	7.16	130.22	121.56
1	a	57	LYS	CA-C-N	7.15	129.74	120.44
1	a	57	LYS	C-N-CA	7.15	129.74	120.44
1	E	207	GLU	CB-CG-CD	-7.15	100.44	112.60
1	G	206	PRO	N-CA-C	-7.15	105.53	114.68
3	M	259	ARG	N-CA-CB	7.15	120.63	110.12
2	6	199	TYR	N-CA-C	7.15	118.72	111.07
3	K	376	THR	CA-C-O	-7.15	111.75	119.97
3	I	211	PHE	N-CA-C	-7.15	101.31	110.53
1	A	182	ASP	N-CA-C	-7.14	101.75	112.54
2	k	112	ILE	N-CA-C	-7.14	98.11	108.11
2	2	195	GLU	CA-C-O	-7.14	113.62	121.33
2	4	64	GLN	OE1-CD-NE2	-7.14	115.46	122.60
2	m	21	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	90	ASP	CA-CB-CG	-7.13	105.47	112.60
2	n	51	ARG	NE-CZ-NH1	-7.13	114.36	121.50
2	k	180	SER	N-CA-C	-7.13	103.68	112.88
1	g	160	LYS	N-CA-CB	7.13	120.41	110.07
1	e	232	TYR	CA-C-N	7.13	130.23	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	232	TYR	C-N-CA	7.13	130.23	120.46
2	h	170	ARG	NE-CZ-NH2	7.13	125.61	119.20
2	3	196	PHE	CA-CB-CG	-7.13	106.67	113.80
3	K	144	GLY	O-C-N	-7.13	115.40	123.67
1	b	18	ASP	N-CA-C	-7.13	105.11	113.88
1	C	20	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	A	142	ASP	CA-CB-CG	7.12	119.72	112.60
1	b	222	LYS	N-CA-C	-7.12	98.19	109.23
1	e	169	ASN	N-CA-C	7.12	119.65	111.11
3	L	219	GLY	CA-C-O	-7.12	113.82	120.80
1	B	151	ASP	CA-C-N	7.12	127.73	119.47
1	B	151	ASP	C-N-CA	7.12	127.73	119.47
3	K	217	GLY	CA-C-O	-7.12	111.12	119.02
2	j	81	ARG	N-CA-C	-7.11	104.87	113.97
2	7	73	GLU	CA-C-N	7.11	130.38	120.29
2	7	73	GLU	C-N-CA	7.11	130.38	120.29
3	J	324	HIS	CG-CD2-NE2	7.11	114.31	107.20
1	A	117	CYS	N-CA-CB	7.10	121.16	110.22
1	F	90	ASP	CA-C-N	7.10	129.80	120.28
1	F	90	ASP	C-N-CA	7.10	129.80	120.28
3	K	264	THR	CA-C-N	7.10	129.67	120.44
3	K	264	THR	C-N-CA	7.10	129.67	120.44
3	M	127	VAL	N-CA-CB	7.10	119.64	110.13
1	a	213	TYR	CB-CG-CD2	7.10	131.45	120.80
3	K	116	VAL	N-CA-C	-7.10	106.58	113.53
3	J	390	PRO	N-CA-C	-7.10	104.69	114.27
2	3	145	LEU	CA-C-N	7.09	129.79	120.28
2	3	145	LEU	C-N-CA	7.09	129.79	120.28
3	J	23	LEU	N-CA-C	7.09	119.01	111.28
2	4	51	ARG	NE-CZ-NH1	-7.09	114.41	121.50
2	7	196	PHE	N-CA-C	-7.09	92.88	107.70
3	K	350	ASP	CA-CB-CG	-7.09	105.51	112.60
2	5	157	PRO	N-CA-C	-7.09	106.49	114.92
2	4	124	SER	N-CA-C	-7.08	98.14	109.76
1	d	84	ASP	CA-C-N	7.08	130.09	120.54
1	d	84	ASP	C-N-CA	7.08	130.09	120.54
3	I	59	ARG	N-CA-C	-7.08	104.52	113.01
2	5	126	ASP	N-CA-C	-7.08	97.93	109.82
1	a	128	GLY	N-CA-C	-7.07	104.63	115.66
1	f	84	ASP	CA-C-N	7.07	129.64	120.44
1	f	84	ASP	C-N-CA	7.07	129.64	120.44
2	7	168	ALA	CA-C-N	7.07	130.46	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	168	ALA	C-N-CA	7.07	130.46	120.42
3	J	391	ASP	O-C-N	-7.07	114.97	122.96
1	e	181	ASP	CA-CB-CG	-7.07	105.53	112.60
2	5	124	SER	O-C-N	-7.07	114.95	123.29
3	H	146	LEU	CA-C-N	7.07	134.42	121.70
3	H	146	LEU	C-N-CA	7.07	134.42	121.70
2	4	209	ALA	N-CA-C	-7.06	103.97	112.59
1	E	188	ALA	CA-C-N	7.06	130.32	120.29
1	E	188	ALA	C-N-CA	7.06	130.32	120.29
2	5	58	GLY	CA-C-O	-7.06	115.26	122.25
2	7	147	ALA	N-CA-CB	7.05	120.49	110.12
3	I	245	ALA	N-CA-C	-7.05	103.85	113.30
1	e	235	ARG	CA-C-N	7.05	129.60	120.44
1	e	235	ARG	C-N-CA	7.05	129.60	120.44
3	K	331	ALA	N-CA-CB	7.05	121.70	110.85
1	E	100	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	e	174	PHE	CA-CB-CG	7.04	120.84	113.80
1	f	232	TYR	O-C-N	7.04	130.93	122.27
2	n	65	PHE	CA-C-N	7.03	130.28	120.29
2	n	65	PHE	C-N-CA	7.03	130.28	120.29
2	n	201	PRO	CA-C-N	7.03	130.04	120.54
2	n	201	PRO	C-N-CA	7.03	130.04	120.54
3	K	358	ALA	CA-C-N	7.03	127.79	119.98
3	K	358	ALA	C-N-CA	7.03	127.79	119.98
1	B	113	ALA	O-C-N	-7.03	114.14	122.15
3	K	77	VAL	N-CA-C	-7.03	97.99	108.46
1	c	93	ARG	N-CA-CB	7.03	120.20	110.01
1	g	171	VAL	CA-C-N	7.03	129.70	120.28
1	g	171	VAL	C-N-CA	7.03	129.70	120.28
3	L	299	ARG	N-CA-C	7.03	119.61	109.84
1	c	83	ALA	CA-C-O	7.03	128.20	120.82
2	3	35	ASN	N-CA-C	-7.03	105.64	114.56
2	4	113	GLY	CA-C-O	7.03	129.08	121.56
2	1	23	VAL	N-CA-C	-7.02	98.06	108.45
1	g	119	PHE	N-CA-C	7.02	118.93	111.28
2	6	24	VAL	N-CA-C	-7.01	98.29	108.11
3	K	75	GLY	N-CA-C	-7.01	105.13	115.72
3	M	396	MET	N-CA-C	-7.01	104.60	113.72
1	A	60	GLU	CA-C-N	7.01	130.61	120.38
1	A	60	GLU	C-N-CA	7.01	130.61	120.38
1	f	207	GLU	N-CA-C	-7.01	104.61	113.02
2	n	198	GLN	CA-C-N	7.00	129.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	198	GLN	C-N-CA	7.00	129.66	120.28
1	E	105	GLU	CA-C-O	7.00	128.37	120.46
1	f	20	ARG	CA-C-N	7.00	130.65	120.71
1	f	20	ARG	C-N-CA	7.00	130.65	120.71
1	B	233	VAL	N-CA-CB	6.99	118.73	110.55
1	a	108	THR	CA-C-N	6.99	130.04	120.46
1	a	108	THR	C-N-CA	6.99	130.04	120.46
1	G	125	GLN	CA-C-O	-6.99	113.01	120.42
3	I	178	VAL	N-CA-C	-6.99	98.69	108.27
3	J	304	ASP	CA-CB-CG	-6.99	105.61	112.60
3	H	230	ALA	N-CA-CB	6.99	120.14	110.01
1	F	28	ARG	N-CA-C	-6.99	103.75	112.90
3	L	88	VAL	N-CA-C	-6.99	97.79	107.99
2	1	62	ASP	CA-CB-CG	-6.98	105.62	112.60
2	m	60	VAL	O-C-N	6.98	129.16	121.90
3	I	196	ALA	CB-CA-C	-6.98	99.20	110.79
3	J	194	ALA	CA-C-N	6.98	130.02	120.46
3	J	194	ALA	C-N-CA	6.98	130.02	120.46
3	H	101	LYS	CA-C-N	6.98	127.40	119.93
3	H	101	LYS	C-N-CA	6.98	127.40	119.93
2	7	104	PHE	CA-CB-CG	-6.98	106.82	113.80
3	J	163	LYS	CA-C-N	6.98	126.58	119.19
3	J	163	LYS	C-N-CA	6.98	126.58	119.19
2	3	208	LEU	N-CA-C	-6.97	104.74	113.18
1	A	221	PHE	CB-CG-CD1	6.97	132.56	120.70
3	L	390	PRO	N-CA-CB	6.97	109.18	103.32
3	L	39	SER	CA-C-N	6.97	129.62	120.28
3	L	39	SER	C-N-CA	6.97	129.62	120.28
1	G	79	SER	N-CA-C	-6.97	98.05	108.99
1	b	182	ASP	CA-C-O	6.96	128.84	120.28
2	3	202	GLU	CA-C-N	6.96	129.61	120.28
2	3	202	GLU	C-N-CA	6.96	129.61	120.28
1	G	12	ILE	N-CA-C	-6.96	106.02	112.43
3	J	316	GLY	CA-C-N	6.96	130.18	120.29
3	J	316	GLY	C-N-CA	6.96	130.18	120.29
1	D	85	ALA	CA-C-N	6.96	129.61	120.28
1	D	85	ALA	C-N-CA	6.96	129.61	120.28
3	J	293	LEU	N-CA-C	-6.96	99.35	110.14
3	H	124	ASP	CA-C-N	6.96	126.93	119.28
3	H	124	ASP	C-N-CA	6.96	126.93	119.28
1	E	57	LYS	N-CA-CB	6.95	121.93	110.39
1	F	112	LEU	CA-C-N	6.95	129.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	112	LEU	C-N-CA	6.95	129.60	120.28
2	i	30	ARG	NE-CZ-NH2	6.95	125.46	119.20
3	M	216	ILE	O-C-N	6.95	130.44	123.00
2	n	47	GLN	CA-C-N	6.95	130.67	120.74
2	n	47	GLN	C-N-CA	6.95	130.67	120.74
1	F	70	ILE	CA-C-O	6.94	129.46	120.78
1	G	121	GLN	N-CA-C	-6.94	104.78	113.18
1	g	228	GLU	CA-C-N	6.94	129.58	120.28
1	g	228	GLU	C-N-CA	6.94	129.58	120.28
2	3	143	GLY	CA-C-N	6.94	129.58	120.28
2	3	143	GLY	C-N-CA	6.94	129.58	120.28
3	H	257	GLY	CA-C-N	6.94	129.58	120.28
3	H	257	GLY	C-N-CA	6.94	129.58	120.28
1	a	150	THR	N-CA-C	-6.93	98.92	109.95
2	3	24	VAL	CA-CB-CG1	6.93	122.18	110.40
3	H	379	ILE	CA-C-N	6.93	129.57	120.28
3	H	379	ILE	C-N-CA	6.93	129.57	120.28
1	c	151	ASP	CA-CB-CG	-6.93	105.67	112.60
2	1	202	GLU	CA-C-N	6.93	130.13	120.29
2	1	202	GLU	C-N-CA	6.93	130.13	120.29
2	i	162	ASP	CA-C-O	-6.93	113.20	120.55
3	L	49	ARG	CA-C-N	6.93	129.86	120.44
3	L	49	ARG	C-N-CA	6.93	129.86	120.44
1	b	142	ASP	N-CA-C	-6.92	104.46	113.12
1	G	84	ASP	N-CA-C	-6.92	103.50	112.23
2	5	122	ILE	CA-C-N	6.92	132.75	122.99
2	5	122	ILE	C-N-CA	6.92	132.75	122.99
2	2	109	GLN	N-CA-C	-6.92	97.13	108.41
2	1	63	ALA	N-CA-CB	6.92	120.04	110.01
2	i	126	ASP	CA-C-N	6.92	126.61	119.56
2	i	126	ASP	C-N-CA	6.92	126.61	119.56
3	K	372	MET	CA-C-N	6.92	129.55	120.28
3	K	372	MET	C-N-CA	6.92	129.55	120.28
2	5	148	TYR	CA-C-N	6.92	127.80	119.99
2	5	148	TYR	C-N-CA	6.92	127.80	119.99
1	b	151	ASP	CA-C-N	6.91	126.88	119.28
1	b	151	ASP	C-N-CA	6.91	126.88	119.28
3	K	320	ILE	CA-C-O	-6.91	114.08	121.27
3	L	281	VAL	CA-C-N	6.91	134.14	121.70
3	L	281	VAL	C-N-CA	6.91	134.14	121.70
1	E	240	ILE	O-C-N	6.91	128.57	121.87
2	7	92	THR	CA-C-N	6.91	129.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	92	THR	C-N-CA	6.91	129.54	120.28
1	G	6	MET	CG-SD-CE	-6.91	85.71	100.90
2	3	55	THR	N-CA-CB	6.91	121.81	110.69
3	M	314	PHE	CA-C-N	6.91	130.10	120.29
3	M	314	PHE	C-N-CA	6.91	130.10	120.29
3	I	65	VAL	N-CA-CB	6.90	118.06	110.53
3	M	273	ASP	N-CA-CB	6.90	121.65	110.40
1	E	224	VAL	N-CA-CB	6.90	118.86	111.00
2	m	24	VAL	N-CA-C	-6.90	98.55	108.48
1	C	170	ALA	CA-C-O	-6.90	113.11	120.42
1	F	124	THR	N-CA-C	-6.89	104.50	113.12
3	M	381	LYS	N-CA-C	6.89	118.45	111.07
3	H	386	THR	N-CA-C	-6.89	98.54	108.60
1	D	16	SER	CA-C-N	6.89	127.46	119.47
1	D	16	SER	C-N-CA	6.89	127.46	119.47
1	a	16	SER	N-CA-CB	6.89	119.85	110.14
1	b	78	THR	O-C-N	-6.89	114.22	123.10
1	b	145	PRO	O-C-N	6.88	131.36	123.10
2	1	209	ALA	N-CA-C	-6.88	104.92	113.38
3	L	355	CYS	CA-C-N	6.88	129.50	120.28
3	L	355	CYS	C-N-CA	6.88	129.50	120.28
2	l	69	ILE	CA-C-N	6.87	129.22	120.56
2	l	69	ILE	C-N-CA	6.87	129.22	120.56
3	I	153	ILE	N-CA-C	6.87	117.66	110.72
1	A	188	ALA	O-C-N	6.87	129.40	122.12
1	a	235	ARG	CD-NE-CZ	-6.87	114.78	124.40
3	I	254	ASP	O-C-N	-6.87	114.15	122.05
3	L	157	VAL	CA-C-N	6.87	129.78	120.44
3	L	157	VAL	C-N-CA	6.87	129.78	120.44
1	c	234	GLU	CB-CG-CD	-6.87	100.93	112.60
3	I	98	GLU	N-CA-C	-6.87	103.03	111.40
3	L	303	PHE	N-CA-C	-6.87	96.17	110.80
3	H	32	ASP	CA-C-N	6.86	129.48	120.28
3	H	32	ASP	C-N-CA	6.86	129.48	120.28
1	c	186	ASP	CA-C-N	6.86	130.03	120.29
1	c	186	ASP	C-N-CA	6.86	130.03	120.29
2	1	69	ILE	CB-CA-C	-6.86	101.53	112.16
3	J	50	ARG	CA-C-N	6.86	129.47	120.28
3	J	50	ARG	C-N-CA	6.86	129.47	120.28
1	B	104	ASP	N-CA-CB	6.86	123.23	112.46
1	E	45	GLY	CA-C-O	6.86	128.27	121.48
3	H	152	GLU	CA-C-O	6.85	127.68	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	142	SER	N-CA-C	-6.85	104.92	113.28
3	J	123	LYS	CB-CA-C	-6.85	108.68	116.63
1	E	240	ILE	CA-C-O	-6.85	113.83	120.95
1	g	70	ILE	N-CA-C	-6.85	106.11	112.96
2	l	165	VAL	CA-C-N	6.85	129.45	120.28
2	l	165	VAL	C-N-CA	6.85	129.45	120.28
1	F	38	ILE	N-CA-C	-6.84	98.33	108.45
3	J	308	GLU	CA-C-O	-6.84	112.81	120.54
1	G	230	LYS	O-C-N	-6.84	114.28	120.71
2	j	148	TYR	N-CA-C	6.84	118.73	111.28
1	g	189	MET	CA-C-N	6.83	129.82	120.46
1	g	189	MET	C-N-CA	6.83	129.82	120.46
1	f	45	GLY	N-CA-C	-6.83	100.68	110.38
1	d	64	ILE	N-CA-CB	6.83	118.60	110.95
1	F	196	MET	CA-C-N	6.83	128.89	120.22
1	F	196	MET	C-N-CA	6.83	128.89	120.22
2	5	134	GLU	N-CA-CB	6.83	121.64	110.17
2	5	85	PRO	CA-C-O	-6.82	113.66	122.12
3	I	337	LYS	CA-C-O	-6.82	113.19	120.42
1	C	109	VAL	O-C-N	6.82	128.48	121.87
2	2	170	ARG	CD-NE-CZ	-6.82	114.86	124.40
2	6	125	ILE	N-CA-C	-6.82	98.63	108.17
1	a	37	ALA	CA-C-O	-6.82	112.39	120.43
1	B	236	ALA	CA-C-O	-6.82	113.33	120.55
2	k	97	LEU	CA-C-O	-6.81	113.67	120.82
1	F	214	VAL	CA-C-O	-6.81	113.39	120.27
1	a	141	VAL	N-CA-C	-6.81	98.23	108.17
1	a	234	GLU	N-CA-CB	6.81	120.13	110.12
1	F	208	ASN	N-CA-C	-6.81	102.88	113.02
2	3	172	ILE	CA-C-N	6.81	130.08	120.28
2	3	172	ILE	C-N-CA	6.81	130.08	120.28
3	K	97	GLU	CB-CG-CD	-6.81	101.03	112.60
1	c	213	TYR	CA-C-N	6.80	132.45	122.99
1	c	213	TYR	C-N-CA	6.80	132.45	122.99
2	h	155	PHE	N-CA-C	6.80	119.59	109.59
3	H	339	LEU	CA-C-N	6.80	129.40	120.28
3	H	339	LEU	C-N-CA	6.80	129.40	120.28
1	G	8	TYR	N-CA-C	-6.80	103.35	112.94
2	4	88	ARG	NE-CZ-NH2	6.80	125.32	119.20
3	L	16	LEU	CA-C-N	6.80	129.39	120.28
3	L	16	LEU	C-N-CA	6.80	129.39	120.28
1	D	172	THR	N-CA-CB	6.80	119.87	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	141	GLY	N-CA-C	-6.80	105.22	112.08
1	d	225	SER	CA-C-N	6.79	128.33	119.84
1	d	225	SER	C-N-CA	6.79	128.33	119.84
3	M	158	GLU	N-CA-C	6.79	119.31	111.02
1	C	41	LYS	CA-C-O	6.79	127.78	120.38
1	B	172	THR	N-CA-C	-6.79	103.81	111.14
2	l	43	LYS	CA-C-O	6.79	127.69	120.36
2	h	95	SER	N-CA-CB	6.79	120.10	110.12
3	L	378	ALA	O-C-N	6.79	129.31	122.12
1	G	181	ASP	CA-CB-CG	-6.78	105.82	112.60
2	2	166	GLU	CB-CA-C	-6.78	100.18	110.90
2	j	176	MET	CA-C-O	6.78	127.74	120.55
2	l	171	ALA	CA-C-O	-6.78	113.70	120.82
1	E	98	ILE	N-CA-CB	6.78	119.76	110.54
2	k	201	PRO	CA-C-N	6.78	129.69	120.54
2	k	201	PRO	C-N-CA	6.78	129.69	120.54
2	6	162	ASP	CA-CB-CG	-6.78	105.82	112.60
2	n	60	VAL	CA-C-N	6.78	127.46	120.00
2	n	60	VAL	C-N-CA	6.78	127.46	120.00
3	L	299	ARG	CA-C-N	6.78	126.54	119.76
3	L	299	ARG	C-N-CA	6.78	126.54	119.76
2	i	187	ASP	N-CA-C	-6.78	98.35	109.40
1	A	221	PHE	CB-CG-CD2	-6.77	109.19	120.70
3	I	48	VAL	CA-C-O	-6.77	113.99	121.17
3	H	324	HIS	CA-C-N	6.77	132.03	120.72
3	H	324	HIS	C-N-CA	6.77	132.03	120.72
1	e	200	ILE	CA-C-N	6.77	131.97	122.36
1	e	200	ILE	C-N-CA	6.77	131.97	122.36
2	6	110	LEU	N-CA-C	-6.77	98.37	109.40
2	7	126	ASP	CA-C-N	6.77	126.91	119.87
2	7	126	ASP	C-N-CA	6.77	126.91	119.87
1	a	152	PRO	N-CA-C	-6.77	106.08	114.20
2	1	29	LYS	N-CA-C	-6.77	104.23	113.30
2	k	126	ASP	N-CA-CB	6.77	117.59	109.74
3	M	311	LEU	CA-C-O	-6.77	113.68	119.36
3	L	383	LEU	CA-C-N	6.76	129.34	120.28
3	L	383	LEU	C-N-CA	6.76	129.34	120.28
1	a	185	PHE	CA-C-N	6.76	129.89	120.29
1	a	185	PHE	C-N-CA	6.76	129.89	120.29
2	2	104	PHE	CA-C-O	-6.76	113.37	120.87
3	L	397	PHE	CA-CB-CG	-6.76	107.04	113.80
2	m	169	VAL	CA-C-N	6.75	129.22	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	169	VAL	C-N-CA	6.75	129.22	120.44
3	H	296	ALA	N-CA-C	-6.75	96.42	110.80
2	6	54	MET	N-CA-C	-6.75	96.74	108.69
3	J	108	LEU	N-CA-C	-6.75	98.84	109.50
1	c	44	GLU	N-CA-C	-6.75	104.74	114.12
1	G	40	ILE	N-CA-CB	6.75	120.73	112.10
2	1	140	THR	N-CA-C	-6.75	96.34	108.48
1	a	223	GLU	CA-C-N	6.75	131.07	122.37
1	a	223	GLU	C-N-CA	6.75	131.07	122.37
1	D	15	PHE	N-CA-C	-6.75	99.07	109.52
3	I	190	LEU	CA-C-N	6.74	129.32	120.28
3	I	190	LEU	C-N-CA	6.74	129.32	120.28
3	I	354	ILE	CA-C-N	6.74	129.21	120.44
3	I	354	ILE	C-N-CA	6.74	129.21	120.44
2	j	29	LYS	N-CA-C	-6.74	105.21	113.50
2	l	200	SER	N-CA-CB	6.74	122.37	110.37
2	7	97	LEU	N-CA-C	6.74	118.70	111.36
1	b	112	LEU	CA-C-N	6.74	129.86	120.29
1	b	112	LEU	C-N-CA	6.74	129.86	120.29
1	C	89	ILE	N-CA-CB	6.73	121.80	110.56
1	C	101	LEU	CA-C-O	-6.73	112.77	120.24
1	d	241	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	D	189	MET	CG-SD-CE	-6.73	86.10	100.90
2	m	128	ILE	CA-C-N	6.73	131.20	121.44
2	m	128	ILE	C-N-CA	6.73	131.20	121.44
1	G	124	THR	CA-C-O	-6.72	113.76	120.82
3	L	163	LYS	CA-C-N	6.72	126.51	119.05
3	L	163	LYS	C-N-CA	6.72	126.51	119.05
1	b	35	ALA	N-CA-C	6.72	119.98	110.23
1	G	38	ILE	O-C-N	6.72	130.29	123.10
3	H	277	PRO	CA-N-CD	6.72	121.41	112.00
1	B	137	LEU	CA-C-N	6.72	130.77	122.37
1	B	137	LEU	C-N-CA	6.72	130.77	122.37
1	A	121	GLN	CA-C-N	6.72	129.95	120.28
1	A	121	GLN	C-N-CA	6.72	129.95	120.28
1	d	118	ASP	CA-C-N	6.72	129.17	120.44
1	d	118	ASP	C-N-CA	6.72	129.17	120.44
1	C	203	GLU	O-C-N	-6.71	115.37	122.96
1	D	185	PHE	N-CA-C	6.71	118.25	111.07
1	E	26	TYR	CB-CG-CD1	-6.71	110.73	120.80
3	J	67	VAL	CA-C-O	6.71	127.48	120.36
2	5	103	TYR	CA-C-N	6.71	128.61	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	103	TYR	C-N-CA	6.71	128.61	122.37
3	M	22	LYS	O-C-N	6.71	129.34	122.09
1	C	184	SER	CA-C-O	-6.71	113.37	121.89
2	4	112	ILE	O-C-N	-6.71	116.30	123.14
3	M	146	LEU	CA-C-N	6.71	129.26	120.28
3	M	146	LEU	C-N-CA	6.71	129.26	120.28
1	a	12	ILE	CA-C-N	6.70	130.23	120.71
1	a	12	ILE	C-N-CA	6.70	130.23	120.71
1	G	219	ARG	N-CA-CB	6.70	121.82	110.49
2	n	99	ASN	CA-C-N	6.70	130.50	120.31
2	n	99	ASN	C-N-CA	6.70	130.50	120.31
3	I	148	VAL	CA-C-O	-6.70	113.98	120.95
3	K	303	PHE	N-CA-CB	6.70	121.82	110.49
1	d	231	PRO	CA-C-N	6.70	129.26	120.28
1	d	231	PRO	C-N-CA	6.70	129.26	120.28
1	e	31	VAL	O-C-N	6.70	128.37	121.87
2	1	146	THR	CA-C-N	6.70	129.26	120.28
2	1	146	THR	C-N-CA	6.70	129.26	120.28
3	J	120	PRO	N-CA-CB	6.70	109.22	103.19
2	3	211	PHE	N-CA-C	-6.70	104.68	114.39
1	C	70	ILE	N-CA-C	-6.69	95.43	109.34
1	E	152	PRO	N-CA-C	-6.69	105.50	113.86
1	e	214	VAL	CA-C-N	6.69	132.49	121.39
1	e	214	VAL	C-N-CA	6.69	132.49	121.39
3	K	298	LEU	CA-C-O	-6.68	111.02	119.31
1	a	114	LYS	CA-CB-CG	6.68	127.46	114.10
2	h	63	ALA	N-CA-C	6.68	118.36	111.14
3	K	138	VAL	O-C-N	-6.68	115.61	123.03
3	L	106	VAL	CA-C-O	-6.68	115.02	121.63
3	L	161	LEU	CA-C-N	6.68	129.53	120.44
3	L	161	LEU	C-N-CA	6.68	129.53	120.44
1	A	109	VAL	N-CA-CB	6.68	118.36	110.55
2	j	200	SER	N-CA-CB	6.68	122.26	110.37
2	6	88	ARG	NE-CZ-NH2	6.68	125.21	119.20
2	1	151	LEU	CA-C-N	6.68	131.28	120.60
2	1	151	LEU	C-N-CA	6.68	131.28	120.60
3	H	265	MET	CA-C-N	6.68	129.23	120.28
3	H	265	MET	C-N-CA	6.68	129.23	120.28
2	i	80	ARG	CB-CA-C	-6.68	99.50	110.85
2	k	55	THR	N-CA-C	-6.68	98.84	109.59
2	7	102	ARG	NE-CZ-NH1	-6.68	114.82	121.50
3	H	198	GLN	CB-CA-C	-6.68	97.80	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	35	LYS	CA-C-N	6.67	129.55	120.54
3	J	35	LYS	C-N-CA	6.67	129.55	120.54
2	2	62	ASP	CA-CB-CG	-6.67	105.93	112.60
2	l	81	ARG	NE-CZ-NH2	6.67	125.20	119.20
3	J	134	GLU	CB-CA-C	-6.67	97.16	110.42
1	C	170	ALA	O-C-N	6.66	129.75	122.15
1	g	31	VAL	N-CA-C	6.66	116.79	110.53
2	5	212	ARG	CA-C-N	6.66	133.69	121.70
2	5	212	ARG	C-N-CA	6.66	133.69	121.70
2	n	24	VAL	CA-C-O	6.66	127.42	120.36
3	L	375	PHE	CA-C-O	-6.66	113.83	120.82
3	J	317	ARG	CA-C-N	6.66	129.88	120.42
3	J	317	ARG	C-N-CA	6.66	129.88	120.42
1	B	157	LEU	CA-C-N	6.66	132.59	122.93
1	B	157	LEU	C-N-CA	6.66	132.59	122.93
1	d	45	GLY	N-CA-C	-6.66	101.11	110.63
3	I	67	VAL	CA-C-N	6.66	130.41	120.69
3	I	67	VAL	C-N-CA	6.66	130.41	120.69
1	c	86	ARG	N-CA-CB	6.66	119.66	110.01
1	c	91	ARG	NE-CZ-NH2	6.66	125.19	119.20
1	f	61	ALA	CA-C-O	6.65	127.14	119.35
2	5	49	ALA	CA-C-N	6.65	129.86	120.28
2	5	49	ALA	C-N-CA	6.65	129.86	120.28
1	d	180	ARG	CA-C-O	-6.65	114.14	121.33
3	I	91	THR	O-C-N	6.65	130.83	122.65
1	C	121	GLN	CA-C-N	6.65	129.85	120.28
1	C	121	GLN	C-N-CA	6.65	129.85	120.28
1	b	202	SER	N-CA-C	-6.65	98.89	108.60
3	H	283	VAL	N-CA-C	-6.64	98.87	108.17
3	I	267	GLN	CA-C-O	-6.64	113.51	120.55
1	f	33	ARG	N-CA-C	-6.64	105.18	113.28
2	k	189	VAL	N-CA-C	-6.64	98.17	107.80
1	e	11	ALA	CA-C-N	6.64	130.44	120.75
1	e	11	ALA	C-N-CA	6.64	130.44	120.75
3	J	55	VAL	N-CA-CB	6.64	118.32	110.55
2	5	102	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	e	216	VAL	CB-CA-C	-6.63	101.13	110.95
3	I	33	GLU	CA-C-N	6.63	132.74	121.14
3	I	33	GLU	C-N-CA	6.63	132.74	121.14
1	D	124	THR	CA-C-N	6.63	129.70	120.29
1	D	124	THR	C-N-CA	6.63	129.70	120.29
3	J	46	ARG	N-CA-C	6.63	118.50	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	145	PRO	N-CA-CB	6.63	109.50	103.34
2	6	70	ILE	CA-C-N	6.63	129.70	120.29
2	6	70	ILE	C-N-CA	6.63	129.70	120.29
2	7	154	ARG	N-CA-C	-6.62	105.17	112.72
1	F	131	PRO	CA-C-O	-6.62	113.59	121.67
2	h	158	GLU	N-CA-C	-6.62	100.47	109.54
1	A	187	ASP	N-CA-CB	6.61	119.84	110.12
2	m	107	LEU	N-CA-C	-6.61	99.13	109.25
3	H	257	GLY	O-C-N	-6.61	115.84	122.19
3	K	319	GLN	CB-CA-C	-6.61	99.82	110.79
1	F	108	THR	N-CA-C	-6.61	101.19	110.50
1	F	114	LYS	CB-CA-C	-6.61	99.82	110.79
2	4	90	ILE	CA-C-N	6.61	129.03	120.44
2	4	90	ILE	C-N-CA	6.61	129.03	120.44
3	H	395	VAL	N-CA-C	-6.61	105.89	112.17
2	6	145	LEU	CA-C-N	6.60	129.67	120.29
2	6	145	LEU	C-N-CA	6.60	129.67	120.29
3	H	329	LYS	N-CA-C	-6.60	98.93	109.76
2	6	40	LYS	O-C-N	6.60	128.93	121.93
2	n	45	ILE	CA-CB-CG1	6.60	121.62	110.40
3	I	389	ILE	O-C-N	-6.60	113.57	121.10
3	K	192	ALA	CA-C-N	6.60	129.13	120.28
3	K	192	ALA	C-N-CA	6.60	129.13	120.28
3	J	294	ASP	CA-C-N	6.60	126.23	119.56
3	J	294	ASP	C-N-CA	6.60	126.23	119.56
3	J	223	VAL	CA-C-O	-6.60	114.08	120.95
1	g	245	LYS	N-CA-C	-6.60	103.19	113.02
2	l	119	GLY	N-CA-C	-6.60	104.90	111.56
2	2	144	SER	N-CA-C	6.59	118.47	111.28
3	J	191	LEU	N-CA-C	6.59	124.85	110.80
1	f	158	GLU	CB-CA-C	6.59	120.56	109.48
1	C	153	SER	N-CA-C	-6.59	104.02	111.14
2	5	184	ASP	N-CA-C	-6.59	98.66	109.40
3	J	324	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
1	B	118	ASP	CA-CB-CG	6.59	119.19	112.60
3	H	90	ASN	CA-CB-CG	6.59	119.19	112.60
2	j	70	ILE	CA-C-N	6.59	129.11	120.28
2	j	70	ILE	C-N-CA	6.59	129.11	120.28
3	I	101	LYS	O-C-N	-6.59	115.72	121.71
1	D	187	ASP	CB-CA-C	-6.58	99.86	110.79
1	f	46	VAL	CA-C-N	6.58	131.59	123.10
1	f	46	VAL	C-N-CA	6.58	131.59	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	96	ASN	CA-CB-CG	-6.58	106.02	112.60
3	I	323	ILE	CA-C-O	-6.58	113.87	120.85
1	b	28	ARG	NE-CZ-NH1	6.58	128.08	121.50
3	I	158	GLU	O-C-N	-6.58	115.14	122.12
2	m	136	ASP	CA-CB-CG	6.58	119.18	112.60
1	F	222	LYS	N-CA-C	-6.58	99.34	109.14
1	a	99	ASN	N-CA-C	6.58	118.45	111.28
1	b	66	LYS	CA-C-N	6.58	132.13	122.99
1	b	66	LYS	C-N-CA	6.58	132.13	122.99
2	6	86	THR	CA-CB-OG1	6.58	119.46	109.60
3	J	273	ASP	CA-C-N	6.58	127.28	119.98
3	J	273	ASP	C-N-CA	6.58	127.28	119.98
3	H	326	ARG	NE-CZ-NH2	6.57	125.12	119.20
3	K	281	VAL	CA-C-N	6.57	133.53	121.70
3	K	281	VAL	C-N-CA	6.57	133.53	121.70
1	G	52	LYS	CA-C-N	6.57	133.38	122.54
1	G	52	LYS	C-N-CA	6.57	133.38	122.54
2	m	84	LYS	CA-C-N	6.57	126.53	119.76
2	m	84	LYS	C-N-CA	6.57	126.53	119.76
3	I	325	THR	N-CA-CB	6.57	119.78	110.12
2	3	177	LYS	O-C-N	6.57	130.35	122.27
3	L	36	PHE	CA-C-N	6.57	129.46	120.46
3	L	36	PHE	C-N-CA	6.57	129.46	120.46
3	J	82	SER	N-CA-CB	6.56	121.05	110.42
1	f	97	GLN	OE1-CD-NE2	6.56	129.16	122.60
2	3	135	LYS	N-CA-C	-6.56	106.02	112.97
3	J	282	LYS	N-CA-CB	6.56	121.65	110.50
1	g	49	ILE	CA-C-O	6.56	128.02	120.67
3	L	61	PRO	N-CA-CB	-6.55	99.52	103.19
2	3	86	THR	CA-C-N	6.55	129.44	120.46
2	3	86	THR	C-N-CA	6.55	129.44	120.46
1	F	132	PHE	O-C-N	6.55	130.36	122.96
3	H	94	TYR	CA-C-O	6.55	127.45	120.70
3	K	221	ARG	CA-C-N	6.55	129.05	120.28
3	K	221	ARG	C-N-CA	6.55	129.05	120.28
1	E	150	THR	N-CA-CB	6.55	121.10	110.43
2	6	156	THR	N-CA-C	-6.55	98.34	108.55
1	c	211	VAL	CA-C-O	6.54	127.96	120.76
2	3	104	PHE	O-C-N	-6.54	114.63	121.04
3	I	376	THR	CA-C-N	6.54	129.04	120.28
3	I	376	THR	C-N-CA	6.54	129.04	120.28
1	E	124	THR	CA-C-N	6.54	128.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	124	THR	C-N-CA	6.54	128.94	120.44
2	m	63	ALA	CA-C-N	6.54	129.33	120.44
2	m	63	ALA	C-N-CA	6.54	129.33	120.44
2	7	58	GLY	N-CA-C	-6.54	101.57	110.20
2	l	49	ALA	N-CA-C	-6.54	100.21	108.45
3	H	73	GLU	CB-CG-CD	-6.54	101.49	112.60
1	F	51	ASP	CA-CB-CG	-6.53	106.07	112.60
2	1	178	ARG	N-CA-C	-6.53	104.24	111.36
2	k	31	ALA	CA-C-O	-6.53	113.31	120.36
3	J	106	VAL	CA-C-O	-6.53	115.16	121.63
3	H	50	ARG	CA-C-O	6.53	127.42	120.70
3	H	337	LYS	CA-C-N	6.53	129.31	120.44
3	H	337	LYS	C-N-CA	6.53	129.31	120.44
1	b	42	CYS	N-CA-C	-6.52	99.66	108.86
1	D	221	PHE	N-CA-CB	6.52	119.31	109.34
3	K	15	LYS	O-C-N	6.52	129.03	122.12
1	D	158	GLU	N-CA-C	-6.52	99.68	110.17
1	D	118	ASP	CA-C-N	6.51	128.91	120.44
1	D	118	ASP	C-N-CA	6.51	128.91	120.44
2	4	96	ASN	CA-CB-CG	-6.51	106.08	112.60
3	K	395	VAL	N-CA-C	-6.51	103.90	111.00
1	b	119	PHE	CA-CB-CG	6.51	120.31	113.80
1	D	70	ILE	CB-CA-C	-6.51	104.53	110.91
3	I	148	VAL	O-C-N	6.51	128.18	121.87
1	a	118	ASP	CA-CB-CG	-6.51	106.09	112.60
1	b	19	GLY	N-CA-C	-6.50	106.35	115.32
2	i	172	ILE	CA-C-N	6.50	128.99	120.28
2	i	172	ILE	C-N-CA	6.50	128.99	120.28
3	I	119	LEU	CA-C-O	-6.50	113.94	120.63
3	L	105	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	23	GLN	CA-C-N	6.50	129.65	120.42
1	A	23	GLN	C-N-CA	6.50	129.65	120.42
3	J	39	SER	N-CA-CB	6.50	119.67	110.12
1	a	68	TYR	CA-C-O	-6.50	113.77	121.11
1	G	97	GLN	CA-C-N	6.49	130.95	120.30
1	G	97	GLN	C-N-CA	6.49	130.95	120.30
1	C	239	ARG	CA-C-N	6.49	129.35	120.46
1	C	239	ARG	C-N-CA	6.49	129.35	120.46
1	D	196	MET	O-C-N	6.49	129.81	122.22
3	I	230	ALA	CA-C-O	-6.49	112.77	120.10
1	G	142	ASP	CA-CB-CG	6.49	119.09	112.60
3	K	309	VAL	CB-CA-C	6.49	118.64	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	186	THR	N-CA-C	-6.49	105.10	114.12
1	e	36	THR	CA-CB-OG1	6.49	119.33	109.60
1	a	170	ALA	CA-C-O	-6.49	114.02	120.70
2	k	104	PHE	CA-C-N	6.49	127.95	119.84
2	k	104	PHE	C-N-CA	6.49	127.95	119.84
3	I	317	ARG	CA-C-N	6.49	129.35	120.46
3	I	317	ARG	C-N-CA	6.49	129.35	120.46
3	M	197	ASN	CA-CB-CG	6.48	119.08	112.60
1	d	65	GLU	CA-C-N	6.48	133.51	122.36
1	d	65	GLU	C-N-CA	6.48	133.51	122.36
2	h	162	ASP	N-CA-C	-6.48	105.19	113.23
2	j	83	ARG	N-CA-C	-6.48	99.18	109.23
1	b	194	VAL	CA-C-N	6.48	128.87	120.44
1	b	194	VAL	C-N-CA	6.48	128.87	120.44
2	n	114	GLY	CA-C-O	-6.48	115.22	121.05
3	H	257	GLY	CA-C-O	6.48	128.16	120.90
3	J	175	PRO	CA-C-O	-6.48	113.85	121.95
1	G	229	LEU	CA-C-N	6.48	128.19	120.09
1	G	229	LEU	C-N-CA	6.48	128.19	120.09
3	J	142	ASP	N-CA-C	-6.48	96.07	107.73
3	H	163	LYS	CA-C-N	6.48	126.18	119.64
3	H	163	LYS	C-N-CA	6.48	126.18	119.64
3	H	32	ASP	N-CA-C	6.47	118.42	111.36
1	A	225	SER	CA-C-O	-6.47	113.36	120.87
1	a	15	PHE	CA-CB-CG	-6.47	107.33	113.80
3	I	154	ARG	NE-CZ-NH2	6.47	125.03	119.20
3	L	30	LEU	CA-C-N	6.47	128.95	120.28
3	L	30	LEU	C-N-CA	6.47	128.95	120.28
1	g	12	ILE	N-CA-C	-6.47	102.99	112.04
1	d	43	LYS	N-CA-C	-6.46	103.91	113.61
1	E	5	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	F	66	LYS	N-CA-C	-6.46	105.52	113.41
1	C	132	PHE	CA-CB-CG	-6.46	107.34	113.80
1	C	100	ARG	N-CA-C	6.46	120.76	113.01
2	i	94	THR	N-CA-C	-6.46	104.24	111.28
2	5	88	ARG	NE-CZ-NH2	6.46	125.02	119.20
2	7	101	TYR	CB-CA-C	-6.46	100.25	111.23
3	K	367	ARG	NE-CZ-NH1	6.46	127.96	121.50
1	C	38	ILE	CA-C-N	-6.46	117.26	121.65
1	C	38	ILE	C-N-CA	-6.46	117.26	121.65
3	M	88	VAL	O-C-N	6.46	129.90	122.99
2	5	18	VAL	N-CA-CB	6.46	117.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	44	LYS	N-CA-C	-6.46	106.61	114.75
2	4	64	GLN	CB-CG-CD	-6.46	101.63	112.60
3	L	395	VAL	N-CA-CB	6.45	122.47	111.50
3	M	52	ARG	N-CA-CB	6.45	119.61	110.12
3	J	170	VAL	CB-CA-C	6.45	120.47	112.02
1	B	105	GLU	CA-C-N	6.45	126.40	119.76
1	B	105	GLU	C-N-CA	6.45	126.40	119.76
1	e	207	GLU	N-CA-C	-6.45	104.33	111.36
3	I	42	ILE	O-C-N	6.45	128.13	121.87
3	K	243	LEU	N-CA-C	-6.45	105.71	112.93
2	3	73	GLU	CA-C-O	-6.45	112.18	119.79
2	n	203	GLU	N-CA-C	-6.44	104.18	111.07
3	K	243	LEU	N-CA-CB	6.44	119.45	110.56
3	M	17	GLU	CA-C-N	6.44	129.20	120.44
3	M	17	GLU	C-N-CA	6.44	129.20	120.44
3	M	341	ARG	CA-C-N	6.44	129.29	120.46
3	M	341	ARG	C-N-CA	6.44	129.29	120.46
3	H	231	LYS	CB-CA-C	-6.44	100.10	110.79
1	A	194	VAL	CA-C-O	-6.44	114.35	121.17
1	B	95	GLU	CB-CG-CD	6.44	123.55	112.60
1	c	237	ASN	CA-C-N	6.44	128.91	120.28
1	c	237	ASN	C-N-CA	6.44	128.91	120.28
1	D	223	GLU	CB-CA-C	6.44	120.86	109.72
1	E	215	LYS	CA-C-N	6.43	129.60	120.53
1	E	215	LYS	C-N-CA	6.43	129.60	120.53
1	E	221	PHE	CA-CB-CG	-6.43	107.36	113.80
3	H	91	THR	CA-C-O	-6.43	114.22	121.81
3	L	352	LYS	CA-C-O	6.43	127.37	120.55
1	e	16	SER	CA-C-O	-6.43	113.30	120.25
2	2	58	GLY	N-CA-C	-6.43	102.06	110.29
2	1	83	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	c	105	GLU	CA-C-N	6.43	126.45	119.89
1	c	105	GLU	C-N-CA	6.43	126.45	119.89
2	h	61	GLY	O-C-N	6.43	128.36	122.19
3	M	348	GLY	CA-C-N	6.43	129.42	120.29
3	M	348	GLY	C-N-CA	6.43	129.42	120.29
1	A	108	THR	CA-C-N	6.42	128.65	120.56
1	A	108	THR	C-N-CA	6.42	128.65	120.56
1	C	117	CYS	N-CA-CB	6.42	120.11	110.22
3	M	176	LYS	N-CA-C	-6.42	103.45	113.02
1	A	11	ALA	N-CA-C	-6.42	99.31	109.07
2	m	85	PRO	N-CD-CG	6.42	112.83	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	ARG	N-CA-C	-6.42	97.32	108.69
2	h	94	THR	CA-C-N	6.42	128.88	120.28
2	h	94	THR	C-N-CA	6.42	128.88	120.28
1	F	240	ILE	CA-C-O	-6.42	114.05	120.85
1	C	89	ILE	N-CA-C	-6.42	104.01	111.00
3	K	127	VAL	CA-C-N	6.42	129.17	120.38
3	K	127	VAL	C-N-CA	6.42	129.17	120.38
3	J	84	GLY	CA-C-N	6.42	127.84	120.98
3	J	84	GLY	C-N-CA	6.42	127.84	120.98
1	f	126	TYR	CB-CG-CD2	-6.41	111.18	120.80
3	M	33	GLU	CA-C-N	6.41	132.37	121.14
3	M	33	GLU	C-N-CA	6.41	132.37	121.14
1	g	131	PRO	CA-C-N	6.41	130.43	120.75
1	g	131	PRO	C-N-CA	6.41	130.43	120.75
2	n	141	GLY	N-CA-C	-6.41	101.95	110.74
3	H	258	ASP	N-CA-C	6.41	118.27	111.28
1	D	30	ALA	N-CA-CB	6.41	119.64	110.16
2	5	166	GLU	CA-C-N	6.41	129.38	120.29
2	5	166	GLU	C-N-CA	6.41	129.38	120.29
2	n	148	TYR	CA-C-O	-6.41	113.63	120.42
2	l	151	LEU	CA-C-N	6.40	129.38	120.29
2	l	151	LEU	C-N-CA	6.40	129.38	120.29
1	b	16	SER	CA-C-N	6.40	127.55	120.45
1	b	16	SER	C-N-CA	6.40	127.55	120.45
1	d	104	ASP	N-CA-C	-6.40	103.35	111.92
2	i	30	ARG	NE-CZ-NH1	-6.40	115.10	121.50
2	7	159	ILE	N-CA-C	-6.40	99.37	108.58
3	I	281	VAL	CA-C-N	6.40	133.22	121.70
3	I	281	VAL	C-N-CA	6.40	133.22	121.70
3	K	12	LYS	CA-C-N	6.40	130.03	120.31
3	K	12	LYS	C-N-CA	6.40	130.03	120.31
1	D	145	PRO	CA-C-O	-6.40	114.35	121.32
1	B	188	ALA	CA-C-N	6.39	128.75	120.44
1	B	188	ALA	C-N-CA	6.39	128.75	120.44
1	D	220	THR	N-CA-C	-6.39	98.47	108.90
1	g	220	THR	CA-C-N	6.39	133.75	121.54
1	g	220	THR	C-N-CA	6.39	133.75	121.54
2	3	46	TYR	CA-CB-CG	-6.39	102.39	113.90
3	M	339	LEU	O-C-N	6.39	128.90	122.12
1	A	56	SER	CA-C-N	6.39	132.33	121.14
1	A	56	SER	C-N-CA	6.39	132.33	121.14
2	1	68	ARG	CA-C-O	6.39	127.33	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	229	LEU	CA-C-N	6.39	130.03	120.31
3	L	229	LEU	C-N-CA	6.39	130.03	120.31
1	B	52	LYS	CA-C-O	6.39	126.84	120.32
1	F	49	ILE	N-CA-C	-6.39	98.92	108.12
1	f	36	THR	CB-CA-C	6.39	121.30	109.54
2	h	90	ILE	O-C-N	6.39	128.41	121.83
2	7	65	PHE	N-CA-CB	6.39	119.28	110.01
1	a	241	ARG	N-CA-C	6.39	117.91	111.07
2	7	42	ALA	N-CA-C	-6.38	98.21	108.55
3	H	207	VAL	N-CA-C	-6.38	99.28	108.53
1	E	237	ASN	CA-C-N	6.38	128.74	120.44
1	E	237	ASN	C-N-CA	6.38	128.74	120.44
1	f	91	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	g	173	GLU	CA-C-N	6.38	128.83	120.28
1	g	173	GLU	C-N-CA	6.38	128.83	120.28
2	i	44	LYS	N-CA-C	-6.38	104.72	114.16
2	j	58	GLY	N-CA-C	-6.38	105.11	111.56
3	K	284	ILE	N-CA-C	-6.38	98.00	107.51
1	A	193	LEU	CA-C-N	6.38	128.60	120.56
1	A	193	LEU	C-N-CA	6.38	128.60	120.56
1	D	22	PHE	CA-C-O	6.38	127.22	119.31
2	3	32	THR	CA-CB-OG1	-6.38	100.03	109.60
2	k	102	ARG	N-CA-CB	6.38	120.80	110.40
1	b	178	GLU	N-CA-C	-6.37	102.73	112.99
3	J	146	LEU	N-CA-CB	6.37	121.33	110.50
2	2	29	LYS	CA-C-N	6.37	131.19	122.34
2	2	29	LYS	C-N-CA	6.37	131.19	122.34
2	7	81	ARG	N-CA-CB	6.37	120.46	110.46
1	A	194	VAL	CA-C-N	6.37	128.81	120.28
1	A	194	VAL	C-N-CA	6.37	128.81	120.28
1	D	204	LEU	CA-C-N	6.37	128.87	123.33
1	D	204	LEU	C-N-CA	6.37	128.87	123.33
3	K	249	ARG	NE-CZ-NH1	6.37	127.87	121.50
1	g	169	ASN	CA-CB-CG	-6.37	106.23	112.60
1	a	131	PRO	CA-C-N	6.36	129.75	120.71
1	a	131	PRO	C-N-CA	6.36	129.75	120.71
2	5	152	GLU	CA-C-N	6.36	129.33	120.29
2	5	152	GLU	C-N-CA	6.36	129.33	120.29
1	d	40	ILE	N-CA-C	-6.36	98.98	108.46
1	F	107	ILE	N-CA-C	6.36	118.78	109.63
2	2	60	VAL	N-CA-C	6.36	116.52	110.42
1	B	85	ALA	O-C-N	-6.36	115.38	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	198	LEU	CA-C-N	6.36	128.80	120.28
1	e	198	LEU	C-N-CA	6.36	128.80	120.28
2	1	204	VAL	CA-C-N	6.36	128.80	120.28
2	1	204	VAL	C-N-CA	6.36	128.80	120.28
1	f	205	VAL	CA-C-O	-6.35	116.64	119.94
2	1	109	GLN	CG-CD-NE2	6.35	125.93	116.40
2	m	60	VAL	CA-CB-CG1	6.35	121.20	110.40
1	a	188	ALA	CA-C-N	6.35	129.08	120.44
1	a	188	ALA	C-N-CA	6.35	129.08	120.44
2	i	163	GLU	CA-C-N	6.35	131.48	120.68
2	i	163	GLU	C-N-CA	6.35	131.48	120.68
3	L	259	ARG	CA-C-O	-6.35	113.69	120.42
3	I	112	THR	N-CA-C	-6.35	105.18	114.39
1	C	9	ASP	N-CA-C	-6.35	103.56	113.02
1	d	151	ASP	CA-C-O	-6.35	114.53	120.94
2	1	43	LYS	CA-C-N	6.35	130.83	120.23
2	1	43	LYS	C-N-CA	6.35	130.83	120.23
3	M	362	ALA	O-C-N	-6.35	114.91	122.15
1	A	85	ALA	CA-C-O	-6.35	114.16	120.82
1	f	212	GLY	N-CA-C	-6.35	98.78	110.97
2	5	81	ARG	CD-NE-CZ	-6.35	115.51	124.40
2	j	180	SER	N-CA-C	-6.34	102.83	110.44
2	m	65	PHE	N-CA-C	6.34	118.27	111.36
2	7	51	ARG	O-C-N	-6.34	114.51	122.19
3	H	304	ASP	CA-C-O	6.34	125.50	118.52
1	E	30	ALA	CA-C-N	6.34	129.15	120.46
1	E	30	ALA	C-N-CA	6.34	129.15	120.46
1	G	181	ASP	CB-CA-C	-6.34	98.60	110.01
2	7	171	ALA	CA-C-N	6.34	129.43	120.42
2	7	171	ALA	C-N-CA	6.34	129.43	120.42
1	c	223	GLU	O-C-N	-6.34	116.11	123.27
1	e	245	LYS	N-CA-C	-6.34	106.18	114.04
2	n	76	LEU	CA-C-O	-6.34	113.83	120.55
1	D	171	VAL	N-CA-C	-6.33	102.95	111.44
2	2	139	ALA	N-CA-C	-6.33	97.31	110.80
1	f	75	CYS	N-CA-C	-6.33	99.70	109.52
3	M	273	ASP	CB-CA-C	-6.33	96.75	109.99
1	a	77	ALA	N-CA-CB	6.33	120.55	111.05
1	F	194	VAL	O-C-N	6.33	128.01	121.87
2	4	107	LEU	N-CA-C	-6.33	97.31	110.80
1	A	105	GLU	CA-C-N	6.33	127.75	119.84
1	A	105	GLU	C-N-CA	6.33	127.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	ASP	CB-CA-C	-6.33	100.94	110.88
2	l	83	ARG	N-CA-CB	6.33	121.19	110.49
2	7	28	GLU	CB-CA-C	6.33	120.67	110.16
1	e	22	PHE	CA-C-O	-6.32	113.72	120.42
2	2	86	THR	N-CA-C	-6.32	102.01	110.55
3	I	357	GLU	CA-C-N	6.32	128.75	120.28
3	I	357	GLU	C-N-CA	6.32	128.75	120.28
3	J	343	THR	N-CA-C	-6.32	105.85	112.93
1	A	48	LEU	O-C-N	6.32	130.71	123.31
1	A	51	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	174	PHE	O-C-N	6.32	128.60	122.03
1	F	64	ILE	CA-C-O	6.32	128.68	120.78
2	l	36	PHE	CA-CB-CG	-6.32	107.48	113.80
2	6	74	ALA	N-CA-CB	6.32	119.41	110.12
1	D	194	VAL	CB-CA-C	-6.32	103.61	112.14
1	c	158	GLU	CB-CA-C	6.32	120.31	109.51
3	L	366	GLU	N-CA-C	-6.32	104.12	113.40
2	6	84	LYS	N-CA-C	6.31	117.66	109.64
1	c	53	ARG	CA-C-N	6.31	132.16	122.25
1	c	53	ARG	C-N-CA	6.31	132.16	122.25
3	M	13	LEU	CA-C-N	6.31	129.25	120.29
3	M	13	LEU	C-N-CA	6.31	129.25	120.29
3	M	71	ILE	O-C-N	-6.31	116.44	123.26
2	3	167	LEU	N-CA-C	6.31	119.14	111.82
1	d	149	GLU	N-CA-C	-6.31	98.62	108.90
2	j	205	GLU	CA-C-N	6.31	129.25	120.29
2	j	205	GLU	C-N-CA	6.31	129.25	120.29
1	a	20	ARG	NE-CZ-NH2	6.30	124.87	119.20
3	M	364	ARG	CD-NE-CZ	-6.30	115.58	124.40
1	f	144	VAL	O-C-N	6.30	128.28	121.10
2	1	203	GLU	CA-C-N	6.30	129.09	120.46
2	1	203	GLU	C-N-CA	6.30	129.09	120.46
1	a	133	GLY	O-C-N	6.30	130.89	122.70
1	B	92	ALA	CB-CA-C	-6.30	100.33	110.79
1	e	93	ARG	CA-C-N	6.30	129.36	120.42
1	e	93	ARG	C-N-CA	6.30	129.36	120.42
1	g	144	VAL	N-CA-C	-6.30	101.02	107.89
1	B	203	GLU	N-CA-CB	6.30	120.02	110.45
1	G	225	SER	CA-C-N	6.30	126.50	119.32
1	G	225	SER	C-N-CA	6.30	126.50	119.32
1	E	207	GLU	N-CA-C	-6.29	105.88	112.93
2	m	55	THR	N-CA-C	-6.29	99.56	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	142	ASP	CA-C-N	6.29	132.40	122.33
3	M	142	ASP	C-N-CA	6.29	132.40	122.33
1	b	105	GLU	CB-CA-C	-6.29	100.22	109.97
1	e	39	GLY	N-CA-C	-6.29	98.27	113.18
1	c	89	ILE	O-C-N	-6.29	113.44	122.12
1	E	97	GLN	CA-C-N	6.29	129.08	120.46
1	E	97	GLN	C-N-CA	6.29	129.08	120.46
2	7	75	ASN	CB-CA-C	-6.29	100.16	110.85
3	H	142	ASP	O-C-N	6.29	129.89	122.34
3	M	136	PRO	CB-CA-C	-6.29	103.34	111.39
1	f	93	ARG	N-CA-C	6.28	118.21	111.36
3	I	89	VAL	N-CA-C	-6.28	98.63	108.81
3	I	386	THR	CA-C-O	-6.28	111.99	119.15
1	e	199	SER	N-CA-C	6.28	118.13	111.28
1	a	71	ASP	CA-CB-CG	-6.28	106.32	112.60
1	c	230	LYS	CA-C-O	-6.28	112.85	118.63
2	6	60	VAL	CA-C-N	6.28	126.91	119.94
2	6	60	VAL	C-N-CA	6.28	126.91	119.94
1	E	134	VAL	CA-CB-CG2	6.28	121.07	110.40
1	g	43	LYS	N-CA-C	-6.28	105.26	113.17
2	7	162	ASP	CA-CB-CG	-6.28	106.32	112.60
3	J	276	ASP	CA-CB-CG	-6.28	106.32	112.60
2	l	86	THR	CA-C-N	6.27	129.06	120.46
2	l	86	THR	C-N-CA	6.27	129.06	120.46
1	D	13	THR	N-CA-C	-6.27	105.78	113.50
2	m	128	ILE	CA-C-O	6.27	126.41	120.14
2	n	104	PHE	CA-CB-CG	-6.27	107.53	113.80
2	j	164	ALA	CA-C-O	-6.27	112.76	119.97
3	I	310	PRO	N-CA-C	-6.27	99.55	112.47
2	h	136	ASP	CA-C-O	-6.27	114.72	121.36
3	K	343	THR	CA-C-N	6.27	129.66	120.82
3	K	343	THR	C-N-CA	6.27	129.66	120.82
3	J	71	ILE	N-CA-CB	6.26	120.67	111.52
3	K	324	HIS	N-CA-CB	6.26	119.53	110.20
3	J	211	PHE	CA-CB-CG	-6.26	107.54	113.80
2	5	88	ARG	NE-CZ-NH1	-6.26	115.24	121.50
3	H	372	MET	CA-C-N	6.26	128.67	120.28
3	H	372	MET	C-N-CA	6.26	128.67	120.28
3	L	269	LEU	CA-C-O	-6.26	113.91	120.55
1	a	40	ILE	N-CA-CB	6.26	121.72	111.45
1	B	17	PRO	N-CA-C	-6.26	106.03	113.86
2	4	108	VAL	N-CA-C	-6.26	99.24	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	44	TYR	CA-C-N	6.26	128.58	120.44
3	L	44	TYR	C-N-CA	6.26	128.58	120.44
1	B	144	VAL	CA-C-O	-6.26	114.33	121.59
1	g	160	LYS	O-C-N	-6.26	115.33	122.09
2	2	97	LEU	CA-C-N	6.25	128.66	120.28
2	2	97	LEU	C-N-CA	6.25	128.66	120.28
2	n	118	GLU	O-C-N	6.25	128.75	122.12
2	n	200	SER	N-CA-CB	6.25	121.50	110.37
1	f	30	ALA	N-CA-C	6.25	118.90	111.71
1	f	53	ARG	N-CA-CB	6.25	119.16	109.97
3	I	57	ARG	NE-CZ-NH2	-6.25	113.57	119.20
3	L	281	VAL	N-CA-C	-6.25	99.36	108.11
3	M	102	PRO	O-C-N	6.25	131.08	122.64
1	g	187	ASP	CA-C-N	6.25	129.28	120.28
1	g	187	ASP	C-N-CA	6.25	129.28	120.28
1	C	62	ASP	N-CA-C	6.25	119.07	111.82
1	G	137	LEU	N-CA-C	-6.25	99.01	109.07
3	J	357	GLU	CA-C-O	-6.25	112.42	119.79
1	f	221	PHE	N-CA-CB	6.25	121.05	110.49
2	i	145	LEU	N-CA-C	-6.25	104.47	111.28
2	4	45	ILE	N-CA-C	-6.25	96.35	109.34
3	L	101	LYS	N-CA-C	-6.25	98.11	108.23
1	B	12	ILE	CA-CB-CG1	6.24	121.01	110.40
1	C	188	ALA	N-CA-C	6.24	118.08	111.28
2	7	28	GLU	N-CA-C	-6.24	98.23	108.41
1	a	166	MET	N-CA-C	-6.24	105.67	113.28
3	H	309	VAL	CA-C-O	-6.24	111.59	119.95
1	b	199	SER	CB-CA-C	-6.24	101.08	110.88
1	e	35	ALA	CA-C-N	6.24	133.46	121.54
1	e	35	ALA	C-N-CA	6.24	133.46	121.54
2	2	146	THR	N-CA-C	-6.24	104.56	111.36
2	i	176	MET	O-C-N	-6.24	114.92	122.22
1	D	216	VAL	N-CA-C	6.23	116.34	110.30
1	G	187	ASP	CA-C-N	6.23	129.14	120.29
1	G	187	ASP	C-N-CA	6.23	129.14	120.29
2	7	28	GLU	N-CA-CB	6.23	120.37	110.65
3	I	109	ASN	CB-CG-ND2	6.23	125.75	116.40
2	6	165	VAL	CA-C-N	6.23	128.63	120.28
2	6	165	VAL	C-N-CA	6.23	128.63	120.28
3	K	137	GLU	N-CA-C	-6.23	104.95	113.30
1	b	117	CYS	CA-C-N	6.23	129.13	120.29
1	b	117	CYS	C-N-CA	6.23	129.13	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	130	PHE	CA-C-N	6.23	129.55	120.71
3	J	130	PHE	C-N-CA	6.23	129.55	120.71
3	H	175	PRO	CA-C-O	-6.23	114.46	121.43
3	J	267	GLN	N-CA-C	6.23	118.07	111.28
1	g	67	ILE	N-CA-CB	6.22	119.73	111.64
1	g	100	ARG	NE-CZ-NH1	-6.22	115.28	121.50
2	j	174	SER	CA-C-N	6.22	128.62	120.28
2	j	174	SER	C-N-CA	6.22	128.62	120.28
2	k	39	SER	CA-C-N	6.22	131.26	122.05
2	k	39	SER	C-N-CA	6.22	131.26	122.05
3	L	40	GLU	N-CA-CB	6.22	119.27	110.12
3	L	96	ASN	CA-C-O	-6.22	114.54	121.51
3	J	183	PRO	CA-C-N	6.22	127.62	119.84
3	J	183	PRO	C-N-CA	6.22	127.62	119.84
2	n	147	ALA	N-CA-C	-6.22	104.42	111.14
1	F	12	ILE	N-CA-C	-6.22	106.65	113.43
1	e	241	ARG	NE-CZ-NH1	-6.21	115.29	121.50
2	2	95	SER	CA-C-N	6.21	128.61	120.28
2	2	95	SER	C-N-CA	6.21	128.61	120.28
3	K	61	PRO	N-CA-CB	6.21	109.11	103.08
3	L	285	GLY	N-CA-C	-6.21	102.83	111.09
2	n	49	ALA	N-CA-C	-6.21	100.36	109.18
3	H	170	VAL	CA-C-O	6.21	127.75	121.17
3	J	191	LEU	CA-C-N	6.21	128.51	120.44
3	J	191	LEU	C-N-CA	6.21	128.51	120.44
1	E	70	ILE	O-C-N	6.20	128.52	122.07
2	k	75	ASN	N-CA-CB	6.20	119.34	110.16
1	D	102	THR	O-C-N	-6.20	114.72	122.35
1	f	123	TYR	N-CA-C	-6.20	105.36	113.17
2	n	65	PHE	N-CA-CB	6.20	119.33	110.16
3	K	360	MET	CA-C-N	6.20	129.09	120.29
3	K	360	MET	C-N-CA	6.20	129.09	120.29
1	G	204	LEU	CA-C-N	6.20	131.98	121.88
1	G	204	LEU	C-N-CA	6.20	131.98	121.88
1	B	205	VAL	O-C-N	-6.20	114.04	121.10
1	c	211	VAL	N-CA-C	-6.20	99.28	108.45
3	H	331	ALA	CA-C-N	6.20	130.16	121.24
3	H	331	ALA	C-N-CA	6.20	130.16	121.24
3	L	182	GLY	CA-C-N	6.19	126.76	120.38
3	L	182	GLY	C-N-CA	6.19	126.76	120.38
1	F	151	ASP	CA-C-O	-6.19	114.47	120.97
1	g	28	ARG	NE-CZ-NH1	6.19	127.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	115	ILE	CA-C-N	6.19	132.02	121.87
2	l	115	ILE	C-N-CA	6.19	132.02	121.87
3	I	46	ARG	O-C-N	6.19	128.68	122.12
1	f	219	ARG	N-CA-C	-6.19	103.63	111.92
2	m	201	PRO	O-C-N	6.19	130.99	122.64
1	b	28	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	e	66	LYS	N-CA-C	-6.18	105.43	114.39
1	g	212	GLY	O-C-N	-6.18	117.86	123.36
2	5	37	ILE	CA-C-O	-6.18	115.51	121.63
1	A	151	ASP	CA-CB-CG	-6.18	106.42	112.60
1	B	172	THR	CA-C-N	6.18	128.56	120.28
1	B	172	THR	C-N-CA	6.18	128.56	120.28
1	G	129	VAL	N-CA-C	-6.18	100.19	108.35
2	2	28	GLU	N-CA-CB	6.18	120.20	110.56
2	3	74	ALA	CA-C-O	6.18	126.97	120.42
3	H	352	LYS	CA-C-N	6.18	128.56	120.28
3	H	352	LYS	C-N-CA	6.18	128.56	120.28
3	K	305	ARG	NE-CZ-NH2	-6.18	113.64	119.20
3	L	52	ARG	N-CA-C	-6.18	104.62	111.36
1	G	93	ARG	CA-C-O	-6.18	113.87	120.42
3	J	28	ARG	CA-C-N	6.18	128.47	120.44
3	J	28	ARG	C-N-CA	6.18	128.47	120.44
2	3	103	TYR	N-CA-C	-6.17	105.75	113.28
2	l	137	ILE	N-CA-CB	6.17	121.42	111.23
3	M	58	LEU	O-C-N	6.17	129.19	122.15
1	e	23	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	f	58	LEU	N-CA-C	-6.17	104.82	112.90
2	j	59	SER	CA-C-N	6.17	129.18	120.42
2	j	59	SER	C-N-CA	6.17	129.18	120.42
3	J	133	GLU	N-CA-C	-6.17	100.16	108.86
1	g	59	LEU	CA-C-N	6.17	130.12	121.24
1	g	59	LEU	C-N-CA	6.17	130.12	121.24
3	I	37	ILE	CA-C-N	6.17	128.54	120.28
3	I	37	ILE	C-N-CA	6.17	128.54	120.28
2	3	209	ALA	CA-C-N	6.16	132.22	122.60
2	3	209	ALA	C-N-CA	6.16	132.22	122.60
3	I	361	PHE	N-CA-CB	6.16	119.28	110.16
3	J	304	ASP	N-CA-C	-6.16	97.67	110.80
1	g	100	ARG	N-CA-CB	6.16	119.28	110.16
2	2	166	GLU	CA-C-N	6.16	128.53	120.28
2	2	166	GLU	C-N-CA	6.16	128.53	120.28
1	F	63	THR	CA-CB-OG1	6.16	118.84	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	214	VAL	N-CA-CB	6.16	119.64	111.64
2	2	24	VAL	N-CA-C	-6.16	99.34	108.45
1	d	33	ARG	CA-C-O	-6.16	112.37	119.14
1	E	52	LYS	CA-C-N	6.16	129.85	121.05
1	E	52	LYS	C-N-CA	6.16	129.85	121.05
1	F	172	THR	CA-C-N	6.16	128.53	120.28
1	F	172	THR	C-N-CA	6.16	128.53	120.28
3	I	334	VAL	CA-C-O	-6.16	113.83	120.85
3	M	210	GLU	CA-C-O	6.16	127.08	120.55
1	b	41	LYS	N-CA-C	-6.15	99.37	109.40
3	M	90	ASN	CA-CB-CG	-6.15	106.45	112.60
1	B	23	GLN	CA-C-O	6.15	126.94	120.42
2	k	67	ALA	CA-C-N	6.15	129.66	120.31
2	k	67	ALA	C-N-CA	6.15	129.66	120.31
3	J	215	TYR	N-CA-CB	6.15	121.94	111.66
1	E	97	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	F	230	LYS	CA-C-O	-6.15	112.97	118.63
1	g	134	VAL	N-CA-C	-6.15	99.62	108.42
2	4	189	VAL	N-CA-C	-6.15	99.19	108.17
2	1	121	SER	O-C-N	-6.15	117.37	123.46
2	6	67	ALA	CA-C-N	6.15	128.52	120.28
2	6	67	ALA	C-N-CA	6.15	128.52	120.28
1	e	146	LYS	N-CA-CB	6.15	120.91	110.71
3	L	224	ARG	NE-CZ-NH1	-6.15	115.35	121.50
3	J	246	ILE	CA-C-N	6.15	130.09	121.24
3	J	246	ILE	C-N-CA	6.15	130.09	121.24
1	c	37	ALA	O-C-N	-6.14	115.78	123.27
2	6	62	ASP	CA-CB-CG	6.14	118.74	112.60
1	f	146	LYS	O-C-N	6.14	130.76	123.27
1	G	237	ASN	N-CA-C	6.14	118.77	111.71
2	n	18	VAL	CB-CA-C	6.14	119.62	111.21
2	j	132	ILE	CA-CB-CG2	-6.14	100.07	110.50
2	6	68	ARG	N-CA-C	6.14	117.97	111.28
3	K	371	THR	CA-C-N	6.14	128.50	120.28
3	K	371	THR	C-N-CA	6.14	128.50	120.28
3	J	35	LYS	N-CA-CB	6.14	118.97	110.07
1	A	190	VAL	O-C-N	6.14	127.92	121.91
1	D	26	TYR	N-CA-C	-6.14	105.83	113.38
1	e	216	VAL	N-CA-C	-6.14	104.37	113.39
1	F	151	ASP	CA-C-N	6.14	126.25	119.87
1	F	151	ASP	C-N-CA	6.14	126.25	119.87
2	6	50	ASP	CA-CB-CG	6.14	118.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	295	PRO	CA-C-O	-6.13	114.67	121.23
3	I	176	LYS	N-CA-C	-6.13	104.97	112.88
1	g	212	GLY	N-CA-C	-6.13	101.52	110.90
1	d	200	ILE	CA-CB-CG2	-6.13	100.08	110.50
2	3	201	PRO	CA-C-N	6.13	128.82	120.54
2	3	201	PRO	C-N-CA	6.13	128.82	120.54
2	k	70	ILE	CA-C-N	6.13	128.41	120.44
2	k	70	ILE	C-N-CA	6.13	128.41	120.44
1	F	57	LYS	CA-C-N	6.13	132.66	122.54
1	F	57	LYS	C-N-CA	6.13	132.66	122.54
3	J	30	LEU	CA-C-N	6.13	128.41	120.44
3	J	30	LEU	C-N-CA	6.13	128.41	120.44
3	K	356	THR	CA-C-N	6.13	128.99	120.29
3	K	356	THR	C-N-CA	6.13	128.99	120.29
1	e	24	VAL	CB-CA-C	-6.13	103.77	112.22
2	1	178	ARG	CA-C-O	6.13	126.91	120.42
2	6	170	ARG	NE-CZ-NH2	6.13	124.71	119.20
3	I	240	ILE	CA-C-O	-6.13	113.98	120.53
2	5	201	PRO	CA-C-N	6.12	128.81	120.54
2	5	201	PRO	C-N-CA	6.12	128.81	120.54
1	B	131	PRO	N-CA-C	-6.12	100.74	112.01
2	3	148	TYR	N-CA-C	6.12	118.75	111.71
3	H	276	ASP	CA-C-O	-6.12	113.03	120.74
3	L	20	TYR	CA-C-N	6.12	128.40	120.44
3	L	20	TYR	C-N-CA	6.12	128.40	120.44
1	G	28	ARG	NE-CZ-NH1	-6.12	115.38	121.50
3	L	373	LEU	N-CA-C	-6.12	104.61	111.28
3	M	67	VAL	N-CA-CB	6.12	123.25	111.93
1	c	185	PHE	CA-C-N	6.12	128.97	120.29
1	c	185	PHE	C-N-CA	6.12	128.97	120.29
1	d	144	VAL	O-C-N	-6.11	115.43	121.12
1	e	83	ALA	CA-C-N	6.11	128.97	120.29
1	e	83	ALA	C-N-CA	6.11	128.97	120.29
2	h	36	PHE	CA-CB-CG	-6.11	107.69	113.80
1	g	160	LYS	CB-CA-C	-6.11	101.24	110.90
1	A	184	SER	CA-C-O	-6.11	114.74	121.89
2	7	136	ASP	CA-C-N	6.11	131.49	123.06
2	7	136	ASP	C-N-CA	6.11	131.49	123.06
2	h	61	GLY	CA-C-O	-6.11	114.06	120.90
1	a	26	TYR	CA-C-O	6.11	127.02	120.55
2	2	145	LEU	CA-C-N	6.11	128.96	120.29
2	2	145	LEU	C-N-CA	6.11	128.96	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	122	ILE	N-CA-C	-6.11	99.41	108.45
3	H	99	GLU	CA-C-N	6.11	133.07	122.81
3	H	99	GLU	C-N-CA	6.11	133.07	122.81
3	H	273	ASP	CB-CA-C	-6.11	100.66	110.79
3	M	257	GLY	CA-C-O	-6.11	113.81	120.40
1	e	115	LYS	CA-C-O	6.10	126.89	120.42
1	G	167	GLY	CA-C-N	6.10	129.98	120.82
1	G	167	GLY	C-N-CA	6.10	129.98	120.82
1	d	83	ALA	CA-C-O	-6.10	114.41	120.82
1	d	168	ARG	O-C-N	6.10	128.61	122.08
1	G	33	ARG	CD-NE-CZ	-6.10	115.86	124.40
2	1	129	GLY	CA-C-O	-6.10	118.06	122.45
2	4	178	ARG	CA-C-O	-6.10	111.67	118.69
2	4	203	GLU	O-C-N	-6.10	114.76	122.27
2	7	180	SER	CA-C-N	6.10	131.96	122.26
2	7	180	SER	C-N-CA	6.10	131.96	122.26
3	L	168	ALA	CA-C-N	6.10	128.45	120.28
3	L	168	ALA	C-N-CA	6.10	128.45	120.28
3	J	17	GLU	CA-C-N	6.10	128.45	120.28
3	J	17	GLU	C-N-CA	6.10	128.45	120.28
1	b	101	LEU	N-CA-C	-6.09	103.96	111.40
2	2	112	ILE	N-CA-CB	6.09	119.56	111.64
1	E	112	LEU	CA-C-N	6.09	128.94	120.29
1	E	112	LEU	C-N-CA	6.09	128.94	120.29
1	D	208	ASN	CA-CB-CG	-6.09	106.51	112.60
3	H	149	GLN	OE1-CD-NE2	6.09	128.69	122.60
2	1	33	MET	N-CA-CB	6.09	120.64	110.59
2	i	53	ALA	CA-C-N	6.09	131.36	122.77
2	i	53	ALA	C-N-CA	6.09	131.36	122.77
3	I	39	SER	N-CA-C	-6.09	104.72	111.36
3	I	302	ARG	N-CA-C	-6.09	104.92	112.72
3	K	9	LEU	CA-C-N	6.09	129.57	120.31
3	K	9	LEU	C-N-CA	6.09	129.57	120.31
1	g	73	HIS	CE1-NE2-CD2	-6.09	102.91	109.00
1	C	168	ARG	CG-CD-NE	-6.08	98.61	112.00
2	1	124	SER	N-CA-C	-6.08	99.80	109.59
2	h	185	GLY	CA-C-N	6.08	131.57	122.75
2	h	185	GLY	C-N-CA	6.08	131.57	122.75
3	H	190	LEU	CA-C-N	6.08	129.56	120.31
3	H	190	LEU	C-N-CA	6.08	129.56	120.31
3	J	374	ASP	N-CA-CB	6.08	119.06	110.12
1	c	46	VAL	N-CA-CB	6.08	121.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLU	N-CA-C	6.08	118.87	111.82
1	D	90	ASP	N-CA-CB	6.08	118.82	110.01
1	F	39	GLY	CA-C-O	-6.08	116.28	121.57
2	2	86	THR	CA-C-N	6.08	128.79	120.46
2	2	86	THR	C-N-CA	6.08	128.79	120.46
1	A	180	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	G	159	TYR	CB-CG-CD1	-6.08	111.69	120.80
1	a	55	GLY	CA-C-N	6.07	131.76	120.95
1	a	55	GLY	C-N-CA	6.07	131.76	120.95
3	L	46	ARG	CB-CA-C	-6.07	100.53	110.85
3	L	71	ILE	N-CA-C	-6.07	99.67	108.17
3	M	303	PHE	N-CA-C	-6.07	95.66	107.62
1	d	135	SER	CA-C-N	6.07	132.12	122.59
1	d	135	SER	C-N-CA	6.07	132.12	122.59
1	G	125	GLN	N-CA-CB	6.07	119.15	110.16
2	l	164	ALA	CA-C-N	6.07	128.78	120.46
2	l	164	ALA	C-N-CA	6.07	128.78	120.46
1	D	118	ASP	CA-C-O	-6.07	113.98	120.42
1	e	173	GLU	CA-C-N	6.07	128.41	120.28
1	e	173	GLU	C-N-CA	6.07	128.41	120.28
3	J	290	ILE	N-CA-C	-6.07	106.84	112.43
2	3	66	LEU	CA-C-N	6.07	128.91	120.29
2	3	66	LEU	C-N-CA	6.07	128.91	120.29
2	j	50	ASP	N-CA-C	6.07	119.52	111.75
1	B	235	ARG	CD-NE-CZ	-6.07	115.91	124.40
2	5	72	ILE	N-CA-C	-6.07	104.83	110.53
2	n	97	LEU	N-CA-C	6.07	117.56	111.07
3	J	319	GLN	CA-C-N	6.07	128.32	120.56
3	J	319	GLN	C-N-CA	6.07	128.32	120.56
3	K	316	GLY	O-C-N	6.06	128.05	122.17
1	G	144	VAL	N-CA-C	-6.06	95.78	108.88
2	7	210	LYS	N-CA-C	-6.06	105.06	112.88
1	E	130	ARG	NE-CZ-NH1	6.06	127.56	121.50
2	4	173	TYR	N-CA-C	-6.06	104.75	111.36
1	E	99	ASN	CA-C-O	-6.06	113.00	119.97
1	g	18	ASP	O-C-N	6.06	129.91	122.34
1	g	142	ASP	CA-C-N	6.06	133.11	121.54
1	g	142	ASP	C-N-CA	6.06	133.11	121.54
2	7	128	ILE	N-CA-C	-6.06	105.77	113.22
3	L	258	ASP	CA-C-N	6.06	128.89	120.29
3	L	258	ASP	C-N-CA	6.06	128.89	120.29
1	E	152	PRO	CA-C-N	6.06	129.52	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	PRO	C-N-CA	6.06	129.52	120.31
1	G	179	TYR	CB-CG-CD2	6.06	129.88	120.80
1	g	113	ALA	O-C-N	6.05	129.72	122.27
3	K	397	PHE	N-CA-CB	6.05	120.01	110.87
3	J	120	PRO	CA-C-O	-6.05	114.72	121.32
1	d	210	GLU	N-CA-C	-6.05	98.53	108.76
2	5	140	THR	N-CA-CB	6.05	121.77	111.66
3	H	220	ALA	N-CA-C	-6.05	104.25	111.69
2	1	206	GLN	O-C-N	-6.05	114.11	122.46
2	5	211	PHE	N-CA-C	-6.05	105.48	112.92
2	7	104	PHE	CA-C-O	-6.05	113.09	120.05
2	n	21	ASP	N-CA-C	-6.05	105.62	114.39
3	H	139	SER	N-CA-C	-6.05	97.92	110.80
1	A	49	ILE	N-CA-CB	6.05	119.76	111.41
3	H	98	GLU	N-CA-C	-6.05	105.55	113.17
3	L	225	GLU	CB-CG-CD	-6.05	102.32	112.60
3	J	145	GLY	CA-C-N	6.05	132.59	121.70
3	J	145	GLY	C-N-CA	6.05	132.59	121.70
1	A	99	ASN	CA-C-N	6.05	129.50	120.31
1	A	99	ASN	C-N-CA	6.05	129.50	120.31
1	f	95	GLU	O-C-N	6.05	128.53	122.12
3	L	28	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	e	190	VAL	CA-C-O	-6.04	114.66	120.95
1	f	190	VAL	CA-CB-CG2	-6.04	100.12	110.40
2	k	142	SER	CB-CA-C	-6.04	100.00	110.09
1	A	18	ASP	CB-CA-C	-6.04	101.35	110.90
3	L	268	LEU	CA-C-N	6.04	128.38	120.28
3	L	268	LEU	C-N-CA	6.04	128.38	120.28
3	J	340	ALA	N-CA-CB	6.04	119.00	110.12
1	B	200	ILE	CA-C-N	6.04	130.71	122.19
1	B	200	ILE	C-N-CA	6.04	130.71	122.19
3	K	275	PHE	CB-CA-C	-6.04	100.76	110.79
1	f	124	THR	N-CA-C	-6.04	106.45	113.88
2	n	212	ARG	N-CA-C	-6.04	99.87	109.59
3	K	361	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	29	GLU	CB-CG-CD	6.04	122.86	112.60
2	1	172	ILE	CB-CA-C	-6.04	103.89	112.22
3	M	224	ARG	CA-C-N	6.04	128.69	120.54
3	M	224	ARG	C-N-CA	6.04	128.69	120.54
1	A	106	PRO	N-CA-CB	6.03	109.58	103.25
1	e	86	ARG	NE-CZ-NH2	6.03	124.63	119.20
3	H	252	ASN	CA-C-N	6.03	132.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	252	ASN	C-N-CA	6.03	132.56	121.70
3	K	115	ILE	CA-C-N	6.03	128.95	121.71
3	K	115	ILE	C-N-CA	6.03	128.95	121.71
1	A	48	LEU	CA-C-O	-6.03	113.62	120.32
1	b	168	ARG	CA-C-O	-6.03	114.49	120.70
2	j	169	VAL	O-C-N	6.03	127.82	121.91
1	F	79	SER	N-CA-C	-6.03	99.53	108.99
3	I	101	LYS	CA-C-O	-6.03	114.53	120.26
2	h	83	ARG	N-CA-C	-6.03	99.36	108.52
3	I	186	THR	N-CA-C	-6.03	105.58	113.17
2	6	161	VAL	CB-CA-C	-6.02	103.91	112.22
2	h	35	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	d	90	ASP	CA-C-N	6.02	128.26	120.44
1	d	90	ASP	C-N-CA	6.02	128.26	120.44
1	d	119	PHE	CA-CB-CG	-6.02	107.78	113.80
1	F	220	THR	O-C-N	-6.02	116.02	123.36
2	m	47	GLN	N-CA-CB	6.02	120.46	110.47
2	m	66	LEU	CA-C-N	6.02	128.34	120.28
2	m	66	LEU	C-N-CA	6.02	128.34	120.28
3	K	95	ILE	N-CA-CB	6.02	119.80	112.10
1	b	18	ASP	CA-CB-CG	-6.02	106.58	112.60
1	C	161	ALA	O-C-N	-6.02	116.56	123.42
2	6	154	ARG	NE-CZ-NH2	-6.01	113.79	119.20
2	m	80	ARG	CB-CA-C	-6.01	101.40	110.90
3	H	164	PRO	N-CA-C	-6.01	105.82	114.18
3	J	305	ARG	CA-C-O	6.01	127.56	120.70
1	E	218	ASP	N-CA-C	-6.01	106.07	113.41
2	2	100	SER	N-CA-CB	6.01	118.79	110.07
2	m	73	GLU	CA-C-N	6.01	128.62	120.44
2	m	73	GLU	C-N-CA	6.01	128.62	120.44
3	L	282	LYS	N-CA-CB	6.01	120.71	110.50
2	1	166	GLU	CA-C-N	6.01	128.82	120.29
2	1	166	GLU	C-N-CA	6.01	128.82	120.29
2	5	87	VAL	CB-CA-C	-6.01	102.85	112.16
3	K	10	LEU	N-CA-C	-6.01	104.85	111.82
1	d	67	ILE	N-CA-C	-6.00	99.09	107.80
2	1	84	LYS	CA-C-N	6.00	126.02	119.90
2	1	84	LYS	C-N-CA	6.00	126.02	119.90
2	6	59	SER	CA-C-N	6.00	128.12	120.56
2	6	59	SER	C-N-CA	6.00	128.12	120.56
1	g	235	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	d	158	GLU	N-CA-C	-6.00	99.41	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	204	VAL	CA-C-N	6.00	128.92	120.28
2	7	204	VAL	C-N-CA	6.00	128.92	120.28
3	K	26	LEU	N-CA-C	6.00	117.49	111.07
3	M	210	GLU	CA-C-N	6.00	129.36	120.90
3	M	210	GLU	C-N-CA	6.00	129.36	120.90
1	C	175	PHE	CB-CG-CD1	6.00	130.89	120.70
1	f	103	TYR	N-CA-C	-6.00	107.78	114.62
2	n	31	ALA	CA-C-O	-6.00	113.67	120.32
3	L	15	LYS	CA-C-N	6.00	128.80	120.29
3	L	15	LYS	C-N-CA	6.00	128.80	120.29
1	E	202	SER	N-CA-C	-5.99	100.41	108.86
2	1	63	ALA	CA-C-N	5.99	128.80	120.29
2	1	63	ALA	C-N-CA	5.99	128.80	120.29
2	l	143	GLY	N-CA-C	-5.99	105.18	115.61
3	I	347	SER	CA-C-N	5.99	127.83	120.22
3	I	347	SER	C-N-CA	5.99	127.83	120.22
3	M	256	SER	N-CA-C	5.99	117.48	111.07
1	E	12	ILE	O-C-N	-5.99	115.76	122.05
3	M	335	ASP	CA-C-O	5.99	126.71	120.30
1	b	186	ASP	O-C-N	-5.99	115.32	122.15
1	c	92	ALA	CA-C-O	-5.99	114.53	120.82
2	2	142	SER	N-CA-C	-5.99	105.46	112.89
2	i	185	GLY	N-CA-C	-5.99	98.98	113.18
2	j	160	GLY	N-CA-C	-5.99	104.54	112.81
3	H	186	THR	N-CA-C	-5.99	105.80	113.23
3	L	372	MET	CA-C-N	5.99	128.31	120.28
3	L	372	MET	C-N-CA	5.99	128.31	120.28
2	1	85	PRO	CA-C-N	5.99	130.34	120.94
2	1	85	PRO	C-N-CA	5.99	130.34	120.94
3	H	159	LEU	CA-C-N	5.99	125.61	119.56
3	H	159	LEU	C-N-CA	5.99	125.61	119.56
2	1	39	SER	N-CA-C	-5.99	98.05	110.80
2	n	56	THR	CA-CB-OG1	5.99	118.58	109.60
3	K	289	ARG	NH1-CZ-NH2	5.99	127.08	119.30
1	B	41	LYS	O-C-N	-5.98	116.23	123.29
1	e	70	ILE	CB-CA-C	5.98	118.86	111.80
3	J	49	ARG	CA-C-N	5.98	128.30	120.28
3	J	49	ARG	C-N-CA	5.98	128.30	120.28
1	e	152	PRO	CA-C-N	5.98	128.57	120.44
1	e	152	PRO	C-N-CA	5.98	128.57	120.44
2	2	191	ILE	N-CA-C	-5.98	96.90	109.34
2	7	144	SER	CA-C-N	5.98	128.78	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	144	SER	C-N-CA	5.98	128.78	120.29
3	J	178	VAL	N-CA-C	-5.98	99.02	107.75
2	4	34	GLY	CA-C-N	5.98	131.08	122.35
2	4	34	GLY	C-N-CA	5.98	131.08	122.35
3	L	45	GLU	N-CA-CB	5.98	118.68	110.01
1	C	77	ALA	N-CA-C	-5.97	100.41	109.85
1	C	106	PRO	CA-C-N	5.97	128.51	120.50
1	C	106	PRO	C-N-CA	5.97	128.51	120.50
2	4	112	ILE	N-CA-C	-5.97	99.87	108.53
1	b	108	THR	CA-C-N	5.97	128.09	120.56
1	b	108	THR	C-N-CA	5.97	128.09	120.56
2	1	58	GLY	O-C-N	-5.97	117.76	122.90
2	i	84	LYS	CA-C-N	5.97	125.94	120.21
2	i	84	LYS	C-N-CA	5.97	125.94	120.21
1	E	194	VAL	CA-C-N	5.97	128.56	120.44
1	E	194	VAL	C-N-CA	5.97	128.56	120.44
2	1	181	ALA	CA-C-O	-5.97	112.08	119.18
3	L	214	LYS	N-CA-CB	5.97	119.63	110.79
1	C	73	HIS	ND1-CE1-NE2	5.97	114.37	108.40
2	i	26	ALA	N-CA-C	-5.97	100.00	109.07
1	E	220	THR	CA-CB-CG2	5.97	120.64	110.50
2	1	45	ILE	N-CA-C	-5.97	99.76	108.11
2	h	169	VAL	O-C-N	5.97	127.66	121.87
2	7	43	LYS	CA-C-N	5.97	131.90	121.52
2	7	43	LYS	C-N-CA	5.97	131.90	121.52
3	M	395	VAL	N-CA-C	-5.97	105.94	112.80
1	g	134	VAL	O-C-N	5.96	129.56	123.00
2	i	166	GLU	N-CA-C	-5.96	104.86	111.36
3	K	397	PHE	N-CA-C	-5.96	101.10	109.69
1	A	150	THR	N-CA-C	-5.96	100.47	109.95
1	G	142	ASP	N-CA-C	-5.96	103.46	112.04
1	G	184	SER	CA-C-N	5.96	128.27	120.28
1	G	184	SER	C-N-CA	5.96	128.27	120.28
3	K	258	ASP	N-CA-CB	5.96	120.56	110.49
1	e	170	ALA	CA-C-N	5.96	130.54	120.29
1	e	170	ALA	C-N-CA	5.96	130.54	120.29
2	4	170	ARG	CA-C-N	5.96	128.27	120.28
2	4	170	ARG	C-N-CA	5.96	128.27	120.28
2	k	68	ARG	NE-CZ-NH1	5.96	127.46	121.50
3	J	232	GLU	CA-C-O	-5.96	114.10	120.42
3	J	374	ASP	CA-C-N	5.96	128.19	120.44
3	J	374	ASP	C-N-CA	5.96	128.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	SER	CA-C-N	5.96	125.64	119.56
1	A	225	SER	C-N-CA	5.96	125.64	119.56
1	D	142	ASP	N-CA-CB	5.96	118.95	110.13
2	i	132	ILE	CA-C-O	-5.96	114.14	120.39
2	m	52	MET	N-CA-C	-5.96	99.29	109.24
3	M	391	ASP	CA-C-O	5.96	126.87	120.38
1	C	214	VAL	N-CA-C	-5.96	97.23	107.24
2	l	125	ILE	CA-C-N	5.96	133.63	121.48
2	l	125	ILE	C-N-CA	5.96	133.63	121.48
3	I	294	ASP	CA-C-N	5.96	126.38	119.47
3	I	294	ASP	C-N-CA	5.96	126.38	119.47
1	F	159	TYR	CG-CD2-CE2	-5.95	112.27	121.20
3	H	13	LEU	CA-C-N	5.95	128.26	120.28
3	H	13	LEU	C-N-CA	5.95	128.26	120.28
1	f	28	ARG	CA-C-N	5.95	128.26	120.28
1	f	28	ARG	C-N-CA	5.95	128.26	120.28
3	I	127	VAL	CA-C-N	5.95	128.53	120.38
3	I	127	VAL	C-N-CA	5.95	128.53	120.38
3	I	192	ALA	CA-C-O	-5.95	114.24	120.55
1	b	173	GLU	CA-C-N	5.95	128.53	120.44
1	b	173	GLU	C-N-CA	5.95	128.53	120.44
1	F	15	PHE	N-CA-C	-5.95	100.56	109.96
1	F	213	TYR	N-CA-CB	5.95	120.62	111.46
1	G	179	TYR	CB-CG-CD1	-5.95	111.87	120.80
2	2	159	ILE	CA-C-O	-5.95	115.06	121.19
2	3	89	ALA	CA-C-N	5.95	128.61	120.46
2	3	89	ALA	C-N-CA	5.95	128.61	120.46
3	H	194	ALA	N-CA-C	5.95	117.44	111.07
3	J	118	VAL	N-CA-C	-5.95	99.78	108.11
1	c	168	ARG	NE-CZ-NH2	-5.95	113.85	119.20
1	a	190	VAL	CA-C-O	-5.95	114.55	120.85
1	C	81	LEU	CA-C-O	-5.95	114.65	121.19
2	h	80	ARG	NE-CZ-NH1	-5.95	115.55	121.50
2	k	116	ASP	CA-CB-CG	5.95	118.55	112.60
2	7	56	THR	N-CA-C	5.95	119.09	109.40
3	L	329	LYS	N-CA-C	-5.95	105.94	112.72
1	d	82	VAL	CA-C-N	5.94	128.17	120.44
1	d	82	VAL	C-N-CA	5.94	128.17	120.44
2	7	171	ALA	N-CA-C	5.94	117.43	111.07
3	M	379	ILE	O-C-N	5.94	127.64	121.87
1	c	21	LEU	CA-C-N	5.94	128.24	120.28
1	c	21	LEU	C-N-CA	5.94	128.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	ALA	N-CA-CB	5.94	120.53	110.49
1	G	7	GLY	O-C-N	-5.94	115.31	122.38
2	1	202	GLU	N-CA-C	5.94	118.24	111.11
3	K	292	ILE	N-CA-C	-5.94	96.98	109.34
1	g	186	ASP	CA-C-N	5.94	128.52	120.44
1	g	186	ASP	C-N-CA	5.94	128.52	120.44
3	K	239	PHE	CB-CA-C	-5.94	101.27	110.78
3	J	220	ALA	CA-C-N	5.94	128.73	120.29
3	J	220	ALA	C-N-CA	5.94	128.73	120.29
1	F	132	PHE	CA-CB-CG	5.94	119.74	113.80
1	f	165	GLY	CA-C-N	5.94	129.34	120.31
1	f	165	GLY	C-N-CA	5.94	129.34	120.31
2	2	104	PHE	CA-C-N	5.94	127.26	119.84
2	2	104	PHE	C-N-CA	5.94	127.26	119.84
2	m	60	VAL	CA-C-N	5.94	126.68	120.03
2	m	60	VAL	C-N-CA	5.94	126.68	120.03
1	A	86	ARG	CB-CA-C	-5.94	101.31	110.81
2	4	102	ARG	CA-C-N	5.94	128.83	120.28
2	4	102	ARG	C-N-CA	5.94	128.83	120.28
3	M	50	ARG	CD-NE-CZ	-5.94	116.09	124.40
1	e	245	LYS	N-CA-CB	5.94	119.60	110.81
3	H	98	GLU	O-C-N	-5.94	114.92	122.34
3	M	365	GLU	CA-C-N	5.94	131.18	122.63
3	M	365	GLU	C-N-CA	5.94	131.18	122.63
1	b	214	VAL	N-CA-C	-5.93	96.05	106.61
1	g	202	SER	CA-C-N	5.93	129.26	120.95
1	g	202	SER	C-N-CA	5.93	129.26	120.95
1	E	70	ILE	N-CA-C	-5.93	107.09	111.90
1	E	135	SER	N-CA-CB	-5.93	100.51	110.83
2	h	168	ALA	N-CA-C	-5.93	104.72	111.07
2	i	106	TYR	CA-C-O	5.93	127.58	120.28
1	B	113	ALA	N-CA-C	-5.93	104.89	111.36
1	e	108	THR	N-CA-CB	5.93	119.30	110.29
2	5	178	ARG	NE-CZ-NH2	-5.93	113.86	119.20
3	K	349	ALA	CA-C-N	5.93	128.23	120.28
3	K	349	ALA	C-N-CA	5.93	128.23	120.28
3	L	182	GLY	O-C-N	5.93	127.70	121.77
1	E	168	ARG	CA-C-N	5.93	128.23	120.28
1	E	168	ARG	C-N-CA	5.93	128.23	120.28
2	1	165	VAL	CA-C-N	5.93	128.15	120.44
2	1	165	VAL	C-N-CA	5.93	128.15	120.44
3	I	114	ALA	O-C-N	-5.93	116.28	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ILE	CA-C-O	-5.93	114.56	120.90
1	F	245	LYS	N-CA-C	-5.93	99.07	108.73
2	k	176	MET	CG-SD-CE	-5.93	87.86	100.90
1	b	214	VAL	CA-C-O	-5.93	114.29	120.51
3	L	101	LYS	O-C-N	5.93	126.00	121.85
1	E	35	ALA	CA-C-N	5.92	132.85	121.54
1	E	35	ALA	C-N-CA	5.92	132.85	121.54
1	F	71	ASP	N-CA-C	-5.92	100.58	108.34
1	f	137	LEU	N-CA-C	-5.92	97.66	108.02
1	g	229	LEU	CA-C-N	5.92	130.91	121.62
1	g	229	LEU	C-N-CA	5.92	130.91	121.62
2	j	150	VAL	O-C-N	5.92	127.93	121.83
2	n	143	GLY	CA-C-N	5.92	128.21	120.28
2	n	143	GLY	C-N-CA	5.92	128.21	120.28
1	e	41	LYS	CA-C-N	5.92	132.06	122.53
1	e	41	LYS	C-N-CA	5.92	132.06	122.53
1	A	38	ILE	N-CA-C	-5.92	99.60	108.12
1	D	118	ASP	N-CA-CB	5.92	118.92	110.16
1	e	61	ALA	O-C-N	5.92	129.70	121.83
1	e	129	VAL	CB-CA-C	5.92	117.16	110.41
1	A	220	THR	N-CA-C	-5.92	97.83	108.48
1	d	34	GLY	O-C-N	5.92	127.90	122.81
2	h	40	LYS	N-CA-C	-5.92	107.05	114.56
3	J	24	ARG	N-CA-C	5.92	117.73	111.28
2	i	148	TYR	N-CA-C	5.92	117.73	111.28
3	K	130	PHE	CA-C-N	5.92	132.84	121.54
3	K	130	PHE	C-N-CA	5.92	132.84	121.54
2	5	74	ALA	CA-C-N	5.91	128.20	120.28
2	5	74	ALA	C-N-CA	5.91	128.20	120.28
2	m	169	VAL	CB-CA-C	-5.91	104.06	112.22
1	D	140	GLY	O-C-N	-5.91	118.26	123.76
2	1	138	VAL	N-CA-CB	5.91	119.74	111.05
2	5	176	MET	N-CA-C	-5.91	103.54	111.87
1	g	103	TYR	N-CA-C	-5.91	105.82	114.39
2	3	179	ASP	CA-CB-CG	-5.91	106.69	112.60
2	6	135	LYS	O-C-N	-5.91	115.98	122.07
3	H	174	PRO	N-CA-C	-5.91	103.49	110.70
3	M	353	ALA	CA-C-N	5.91	128.81	120.42
3	M	353	ALA	C-N-CA	5.91	128.81	120.42
2	6	88	ARG	NE-CZ-NH1	-5.91	115.59	121.50
2	7	27	THR	CA-CB-OG1	5.91	118.46	109.60
3	H	362	ALA	N-CA-CB	5.90	118.80	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLY	N-CA-C	-5.90	106.33	116.01
1	c	219	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	E	40	ILE	N-CA-C	-5.90	99.55	108.17
3	I	91	THR	CA-C-O	-5.90	115.15	121.94
3	I	382	VAL	CG1-CB-CG2	5.90	123.78	110.80
1	a	243	LEU	N-CA-CB	5.90	118.79	110.12
2	7	39	SER	CA-C-N	5.90	128.46	120.38
2	7	39	SER	C-N-CA	5.90	128.46	120.38
1	f	141	VAL	N-CA-C	-5.90	97.33	107.24
3	K	302	ARG	NE-CZ-NH2	-5.90	113.89	119.20
3	L	93	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	C	198	LEU	CA-C-N	5.90	128.66	120.29
1	C	198	LEU	C-N-CA	5.90	128.66	120.29
1	E	76	ALA	N-CA-CB	5.90	121.51	111.66
2	4	25	MET	N-CA-C	-5.89	100.29	109.72
2	l	40	LYS	CA-C-N	5.89	129.25	120.17
2	l	40	LYS	C-N-CA	5.89	129.25	120.17
3	I	325	THR	CA-C-N	5.89	128.45	120.38
3	I	325	THR	C-N-CA	5.89	128.45	120.38
3	M	224	ARG	NE-CZ-NH2	5.89	124.50	119.20
3	M	375	PHE	N-CA-CB	5.89	118.79	110.12
2	j	202	GLU	CA-C-N	5.89	128.18	120.28
2	j	202	GLU	C-N-CA	5.89	128.18	120.28
3	K	153	ILE	O-C-N	5.89	127.90	121.83
3	K	188	LYS	N-CA-C	5.89	117.70	111.28
3	H	143	ILE	N-CA-C	-5.89	100.00	108.48
3	M	130	PHE	N-CA-C	5.89	118.60	110.35
1	B	105	GLU	CA-C-O	-5.89	114.20	119.86
1	C	24	VAL	CA-C-N	5.89	128.17	120.28
1	C	24	VAL	C-N-CA	5.89	128.17	120.28
2	k	127	PRO	CA-C-N	5.89	132.01	122.76
2	k	127	PRO	C-N-CA	5.89	132.01	122.76
3	J	321	PHE	N-CA-CB	5.89	118.78	110.12
3	L	353	ALA	CA-C-N	5.89	127.98	120.56
3	L	353	ALA	C-N-CA	5.89	127.98	120.56
2	7	201	PRO	CA-C-N	5.89	128.97	120.79
2	7	201	PRO	C-N-CA	5.89	128.97	120.79
3	L	326	ARG	CD-NE-CZ	-5.89	116.16	124.40
1	c	196	MET	N-CA-C	-5.88	104.95	111.36
1	A	227	GLU	CA-C-N	5.88	128.16	120.28
1	A	227	GLU	C-N-CA	5.88	128.16	120.28
2	h	23	VAL	N-CA-C	-5.88	99.58	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	CA-C-N	5.88	128.75	120.28
1	A	116	ILE	C-N-CA	5.88	128.75	120.28
2	l	163	GLU	CB-CG-CD	-5.88	102.60	112.60
2	6	181	ALA	CA-C-O	-5.88	112.58	119.05
3	H	218	GLU	O-C-N	-5.88	115.04	122.27
2	k	155	PHE	CA-CB-CG	5.88	119.68	113.80
1	e	52	LYS	CA-C-O	-5.88	114.32	120.32
3	H	277	PRO	N-CA-CB	-5.88	97.29	103.52
2	3	148	TYR	CB-CA-C	-5.88	99.76	110.63
3	M	152	GLU	N-CA-C	5.88	117.77	111.36
1	A	65	GLU	N-CA-CB	5.88	120.49	110.50
2	h	192	THR	CA-CB-OG1	5.88	118.41	109.60
2	j	207	ILE	CA-C-O	-5.87	114.84	120.95
2	4	21	ASP	CB-CA-C	-5.87	100.54	110.64
3	I	278	ARG	CA-C-O	5.87	125.60	119.14
2	j	64	GLN	CB-CA-C	-5.87	101.62	110.90
3	J	65	VAL	N-CA-C	-5.87	100.12	108.58
1	a	28	ARG	CA-C-N	5.87	128.15	120.28
1	a	28	ARG	C-N-CA	5.87	128.15	120.28
1	F	241	ARG	N-CA-CB	5.87	119.26	110.22
1	G	133	GLY	N-CA-C	-5.87	99.27	113.18
2	4	130	GLY	N-CA-C	-5.87	104.21	112.60
2	5	169	VAL	N-CA-CB	5.87	118.52	110.54
1	c	205	VAL	N-CA-CB	-5.87	106.15	112.37
2	1	86	THR	N-CA-C	-5.87	102.23	110.50
2	6	115	ILE	CA-C-N	5.87	131.50	121.87
2	6	115	ILE	C-N-CA	5.87	131.50	121.87
3	H	94	TYR	N-CA-C	-5.87	104.80	111.14
1	e	35	ALA	N-CA-C	5.87	118.56	110.35
2	3	207	ILE	CB-CA-C	-5.87	102.60	112.16
2	3	72	ILE	CA-CB-CG2	5.87	120.47	110.50
2	m	145	LEU	CA-C-N	5.87	128.62	120.29
2	m	145	LEU	C-N-CA	5.87	128.62	120.29
3	K	52	ARG	CD-NE-CZ	-5.87	116.19	124.40
2	3	192	THR	CA-CB-CG2	5.86	120.47	110.50
2	m	80	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	F	190	VAL	CB-CA-C	-5.86	104.23	112.14
2	1	68	ARG	NE-CZ-NH2	5.86	124.48	119.20
1	c	135	SER	N-CA-C	-5.86	100.24	109.50
2	2	143	GLY	CA-C-N	5.86	128.13	120.28
2	2	143	GLY	C-N-CA	5.86	128.13	120.28
2	1	92	THR	CA-C-O	5.86	126.63	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	GLY	N-CA-C	-5.86	103.86	114.46
1	f	108	THR	O-C-N	5.86	129.58	122.96
1	d	74	ILE	N-CA-C	-5.86	99.10	107.77
1	E	106	PRO	CB-CA-C	-5.86	104.26	111.64
1	e	142	ASP	N-CA-C	-5.86	107.37	114.75
1	g	54	VAL	N-CA-C	-5.86	99.69	108.12
2	m	27	THR	CA-CB-CG2	-5.86	100.55	110.50
3	I	70	ASP	CA-CB-CG	5.86	118.46	112.60
3	L	247	ALA	CA-C-O	-5.86	114.04	120.36
3	M	333	ASP	CA-CB-CG	-5.85	106.75	112.60
1	b	100	ARG	N-CA-CB	5.85	119.23	110.22
1	D	120	LYS	CA-C-N	5.85	128.12	120.28
1	D	120	LYS	C-N-CA	5.85	128.12	120.28
1	F	154	GLY	N-CA-C	-5.85	99.31	113.18
2	i	78	GLU	CA-C-N	5.85	128.73	120.42
2	i	78	GLU	C-N-CA	5.85	128.73	120.42
2	n	87	VAL	N-CA-C	5.85	116.59	110.62
2	2	109	GLN	CA-C-O	5.85	126.56	120.30
2	i	30	ARG	CA-C-N	5.85	131.72	122.94
2	i	30	ARG	C-N-CA	5.85	131.72	122.94
2	6	49	ALA	N-CA-C	-5.85	100.67	108.74
3	L	303	PHE	N-CA-CB	5.85	120.37	110.49
3	J	42	ILE	N-CA-C	5.85	116.59	110.62
3	J	167	PHE	CA-C-N	5.85	128.60	120.29
3	J	167	PHE	C-N-CA	5.85	128.60	120.29
1	C	206	PRO	N-CA-C	-5.85	106.55	113.86
1	d	67	ILE	CB-CA-C	5.85	119.50	110.96
3	I	324	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	147	LEU	N-CA-C	-5.85	98.34	108.69
2	3	59	SER	CA-C-N	5.85	128.47	120.46
2	3	59	SER	C-N-CA	5.85	128.47	120.46
1	a	49	ILE	N-CA-CB	5.84	119.48	111.41
1	B	216	VAL	N-CA-C	-5.84	106.02	111.45
3	I	354	ILE	N-CA-C	5.84	116.03	110.42
3	M	115	ILE	CA-C-O	-5.84	114.38	121.04
3	J	339	LEU	O-C-N	5.84	128.31	122.12
1	e	129	VAL	N-CA-CB	5.84	119.93	112.34
3	K	293	LEU	CA-C-N	5.84	128.79	120.49
3	K	293	LEU	C-N-CA	5.84	128.79	120.49
3	H	306	ILE	CA-C-O	-5.84	114.32	120.39
3	H	347	SER	N-CA-CB	5.84	119.30	110.42
1	a	104	ASP	CA-CB-CG	-5.84	106.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	46	ARG	CA-C-N	5.84	128.10	120.28
3	H	46	ARG	C-N-CA	5.84	128.10	120.28
3	J	303	PHE	O-C-N	-5.84	117.18	123.42
2	5	93	LEU	N-CA-C	-5.83	104.92	111.28
1	A	160	LYS	N-CA-C	-5.83	106.81	114.04
1	D	150	THR	N-CA-C	-5.83	100.20	109.59
1	E	70	ILE	CB-CA-C	-5.83	105.70	111.30
1	e	17	PRO	N-CA-C	-5.83	104.83	114.75
1	g	214	VAL	O-C-N	-5.83	117.72	122.97
1	g	233	VAL	CA-C-N	5.83	128.57	120.29
1	g	233	VAL	C-N-CA	5.83	128.57	120.29
1	B	168	ARG	CA-C-O	5.83	126.94	120.82
1	g	153	SER	N-CA-C	-5.83	106.21	113.38
2	1	144	SER	CA-C-O	-5.83	114.37	120.55
2	i	30	ARG	CA-C-O	5.83	127.69	121.16
3	M	316	GLY	N-CA-C	5.83	119.26	112.50
1	c	219	ARG	N-CA-C	-5.83	103.87	111.74
1	c	233	VAL	CA-C-N	5.83	128.09	120.28
1	c	233	VAL	C-N-CA	5.83	128.09	120.28
2	1	129	GLY	N-CA-C	-5.83	106.09	112.04
3	J	107	ALA	N-CA-C	-5.83	100.20	109.59
2	h	175	ALA	CB-CA-C	-5.83	99.48	110.67
2	5	125	ILE	CA-CB-CG2	-5.83	100.59	110.50
2	7	96	ASN	CA-C-N	5.83	128.57	120.29
2	7	96	ASN	C-N-CA	5.83	128.57	120.29
1	d	202	SER	O-C-N	-5.83	116.75	123.33
1	E	70	ILE	CA-C-O	-5.83	114.83	120.30
3	M	15	LYS	N-CA-C	-5.83	104.84	111.07
1	f	196	MET	CA-C-N	5.82	127.47	120.13
1	f	196	MET	C-N-CA	5.82	127.47	120.13
2	2	81	ARG	CA-CB-CG	-5.82	102.45	114.10
2	j	70	ILE	O-C-N	5.82	127.52	121.87
3	L	347	SER	N-CA-CB	5.82	120.93	111.21
1	D	104	ASP	CA-CB-CG	5.82	118.42	112.60
3	K	128	TYR	CA-CB-CG	-5.82	103.43	113.90
3	M	129	GLY	O-C-N	-5.82	115.25	122.34
2	i	71	LYS	O-C-N	-5.81	116.08	122.07
3	M	119	LEU	O-C-N	-5.81	116.00	121.35
1	e	118	ASP	CA-C-N	5.81	128.54	120.29
1	e	118	ASP	C-N-CA	5.81	128.54	120.29
1	G	234	GLU	CA-C-O	5.81	126.66	120.10
1	a	191	LEU	CA-C-N	5.81	127.59	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	191	LEU	C-N-CA	5.81	127.59	120.22
1	A	21	LEU	O-C-N	5.81	130.31	122.59
1	F	94	ILE	CA-C-O	-5.81	114.69	120.85
1	f	53	ARG	NE-CZ-NH1	-5.80	115.69	121.50
2	k	139	ALA	N-CA-C	-5.80	98.03	108.48
2	l	43	LYS	N-CA-C	-5.80	99.44	108.90
3	M	135	LYS	N-CA-C	5.80	122.64	109.81
3	J	289	ARG	CA-C-O	5.80	127.66	121.45
1	f	184	SER	N-CA-CB	5.80	118.74	110.44
2	2	154	ARG	N-CA-C	-5.80	104.72	113.89
1	D	168	ARG	N-CA-CB	5.80	118.65	110.12
2	4	133	GLU	N-CA-C	-5.80	101.89	110.48
2	l	206	GLN	CA-C-O	5.80	126.08	119.18
1	C	67	ILE	O-C-N	5.80	129.82	122.57
1	C	194	VAL	N-CA-CB	5.80	117.33	110.55
1	F	93	ARG	CA-C-N	5.80	128.65	120.42
1	F	93	ARG	C-N-CA	5.80	128.65	120.42
3	K	283	VAL	CA-C-O	5.80	126.74	120.53
1	a	16	SER	CA-C-N	5.80	125.66	119.28
1	a	16	SER	C-N-CA	5.80	125.66	119.28
1	F	64	ILE	CA-C-N	5.80	129.50	120.75
1	F	64	ILE	C-N-CA	5.80	129.50	120.75
1	f	111	GLU	N-CA-C	-5.80	106.04	113.23
2	j	181	ALA	N-CA-C	-5.80	104.39	113.02
3	H	44	TYR	CA-C-N	5.80	128.05	120.28
3	H	44	TYR	C-N-CA	5.80	128.05	120.28
3	L	141	GLU	N-CA-C	-5.80	105.52	112.59
1	b	124	THR	N-CA-C	-5.79	104.40	112.45
3	K	61	PRO	N-CA-C	5.79	117.77	110.70
1	b	241	ARG	CA-C-N	5.79	127.97	120.44
1	b	241	ARG	C-N-CA	5.79	127.97	120.44
1	D	86	ARG	CD-NE-CZ	-5.79	116.29	124.40
1	E	97	GLN	N-CA-C	5.79	117.59	111.28
1	g	67	ILE	N-CA-C	-5.79	99.29	107.75
2	n	151	LEU	CB-CA-C	-5.79	101.78	110.88
1	e	34	GLY	CA-C-N	5.79	129.94	121.31
1	e	34	GLY	C-N-CA	5.79	129.94	121.31
1	G	149	GLU	N-CA-C	-5.79	99.96	109.40
2	n	133	GLU	N-CA-C	-5.79	99.90	108.99
3	K	276	ASP	CA-C-N	5.79	125.80	119.89
3	K	276	ASP	C-N-CA	5.79	125.80	119.89
3	L	385	LYS	N-CA-C	-5.79	105.05	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	93	LEU	CA-C-N	5.79	128.04	120.28
2	2	93	LEU	C-N-CA	5.79	128.04	120.28
1	A	125	GLN	CA-C-O	-5.79	113.81	120.24
1	b	214	VAL	O-C-N	5.79	128.32	122.71
1	c	80	GLY	O-C-N	5.79	129.18	123.10
1	G	121	GLN	CG-CD-OE1	-5.79	109.22	120.80
2	3	161	VAL	CA-C-N	5.79	128.51	120.29
2	3	161	VAL	C-N-CA	5.79	128.51	120.29
2	j	15	VAL	O-C-N	-5.79	116.53	122.95
2	l	178	ARG	N-CA-C	-5.79	105.80	112.92
3	I	252	ASN	N-CA-C	-5.79	100.15	108.60
3	K	307	ILE	CA-C-O	-5.79	114.03	120.74
3	L	245	ALA	N-CA-C	-5.79	103.71	111.87
1	A	145	PRO	N-CA-CB	5.79	108.76	103.15
1	C	185	PHE	O-C-N	5.79	128.25	122.12
2	2	98	LEU	CA-C-O	-5.79	114.42	120.55
2	m	180	SER	O-C-N	5.79	129.14	122.25
1	C	107	ILE	CA-C-N	5.79	129.09	120.87
1	C	107	ILE	C-N-CA	5.79	129.09	120.87
1	C	151	ASP	CA-C-O	-5.79	113.53	120.41
1	F	28	ARG	CA-C-O	5.79	126.37	119.60
1	f	67	ILE	N-CA-CB	5.79	119.39	111.41
2	3	140	THR	N-CA-CB	5.79	121.34	111.50
3	H	28	ARG	CD-NE-CZ	-5.79	116.30	124.40
1	c	196	MET	CA-C-N	5.78	126.53	119.99
1	c	196	MET	C-N-CA	5.78	126.53	119.99
1	D	172	THR	CA-C-N	5.78	128.50	120.29
1	D	172	THR	C-N-CA	5.78	128.50	120.29
2	4	212	ARG	CA-C-O	-5.78	112.44	119.32
3	H	133	GLU	CA-C-N	5.78	130.34	122.07
3	H	133	GLU	C-N-CA	5.78	130.34	122.07
3	H	286	ALA	O-C-N	-5.78	117.51	123.29
3	L	146	LEU	CA-C-N	5.78	128.30	120.38
3	L	146	LEU	C-N-CA	5.78	128.30	120.38
1	g	239	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	a	218	ASP	N-CA-C	-5.78	108.03	114.62
2	6	118	GLU	CA-C-O	-5.78	112.59	119.35
2	m	87	VAL	CA-C-N	5.78	128.50	120.29
2	m	87	VAL	C-N-CA	5.78	128.50	120.29
3	K	288	ASN	CA-CB-CG	-5.78	106.82	112.60
3	M	251	THR	N-CA-C	-5.78	99.58	109.24
3	M	112	THR	CA-C-O	5.78	125.65	118.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	379	ILE	O-C-N	5.78	127.78	121.83
1	b	105	GLU	N-CA-C	-5.78	101.55	108.25
1	F	100	ARG	CA-C-N	5.78	127.95	120.44
1	F	100	ARG	C-N-CA	5.78	127.95	120.44
2	i	207	ILE	CA-CB-CG1	5.77	120.22	110.40
2	m	176	MET	N-CA-C	5.77	118.79	111.69
3	M	224	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	d	65	GLU	N-CA-C	5.77	118.96	110.30
3	I	17	GLU	O-C-N	5.77	128.32	122.09
3	I	172	ILE	N-CA-C	-5.77	101.50	109.46
3	J	387	THR	CA-C-O	-5.77	114.32	119.86
1	b	85	ALA	O-C-N	5.77	128.24	122.12
1	f	73	HIS	CA-CB-CG	5.77	119.57	113.80
2	m	24	VAL	CA-C-O	5.77	127.42	120.67
3	K	28	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	f	245	LYS	N-CA-C	-5.77	106.22	113.72
2	m	211	PHE	CA-CB-CG	-5.77	108.03	113.80
1	C	162	THR	CA-CB-CG2	5.77	120.30	110.50
2	1	104	PHE	CB-CA-C	-5.77	102.14	111.14
3	L	96	ASN	CA-CB-CG	-5.77	106.83	112.60
3	J	17	GLU	CA-C-O	-5.77	114.77	120.82
2	5	87	VAL	N-CA-CB	5.76	120.51	110.65
2	m	177	LYS	N-CA-CB	5.76	119.12	110.53
1	d	25	GLU	CA-C-N	5.76	127.93	120.44
1	d	25	GLU	C-N-CA	5.76	127.93	120.44
3	K	196	ALA	N-CA-C	5.76	117.56	111.28
3	M	101	LYS	O-C-N	5.76	125.88	121.85
1	d	70	ILE	N-CA-C	-5.76	106.09	111.45
1	F	44	GLU	N-CA-C	-5.76	104.79	113.89
2	1	114	GLY	N-CA-C	-5.76	103.01	110.38
2	i	54	MET	N-CA-C	-5.76	98.89	108.34
1	f	219	ARG	CD-NE-CZ	-5.76	116.34	124.40
3	L	357	GLU	N-CA-CB	5.76	118.68	110.16
2	h	206	GLN	OE1-CD-NE2	5.76	128.36	122.60
2	6	184	ASP	CA-CB-CG	5.76	118.36	112.60
3	I	109	ASN	CB-CA-C	5.76	118.89	110.26
3	I	283	VAL	N-CA-C	-5.76	99.42	108.23
2	2	169	VAL	CA-CB-CG1	5.75	120.18	110.40
2	3	101	TYR	CB-CG-CD2	-5.75	112.17	120.80
1	C	237	ASN	OD1-CG-ND2	5.75	128.35	122.60
2	5	90	ILE	N-CA-C	-5.75	105.12	110.53
1	C	230	LYS	CA-C-O	-5.75	112.28	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	SER	N-CA-C	-5.75	103.42	110.31
1	F	40	ILE	N-CA-C	-5.75	99.90	108.46
2	h	186	ILE	N-CA-C	-5.75	99.78	108.17
2	i	101	TYR	CB-CA-C	-5.75	101.77	111.02
3	L	41	ARG	CA-C-N	5.75	128.33	120.46
3	L	41	ARG	C-N-CA	5.75	128.33	120.46
1	A	34	GLY	CA-C-N	5.74	129.26	120.82
1	A	34	GLY	C-N-CA	5.74	129.26	120.82
1	C	118	ASP	CA-CB-CG	-5.74	106.86	112.60
1	e	179	TYR	CA-C-N	5.74	131.61	122.59
1	e	179	TYR	C-N-CA	5.74	131.61	122.59
2	i	193	GLU	N-CA-CB	5.74	120.20	110.49
2	n	28	GLU	CB-CG-CD	-5.74	102.84	112.60
3	M	264	THR	CA-CB-OG1	5.74	118.22	109.60
2	3	170	ARG	NE-CZ-NH2	5.74	124.37	119.20
2	7	170	ARG	NE-CZ-NH1	-5.74	115.76	121.50
3	K	222	LEU	CA-C-O	-5.74	114.46	120.55
1	C	31	VAL	CA-CB-CG2	-5.74	100.64	110.40
1	f	101	LEU	N-CA-C	-5.74	104.63	111.69
2	7	156	THR	CA-C-O	-5.74	113.28	120.23
3	I	311	LEU	CA-C-N	5.74	125.71	120.03
3	I	311	LEU	C-N-CA	5.74	125.71	120.03
3	L	180	LEU	N-CA-C	-5.74	99.88	109.24
3	M	31	GLU	CA-C-N	5.74	128.54	120.28
3	M	31	GLU	C-N-CA	5.74	128.54	120.28
1	d	45	GLY	CA-C-N	5.74	131.51	122.33
1	d	45	GLY	C-N-CA	5.74	131.51	122.33
2	4	46	TYR	N-CA-C	-5.74	98.93	108.34
3	K	335	ASP	N-CA-CB	5.74	119.77	110.42
1	E	123	TYR	N-CA-C	-5.74	105.94	113.17
1	f	93	ARG	NE-CZ-NH2	5.74	124.36	119.20
3	K	194	ALA	N-CA-C	5.74	117.33	111.14
3	M	60	SER	O-C-N	-5.74	115.39	121.30
2	6	81	ARG	CA-C-N	5.73	130.50	122.36
2	6	81	ARG	C-N-CA	5.73	130.50	122.36
1	B	151	ASP	CA-C-O	-5.73	115.31	121.27
2	h	25	MET	CG-SD-CE	-5.73	88.29	100.90
2	i	162	ASP	O-C-N	5.73	128.19	122.12
2	4	69	ILE	CA-C-N	5.73	128.56	120.42
2	4	69	ILE	C-N-CA	5.73	128.56	120.42
2	h	63	ALA	CA-C-O	-5.73	114.80	120.70
2	l	145	LEU	CB-CA-C	-5.73	101.89	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	219	GLY	CA-C-N	5.73	128.23	120.44
3	K	219	GLY	C-N-CA	5.73	128.23	120.44
2	l	132	ILE	CB-CA-C	-5.73	103.29	111.31
1	a	76	ALA	O-C-N	-5.72	116.25	123.17
1	g	160	LYS	CA-C-O	5.72	126.60	120.70
2	7	173	TYR	O-C-N	5.72	128.19	122.12
3	M	244	ASP	CA-C-N	5.72	131.22	122.29
3	M	244	ASP	C-N-CA	5.72	131.22	122.29
1	B	230	LYS	CA-C-N	5.72	125.40	119.05
1	B	230	LYS	C-N-CA	5.72	125.40	119.05
2	j	100	SER	N-CA-C	5.72	117.60	111.36
3	H	148	VAL	N-CA-C	-5.72	104.28	112.35
3	I	303	PHE	CB-CA-C	-5.72	103.65	111.95
1	f	32	LYS	N-CA-C	-5.72	106.26	113.18
3	M	360	MET	O-C-N	5.72	128.67	122.15
1	g	91	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	5	105	PRO	CA-C-O	-5.72	114.90	121.36
2	n	41	ALA	CB-CA-C	-5.72	102.33	110.34
3	L	338	GLU	N-CA-CB	5.72	118.53	110.12
2	7	31	ALA	N-CA-C	-5.72	100.57	109.72
3	J	24	ARG	CA-C-N	5.72	127.94	120.28
3	J	24	ARG	C-N-CA	5.72	127.94	120.28
1	A	190	VAL	N-CA-CB	5.72	117.24	110.55
2	h	60	VAL	N-CA-C	-5.72	105.28	110.82
2	l	116	ASP	CA-C-N	5.72	128.51	120.28
2	l	116	ASP	C-N-CA	5.72	128.51	120.28
3	H	195	VAL	CA-C-N	5.72	127.94	120.28
3	H	195	VAL	C-N-CA	5.72	127.94	120.28
3	I	85	PRO	N-CA-C	5.71	120.18	111.15
1	e	47	ILE	N-CA-C	-5.71	100.11	108.11
2	6	111	LEU	CB-CA-C	-5.71	99.36	109.70
1	F	190	VAL	CA-C-N	5.71	128.50	120.28
1	F	190	VAL	C-N-CA	5.71	128.50	120.28
3	H	39	SER	N-CA-CB	5.71	118.52	110.12
3	M	371	THR	CA-CB-CG2	-5.71	100.79	110.50
1	E	18	ASP	CB-CA-C	-5.71	101.15	110.85
2	h	65	PHE	CA-CB-CG	-5.71	108.09	113.80
2	n	193	GLU	CA-C-O	5.71	128.19	121.40
3	J	222	LEU	CA-C-N	5.71	128.28	120.46
3	J	222	LEU	C-N-CA	5.71	128.28	120.46
1	f	24	VAL	N-CA-CB	5.71	118.30	110.54
2	j	99	ASN	CA-C-O	-5.71	114.83	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	397	PHE	CA-CB-CG	-5.71	108.09	113.80
1	C	175	PHE	CB-CG-CD2	-5.71	111.00	120.70
1	F	176	GLU	CA-C-O	-5.71	114.37	120.42
2	5	45	ILE	CA-CB-CG1	5.71	120.10	110.40
2	i	114	GLY	CA-C-O	-5.70	115.88	120.79
2	6	62	ASP	N-CA-C	-5.70	105.14	111.36
3	I	60	SER	N-CA-C	-5.70	102.42	110.29
1	A	56	SER	N-CA-CB	5.70	118.19	110.38
2	h	50	ASP	CA-CB-CG	-5.70	106.90	112.60
1	e	125	GLN	OE1-CD-NE2	-5.70	116.90	122.60
2	5	27	THR	N-CA-C	-5.70	100.65	109.14
3	I	94	TYR	N-CA-C	-5.70	105.53	112.88
3	K	389	ILE	CA-C-O	-5.70	112.31	119.95
3	M	300	PRO	O-C-N	-5.70	116.13	123.03
2	h	142	SER	CA-C-O	5.70	125.96	119.18
2	6	95	SER	N-CA-C	5.70	117.17	111.07
2	7	74	ALA	N-CA-C	-5.70	105.15	111.36
2	n	13	THR	CA-CB-OG1	5.70	118.15	109.60
3	L	104	ALA	N-CA-CB	5.70	119.75	110.17
1	A	107	ILE	CA-CB-CG1	5.70	120.08	110.40
1	c	105	GLU	N-CA-CB	5.70	120.85	111.17
2	2	116	ASP	N-CA-C	-5.69	100.88	108.74
2	5	143	GLY	CA-C-N	5.69	128.48	120.28
2	5	143	GLY	C-N-CA	5.69	128.48	120.28
1	B	109	VAL	CA-C-N	5.69	127.91	120.28
1	B	109	VAL	C-N-CA	5.69	127.91	120.28
1	D	80	GLY	N-CA-C	-5.69	103.62	111.76
1	e	79	SER	N-CA-C	-5.69	100.05	108.99
2	2	51	ARG	NE-CZ-NH1	-5.69	115.81	121.50
2	4	168	ALA	CA-C-N	5.69	127.85	120.56
2	4	168	ALA	C-N-CA	5.69	127.85	120.56
2	l	66	LEU	CA-C-N	5.69	127.91	120.28
2	l	66	LEU	C-N-CA	5.69	127.91	120.28
3	H	266	MET	CA-C-N	5.69	127.91	120.28
3	H	266	MET	C-N-CA	5.69	127.91	120.28
1	a	237	ASN	CA-C-O	-5.69	113.67	120.10
1	B	168	ARG	N-CA-C	5.69	117.16	111.07
1	G	67	ILE	CB-CA-C	5.69	117.41	111.09
1	G	67	ILE	N-CA-C	-5.69	96.48	106.61
2	1	111	LEU	CA-C-O	-5.69	113.26	120.20
2	n	30	ARG	N-CA-CB	5.69	120.11	110.49
1	E	143	GLU	N-CA-CB	5.68	118.73	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	289	ARG	CA-C-N	5.68	127.93	120.60
3	I	289	ARG	C-N-CA	5.68	127.93	120.60
3	M	73	GLU	N-CA-C	-5.68	106.20	113.02
2	1	191	ILE	CB-CA-C	-5.68	101.97	111.29
2	1	209	ALA	CA-C-O	5.68	125.63	119.15
2	3	92	THR	OG1-CB-CG2	-5.68	97.93	109.30
2	6	75	ASN	N-CA-C	-5.68	105.00	111.14
2	n	164	ALA	O-C-N	-5.68	115.67	122.15
3	K	296	ALA	CA-C-N	5.68	128.25	120.46
3	K	296	ALA	C-N-CA	5.68	128.25	120.46
3	M	54	GLU	CA-C-N	5.68	127.72	120.56
3	M	54	GLU	C-N-CA	5.68	127.72	120.56
2	m	19	CYS	N-CA-CB	5.68	119.16	110.70
1	C	90	ASP	CA-CB-CG	-5.68	106.92	112.60
1	F	139	ALA	CA-C-O	5.68	126.49	120.36
2	1	191	ILE	N-CA-CB	5.68	120.60	111.23
3	L	292	ILE	O-C-N	-5.68	116.63	122.14
3	J	16	LEU	CA-C-N	5.68	127.82	120.44
3	J	16	LEU	C-N-CA	5.68	127.82	120.44
1	A	7	GLY	CA-C-N	5.68	131.92	121.70
1	A	7	GLY	C-N-CA	5.68	131.92	121.70
1	G	241	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	b	17	PRO	N-CA-C	-5.68	107.25	114.35
1	e	137	LEU	N-CA-CB	5.68	119.89	110.47
2	i	75	ASN	N-CA-C	-5.68	105.17	111.36
2	i	150	VAL	CA-C-O	-5.68	114.64	120.71
2	6	139	ALA	N-CA-C	-5.68	98.71	110.80
3	M	298	LEU	N-CA-C	-5.68	104.77	112.26
3	M	360	MET	N-CA-C	-5.68	105.17	111.36
2	3	157	PRO	N-CA-C	-5.67	107.26	114.35
3	L	44	TYR	N-CA-CB	5.67	118.57	110.06
1	e	66	LYS	CA-C-N	-5.67	115.75	123.12
1	e	66	LYS	C-N-CA	-5.67	115.75	123.12
2	h	55	THR	CB-CA-C	5.67	120.21	109.37
1	C	105	GLU	N-CA-C	-5.67	98.19	108.85
3	M	321	PHE	N-CA-C	5.67	117.46	111.28
3	J	53	SER	O-C-N	5.67	128.13	122.12
1	A	221	PHE	N-CA-C	5.67	118.70	110.42
2	h	122	ILE	N-CA-CB	5.67	120.74	111.44
2	5	190	LYS	N-CA-CB	-5.67	101.69	111.55
1	f	63	THR	N-CA-C	-5.67	106.35	113.72
1	a	116	ILE	N-CA-CB	5.67	119.08	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	VAL	CA-C-O	5.67	126.86	120.85
1	g	18	ASP	N-CA-C	-5.67	106.03	113.17
3	H	231	LYS	N-CA-CB	5.67	118.45	110.12
3	L	358	ALA	CB-CA-C	-5.67	101.38	110.79
3	L	390	PRO	O-C-N	5.67	130.19	122.99
3	J	169	GLU	CB-CA-C	-5.67	101.22	110.85
3	I	345	GLY	N-CA-C	-5.67	106.94	115.32
3	L	353	ALA	N-CA-C	5.67	117.53	111.36
1	F	82	VAL	CB-CA-C	-5.66	104.41	112.22
1	F	141	VAL	CB-CA-C	-5.66	101.33	110.28
3	M	391	ASP	N-CA-CB	5.66	119.46	110.57
1	b	229	LEU	N-CA-C	-5.66	105.10	112.23
1	D	182	ASP	N-CA-CB	5.66	118.82	110.56
1	F	109	VAL	CA-C-N	5.66	128.14	120.44
1	F	109	VAL	C-N-CA	5.66	128.14	120.44
2	h	28	GLU	N-CA-C	-5.66	101.06	110.17
2	l	52	MET	CA-C-O	5.66	126.81	120.70
1	b	172	THR	CA-C-N	5.66	128.32	120.29
1	b	172	THR	C-N-CA	5.66	128.32	120.29
1	d	100	ARG	CA-C-N	5.66	128.33	120.29
1	d	100	ARG	C-N-CA	5.66	128.33	120.29
1	d	168	ARG	CA-C-O	-5.66	114.84	121.07
2	2	128	ILE	N-CA-C	-5.66	107.23	112.83
2	j	63	ALA	CA-C-N	5.66	128.13	120.44
2	j	63	ALA	C-N-CA	5.66	128.13	120.44
3	L	132	VAL	CA-C-N	5.66	131.52	122.86
3	L	132	VAL	C-N-CA	5.66	131.52	122.86
1	a	188	ALA	O-C-N	5.66	128.12	122.12
1	d	195	ALA	O-C-N	5.66	128.12	122.12
2	3	166	GLU	O-C-N	-5.66	116.25	122.07
3	J	303	PHE	CB-CA-C	-5.66	100.10	110.62
3	H	220	ALA	CA-C-N	5.65	128.17	120.54
3	H	220	ALA	C-N-CA	5.65	128.17	120.54
3	L	369	LYS	N-CA-C	-5.65	99.45	109.06
3	J	395	VAL	N-CA-C	-5.65	104.64	112.50
1	e	40	ILE	CA-CB-CG1	5.65	120.01	110.40
2	n	40	LYS	N-CA-C	-5.65	105.11	112.23
3	H	317	ARG	O-C-N	-5.65	116.25	122.07
3	M	134	GLU	N-CA-C	-5.65	101.28	109.59
3	J	13	LEU	N-CA-CB	5.65	118.53	110.16
1	D	216	VAL	CB-CA-C	-5.65	104.75	111.81
1	F	56	SER	CA-C-O	5.65	128.05	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	29	ARG	N-CA-CB	5.65	118.52	110.16
1	B	144	VAL	O-C-N	-5.65	118.13	121.69
1	d	107	ILE	CA-C-N	5.65	129.28	120.75
1	d	107	ILE	C-N-CA	5.65	129.28	120.75
1	d	193	LEU	N-CA-CB	5.65	118.52	110.16
3	J	348	GLY	CA-C-N	5.65	128.90	120.31
3	J	348	GLY	C-N-CA	5.65	128.90	120.31
1	c	100	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	D	122	GLN	N-CA-CB	5.65	118.20	110.01
2	2	37	ILE	N-CA-CB	5.65	117.70	110.13
2	l	70	ILE	N-CA-CB	5.65	117.16	110.55
2	n	73	GLU	N-CA-C	-5.65	105.89	112.89
3	I	53	SER	CA-CB-OG	5.65	122.39	111.10
3	K	40	GLU	CA-C-N	5.65	127.85	120.28
3	K	40	GLU	C-N-CA	5.65	127.85	120.28
3	M	207	VAL	N-CA-C	5.65	116.21	110.05
2	2	136	ASP	CA-CB-CG	-5.65	106.95	112.60
3	L	273	ASP	CA-CB-CG	-5.65	106.95	112.60
1	C	56	SER	N-CA-C	-5.64	103.25	110.53
1	E	190	VAL	N-CA-CB	5.64	117.16	110.55
2	h	154	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	4	50	ASP	CA-CB-CG	-5.64	106.96	112.60
2	k	190	LYS	CG-CD-CE	5.64	124.28	111.30
1	d	176	GLU	O-C-N	5.64	129.21	122.27
2	3	79	ILE	N-CA-CB	-5.64	102.11	110.58
2	3	177	LYS	CA-C-O	-5.64	113.48	119.97
2	7	108	VAL	CA-C-N	5.64	130.79	123.00
2	7	108	VAL	C-N-CA	5.64	130.79	123.00
1	g	71	ASP	N-CA-CB	5.64	120.15	111.46
3	K	322	LYS	CA-C-O	-5.64	113.48	119.97
1	F	110	LYS	CA-C-O	-5.64	114.89	120.70
1	b	73	HIS	ND1-CE1-NE2	5.64	114.04	108.40
3	H	364	ARG	NH1-CZ-NH2	5.64	126.63	119.30
3	M	153	ILE	CA-C-N	5.64	128.29	120.29
3	M	153	ILE	C-N-CA	5.64	128.29	120.29
2	j	18	VAL	N-CA-CB	5.63	116.86	110.72
2	h	134	GLU	N-CA-C	-5.63	99.24	108.76
1	C	50	ALA	CB-CA-C	5.63	120.47	110.16
1	c	203	GLU	CA-C-O	5.63	127.40	120.92
1	d	110	LYS	N-CA-C	5.63	117.42	111.28
1	E	148	TYR	CA-C-N	5.63	130.93	123.05
1	E	148	TYR	C-N-CA	5.63	130.93	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	159	ILE	CA-C-N	5.63	126.58	120.44
2	l	159	ILE	C-N-CA	5.63	126.58	120.44
2	m	59	SER	CA-C-N	5.63	127.77	120.56
2	m	59	SER	C-N-CA	5.63	127.77	120.56
3	K	50	ARG	N-CA-C	5.63	117.22	111.14
3	J	17	GLU	N-CA-CB	5.63	118.18	110.01
2	6	63	ALA	CA-C-N	5.63	128.87	120.31
2	6	63	ALA	C-N-CA	5.63	128.87	120.31
2	3	104	PHE	CA-CB-CG	-5.63	108.17	113.80
2	6	205	GLU	CA-C-N	5.63	130.25	120.68
2	6	205	GLU	C-N-CA	5.63	130.25	120.68
2	m	92	THR	CA-C-N	5.63	127.82	120.28
2	m	92	THR	C-N-CA	5.63	127.82	120.28
3	J	297	ILE	N-CA-C	-5.63	107.33	112.96
1	e	145	PRO	CA-C-O	-5.63	114.93	121.34
2	3	105	PRO	N-CA-CB	5.63	108.57	103.34
3	I	195	VAL	CA-C-N	5.62	127.82	120.28
3	I	195	VAL	C-N-CA	5.62	127.82	120.28
1	A	59	LEU	N-CA-CB	5.62	118.27	110.17
1	F	142	ASP	N-CA-C	-5.62	104.03	111.96
1	G	71	ASP	N-CA-CB	5.62	115.25	109.51
2	h	163	GLU	CB-CG-CD	-5.62	103.04	112.60
3	M	142	ASP	N-CA-C	-5.62	106.31	112.72
3	J	65	VAL	CB-CA-C	-5.62	103.94	110.91
1	A	105	GLU	N-CA-C	-5.62	101.50	110.10
2	i	105	PRO	CA-N-CD	-5.62	104.13	112.00
2	3	191	ILE	CA-C-O	-5.62	114.61	120.51
2	j	166	GLU	CA-C-N	5.62	128.37	120.28
2	j	166	GLU	C-N-CA	5.62	128.37	120.28
2	k	107	LEU	O-C-N	-5.62	116.05	123.13
2	6	69	ILE	CA-C-N	5.62	128.16	120.46
2	6	69	ILE	C-N-CA	5.62	128.16	120.46
2	n	26	ALA	CA-C-O	-5.62	115.06	121.58
3	K	42	ILE	O-C-N	5.62	127.32	121.87
1	C	148	TYR	CA-CB-CG	-5.62	103.78	113.90
1	E	172	THR	CA-C-O	5.62	126.38	120.42
2	5	25	MET	N-CA-C	-5.62	100.53	109.07
1	D	145	PRO	N-CA-C	5.62	120.42	111.26
3	L	231	LYS	CA-C-N	5.62	128.27	120.29
3	L	231	LYS	C-N-CA	5.62	128.27	120.29
3	J	205	ARG	N-CA-C	-5.62	98.05	107.99
1	d	231	PRO	N-CA-CB	5.62	109.47	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	151	ASP	CA-C-N	5.62	126.35	120.12
1	g	151	ASP	C-N-CA	5.62	126.35	120.12
2	i	72	ILE	CA-C-O	5.62	126.79	120.95
3	L	333	ASP	N-CA-C	-5.62	98.63	109.24
1	E	66	LYS	N-CA-C	-5.61	106.78	113.97
1	F	20	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	f	42	CYS	CA-C-O	-5.61	115.22	121.51
2	5	157	PRO	CA-C-N	5.61	131.63	122.65
2	5	157	PRO	C-N-CA	5.61	131.63	122.65
1	C	215	LYS	CA-C-N	5.61	128.15	120.46
1	C	215	LYS	C-N-CA	5.61	128.15	120.46
2	3	66	LEU	N-CA-CB	5.61	118.37	110.12
3	K	48	VAL	CB-CA-C	-5.61	104.57	112.14
3	L	49	ARG	N-CA-C	5.61	117.39	111.28
3	J	12	LYS	CA-C-N	5.61	128.26	120.29
3	J	12	LYS	C-N-CA	5.61	128.26	120.29
1	F	173	GLU	CA-C-N	5.61	127.80	120.28
1	F	173	GLU	C-N-CA	5.61	127.80	120.28
2	n	147	ALA	CA-C-N	5.61	128.25	120.29
2	n	147	ALA	C-N-CA	5.61	128.25	120.29
1	b	230	LYS	CA-C-O	-5.61	112.48	120.16
1	c	172	THR	N-CA-C	-5.61	105.25	111.36
1	f	64	ILE	N-CA-CB	5.61	118.30	110.56
2	j	62	ASP	CA-C-N	5.61	127.73	120.44
2	j	62	ASP	C-N-CA	5.61	127.73	120.44
2	2	96	ASN	CA-CB-CG	-5.61	106.99	112.60
2	i	102	ARG	N-CA-C	-5.61	106.03	112.92
3	K	291	ASP	CB-CA-C	-5.60	101.25	110.72
1	B	159	TYR	CA-CB-CG	-5.60	103.81	113.90
1	C	73	HIS	CE1-NE2-CD2	-5.60	103.40	109.00
1	C	211	VAL	CA-C-N	5.60	125.92	121.61
1	C	211	VAL	C-N-CA	5.60	125.92	121.61
1	E	208	ASN	N-CA-C	-5.60	105.37	113.21
1	F	238	GLU	CA-C-O	5.60	126.49	120.55
2	l	160	GLY	N-CA-C	-5.60	106.17	112.33
3	I	262	GLN	CA-C-N	5.60	127.72	120.44
3	I	262	GLN	C-N-CA	5.60	127.72	120.44
3	L	30	LEU	O-C-N	5.60	129.16	122.27
3	J	381	LYS	N-CA-C	5.60	117.19	111.14
1	e	15	PHE	CA-C-O	-5.60	114.58	120.80
3	I	329	LYS	N-CA-C	-5.60	99.89	109.24
1	A	80	GLY	O-C-N	-5.60	118.08	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	99	ASN	CA-CB-CG	5.60	118.20	112.60
3	L	208	GLY	N-CA-C	-5.60	107.98	115.32
1	c	101	LEU	CA-C-O	-5.60	114.03	120.24
3	J	281	VAL	N-CA-C	-5.60	100.06	108.12
1	F	173	GLU	N-CA-C	-5.60	105.18	111.28
2	l	99	ASN	N-CA-C	5.60	117.46	111.36
3	H	360	MET	CA-C-N	5.59	127.78	120.28
3	H	360	MET	C-N-CA	5.59	127.78	120.28
1	G	50	ALA	CA-C-N	5.59	129.20	120.75
1	G	50	ALA	C-N-CA	5.59	129.20	120.75
3	I	209	SER	N-CA-C	-5.59	106.12	113.17
1	c	176	GLU	N-CA-C	-5.59	105.57	112.90
1	E	38	ILE	CA-C-O	-5.59	114.13	120.67
2	3	107	LEU	N-CA-C	-5.59	96.65	107.44
2	j	158	GLU	CA-C-N	5.59	128.85	120.69
2	j	158	GLU	C-N-CA	5.59	128.85	120.69
2	7	211	PHE	CA-CB-CG	5.59	119.39	113.80
3	J	149	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	f	197	GLY	CA-C-N	5.59	127.77	120.28
1	f	197	GLY	C-N-CA	5.59	127.77	120.28
1	f	242	GLU	CB-CA-C	-5.59	102.10	110.88
2	4	65	PHE	CA-CB-CG	-5.59	108.21	113.80
2	l	198	GLN	O-C-N	-5.59	116.73	123.27
3	I	324	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
3	M	301	GLY	N-CA-C	-5.59	107.93	115.36
2	2	24	VAL	CA-C-N	5.59	131.42	121.75
2	2	24	VAL	C-N-CA	5.59	131.42	121.75
2	k	112	ILE	CA-C-O	-5.59	114.52	120.39
3	I	158	GLU	CB-CG-CD	-5.59	103.10	112.60
3	L	173	GLU	CA-C-O	-5.59	115.16	119.46
1	B	225	SER	CA-C-O	-5.59	114.87	120.96
1	d	171	VAL	O-C-N	-5.59	116.08	121.83
1	E	169	ASN	N-CA-C	5.59	117.37	111.28
1	E	218	ASP	CA-CB-CG	-5.58	107.02	112.60
1	G	69	LYS	CA-C-O	-5.58	114.91	121.16
1	G	213	TYR	O-C-N	5.58	129.40	123.42
2	6	143	GLY	CA-C-N	5.58	128.03	120.38
2	6	143	GLY	C-N-CA	5.58	128.03	120.38
2	1	160	GLY	CA-C-O	-5.58	116.70	122.28
2	3	150	VAL	CA-C-N	5.58	128.03	120.38
2	3	150	VAL	C-N-CA	5.58	128.03	120.38
2	l	192	THR	N-CA-CB	-5.58	102.18	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	44	LYS	N-CA-C	-5.58	104.71	112.30
2	7	158	GLU	CA-C-N	5.58	129.57	122.37
2	7	158	GLU	C-N-CA	5.58	129.57	122.37
3	M	380	GLU	CA-C-N	5.58	127.70	120.44
3	M	380	GLU	C-N-CA	5.58	127.70	120.44
1	D	73	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	G	6	MET	N-CA-C	-5.58	98.91	110.80
2	j	127	PRO	N-CA-C	-5.58	107.16	114.03
2	7	93	LEU	CA-C-N	5.58	128.22	120.29
2	7	93	LEU	C-N-CA	5.58	128.22	120.29
3	H	282	LYS	CB-CA-C	-5.58	100.32	109.53
3	H	383	LEU	O-C-N	5.58	128.04	122.12
3	I	70	ASP	CA-C-O	-5.58	115.47	121.38
3	I	323	ILE	O-C-N	5.58	127.58	121.83
3	K	32	ASP	CA-CB-CG	-5.58	107.02	112.60
3	L	277	PRO	CA-C-O	-5.58	114.86	121.67
1	d	120	LYS	O-C-N	5.58	128.51	122.15
2	m	101	TYR	CB-CA-C	-5.58	101.16	110.81
3	M	316	GLY	CA-C-N	5.58	127.75	120.28
3	M	316	GLY	C-N-CA	5.58	127.75	120.28
2	7	195	GLU	O-C-N	-5.58	117.40	123.26
3	L	340	ALA	O-C-N	5.58	128.75	122.22
1	c	187	ASP	N-CA-CB	5.58	118.41	110.16
2	h	96	ASN	OD1-CG-ND2	5.58	128.18	122.60
2	6	47	GLN	OE1-CD-NE2	5.58	128.18	122.60
2	7	170	ARG	CA-C-N	5.58	127.69	120.44
2	7	170	ARG	C-N-CA	5.58	127.69	120.44
1	e	185	PHE	N-CA-C	5.57	117.03	111.07
2	h	111	LEU	N-CA-CB	5.57	119.35	110.65
3	I	349	ALA	CA-C-N	5.57	128.20	120.29
3	I	349	ALA	C-N-CA	5.57	128.20	120.29
3	L	205	ARG	CA-C-O	-5.57	114.19	120.32
3	J	150	ILE	O-C-N	5.57	127.57	121.83
1	A	64	ILE	CA-C-N	5.57	131.72	121.70
1	A	64	ILE	C-N-CA	5.57	131.72	121.70
1	D	57	LYS	N-CA-C	-5.57	106.25	113.16
1	e	220	THR	CA-CB-CG2	-5.57	101.03	110.50
2	i	20	LYS	N-CA-C	-5.57	106.84	113.97
1	b	134	VAL	CA-C-N	5.57	131.31	122.62
1	b	134	VAL	C-N-CA	5.57	131.31	122.62
1	B	20	ARG	CD-NE-CZ	-5.57	116.61	124.40
1	C	158	GLU	CA-C-N	5.57	131.00	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	GLU	C-N-CA	5.57	131.00	121.87
1	f	230	LYS	CA-C-O	-5.57	113.21	118.44
3	H	239	PHE	CA-CB-CG	5.57	119.37	113.80
1	c	118	ASP	CB-CA-C	-5.57	101.55	110.79
2	i	201	PRO	CA-C-N	5.57	128.05	120.54
2	i	201	PRO	C-N-CA	5.57	128.05	120.54
2	n	204	VAL	CA-C-N	5.57	128.29	120.28
2	n	204	VAL	C-N-CA	5.57	128.29	120.28
3	J	189	THR	N-CA-C	-5.57	104.90	110.97
3	J	226	VAL	N-CA-C	-5.57	105.08	110.42
1	a	227	GLU	CB-CG-CD	5.56	122.06	112.60
1	F	223	GLU	CA-C-N	5.56	129.91	122.01
1	F	223	GLU	C-N-CA	5.56	129.91	122.01
2	2	111	LEU	CA-C-N	5.56	130.50	123.10
2	2	111	LEU	C-N-CA	5.56	130.50	123.10
2	2	165	VAL	N-CA-C	-5.56	103.98	111.44
3	H	42	ILE	CA-C-N	5.56	127.67	120.44
3	H	42	ILE	C-N-CA	5.56	127.67	120.44
3	J	227	PHE	CA-C-O	-5.56	114.65	120.55
1	c	33	ARG	O-C-N	5.56	129.11	122.27
1	g	146	LYS	CA-C-O	5.56	127.22	120.99
2	m	90	ILE	N-CA-CB	5.56	118.92	110.58
1	a	168	ARG	CA-C-O	-5.56	115.16	121.00
1	b	124	THR	CA-CB-CG2	5.56	119.95	110.50
2	1	103	TYR	N-CA-C	-5.56	106.50	113.28
2	h	104	PHE	CA-C-N	5.56	126.79	119.84
2	h	104	PHE	C-N-CA	5.56	126.79	119.84
3	K	111	GLN	N-CA-CB	5.56	118.03	109.91
1	a	179	TYR	N-CA-C	-5.56	100.62	109.96
1	D	232	TYR	CA-C-N	5.56	128.07	120.46
1	D	232	TYR	C-N-CA	5.56	128.07	120.46
1	e	70	ILE	N-CA-C	-5.56	106.39	111.67
1	g	42	CYS	CA-C-O	5.56	127.57	121.40
2	1	143	GLY	CA-C-N	5.56	127.73	120.28
2	1	143	GLY	C-N-CA	5.56	127.73	120.28
3	H	112	THR	CA-CB-OG1	5.56	117.94	109.60
3	H	269	LEU	O-C-N	5.56	128.49	122.15
1	c	240	ILE	CB-CA-C	-5.56	104.64	112.14
1	a	115	LYS	CA-C-N	5.55	128.31	120.42
1	a	115	LYS	C-N-CA	5.55	128.31	120.42
1	E	198	LEU	N-CA-C	-5.55	104.86	111.69
2	6	168	ALA	N-CA-C	5.55	117.41	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	227	PHE	CA-CB-CG	-5.55	108.25	113.80
1	B	235	ARG	NE-CZ-NH2	5.55	124.20	119.20
2	j	129	GLY	CA-C-N	5.55	129.49	121.44
2	j	129	GLY	C-N-CA	5.55	129.49	121.44
2	k	194	ASP	CB-CA-C	-5.55	99.37	110.42
3	J	154	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	B	184	SER	N-CA-C	-5.55	100.92	109.52
1	F	217	ASP	CA-C-O	-5.55	112.71	119.43
3	I	118	VAL	CA-C-O	5.55	127.37	121.04
3	K	189	THR	N-CA-C	-5.55	105.15	111.14
3	K	239	PHE	CA-CB-CG	-5.55	108.25	113.80
1	G	214	VAL	CA-CB-CG2	-5.55	100.97	110.40
3	H	70	ASP	N-CA-CB	5.55	120.00	111.46
2	h	165	VAL	N-CA-C	-5.55	105.44	110.82
2	k	146	THR	O-C-N	5.55	128.47	122.15
2	5	23	VAL	N-CA-C	-5.55	100.07	108.17
3	H	240	ILE	CA-C-O	-5.55	114.39	120.43
3	L	71	ILE	CA-C-O	5.55	126.36	120.48
3	J	34	LYS	CA-C-N	5.55	127.98	120.44
3	J	34	LYS	C-N-CA	5.55	127.98	120.44
1	a	83	ALA	CA-C-N	5.54	128.16	120.29
1	a	83	ALA	C-N-CA	5.54	128.16	120.29
1	F	130	ARG	CA-C-N	5.54	125.45	119.85
1	F	130	ARG	C-N-CA	5.54	125.45	119.85
2	3	63	ALA	CA-C-O	-5.54	115.00	120.82
2	4	109	GLN	CB-CA-C	-5.54	100.13	109.72
2	4	166	GLU	N-CA-CB	5.54	118.27	110.12
2	l	202	GLU	CA-C-O	-5.54	114.97	121.07
3	K	119	LEU	CA-C-N	5.54	125.47	119.76
3	K	119	LEU	C-N-CA	5.54	125.47	119.76
1	c	227	GLU	CA-C-N	5.54	128.74	120.31
1	c	227	GLU	C-N-CA	5.54	128.74	120.31
1	A	181	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	169	ASN	CA-C-O	-5.54	115.00	120.82
1	F	182	ASP	N-CA-C	-5.54	105.13	112.94
3	I	71	ILE	CA-CB-CG1	5.54	119.82	110.40
3	K	353	ALA	CA-C-N	5.54	127.54	120.56
3	K	353	ALA	C-N-CA	5.54	127.54	120.56
3	M	294	ASP	N-CA-C	-5.54	102.22	110.20
1	D	12	ILE	N-CA-C	-5.54	106.91	112.17
3	K	28	ARG	CA-C-N	5.54	127.64	120.44
3	K	28	ARG	C-N-CA	5.54	127.64	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	LYS	N-CA-CB	5.54	118.04	110.01
1	F	64	ILE	O-C-N	-5.54	115.65	122.57
3	I	9	LEU	CA-C-N	5.54	127.70	120.28
3	I	9	LEU	C-N-CA	5.54	127.70	120.28
3	L	223	VAL	CA-C-N	5.54	128.15	120.29
3	L	223	VAL	C-N-CA	5.54	128.15	120.29
3	M	71	ILE	CA-C-O	5.54	126.20	120.39
1	C	166	MET	CG-SD-CE	-5.53	88.73	100.90
2	7	80	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	C	179	TYR	CB-CG-CD2	-5.53	112.50	120.80
1	F	194	VAL	CA-C-O	-5.53	115.20	120.95
1	F	217	ASP	CA-CB-CG	5.53	118.13	112.60
3	K	309	VAL	N-CA-CB	-5.53	104.05	111.40
3	M	155	GLU	CB-CG-CD	-5.53	103.20	112.60
1	B	178	GLU	CA-C-N	5.53	128.56	120.71
1	B	178	GLU	C-N-CA	5.53	128.56	120.71
3	K	26	LEU	CA-C-N	5.53	128.14	120.29
3	K	26	LEU	C-N-CA	5.53	128.14	120.29
2	n	69	ILE	CA-C-O	-5.53	115.31	121.17
1	d	122	GLN	CB-CG-CD	-5.53	103.21	112.60
2	1	98	LEU	O-C-N	-5.53	115.85	122.15
2	1	104	PHE	N-CA-C	-5.53	99.21	108.94
2	n	87	VAL	CB-CA-C	-5.53	104.68	112.14
3	M	195	VAL	N-CA-C	-5.53	104.98	110.62
1	a	223	GLU	CB-CA-C	5.52	119.25	110.19
1	g	63	THR	N-CA-C	-5.52	107.54	114.56
1	E	24	VAL	CA-C-N	5.52	128.23	120.28
1	E	24	VAL	C-N-CA	5.52	128.23	120.28
1	F	61	ALA	CB-CA-C	-5.52	102.17	110.90
2	k	200	SER	CA-C-N	5.52	125.62	119.32
2	k	200	SER	C-N-CA	5.52	125.62	119.32
2	m	202	GLU	N-CA-C	5.52	117.74	111.11
3	H	272	LEU	N-CA-C	5.52	117.30	111.28
1	D	229	LEU	CA-C-N	5.52	129.14	120.97
1	D	229	LEU	C-N-CA	5.52	129.14	120.97
2	k	123	TYR	CB-CA-C	5.52	119.81	109.71
2	5	89	ALA	CA-C-N	5.52	127.62	120.56
2	5	89	ALA	C-N-CA	5.52	127.62	120.56
1	d	62	ASP	N-CA-C	-5.52	105.91	113.30
2	h	101	TYR	CB-CA-C	-5.52	102.14	111.02
2	4	185	GLY	N-CA-C	-5.52	104.49	111.72
3	M	360	MET	CA-C-O	-5.52	114.57	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	165	GLY	CA-C-N	5.52	128.12	120.29
1	G	165	GLY	C-N-CA	5.52	128.12	120.29
2	i	128	ILE	N-CA-C	-5.52	106.93	112.17
2	5	199	TYR	CB-CA-C	-5.52	101.63	110.79
1	a	124	THR	N-CA-C	-5.51	105.28	112.23
3	K	372	MET	O-C-N	-5.51	116.27	122.12
1	c	42	CYS	CA-C-O	-5.51	115.10	121.49
1	g	41	LYS	N-CA-CB	5.51	119.16	110.23
2	h	186	ILE	N-CA-CB	5.51	120.51	111.58
2	n	167	LEU	CA-C-N	5.51	127.66	120.28
2	n	167	LEU	C-N-CA	5.51	127.66	120.28
3	H	104	ALA	CA-C-O	-5.51	114.10	120.49
3	L	17	GLU	CA-C-N	5.51	127.66	120.28
3	L	17	GLU	C-N-CA	5.51	127.66	120.28
3	L	23	LEU	N-CA-C	5.51	117.28	111.28
1	e	175	PHE	N-CA-C	-5.51	106.52	113.18
2	j	119	GLY	N-CA-C	-5.51	103.14	110.58
2	n	170	ARG	CA-C-N	5.51	128.11	120.29
2	n	170	ARG	C-N-CA	5.51	128.11	120.29
3	I	298	LEU	N-CA-CB	5.51	118.22	110.12
3	L	175	PRO	N-CA-CB	5.51	108.57	103.39
1	d	54	VAL	CA-C-N	5.51	128.61	122.55
1	d	54	VAL	C-N-CA	5.51	128.61	122.55
2	3	194	ASP	CA-CB-CG	-5.51	107.09	112.60
2	i	44	LYS	N-CA-CB	5.50	121.23	110.88
3	H	101	LYS	N-CA-C	-5.50	101.81	108.14
3	J	373	LEU	CA-C-O	5.50	126.39	120.55
1	G	33	ARG	CG-CD-NE	-5.50	99.89	112.00
2	1	98	LEU	CA-C-N	5.50	128.11	120.29
2	1	98	LEU	C-N-CA	5.50	128.11	120.29
2	7	167	LEU	CA-C-N	5.50	128.21	120.28
2	7	167	LEU	C-N-CA	5.50	128.21	120.28
1	c	123	TYR	CB-CG-CD2	5.50	129.05	120.80
1	g	36	THR	CA-CB-OG1	5.50	117.85	109.60
2	2	104	PHE	N-CA-C	-5.50	102.14	110.50
3	K	148	VAL	CA-C-N	5.50	128.10	120.29
3	K	148	VAL	C-N-CA	5.50	128.10	120.29
3	K	175	PRO	CA-C-O	-5.50	115.30	122.12
1	e	90	ASP	O-C-N	-5.50	116.29	122.12
3	L	341	ARG	CB-CA-C	-5.50	101.66	110.79
1	A	60	GLU	N-CA-C	-5.50	102.75	110.50
1	c	185	PHE	CA-C-O	5.50	126.38	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	171	VAL	CA-C-N	5.50	127.59	120.44
1	G	171	VAL	C-N-CA	5.50	127.59	120.44
3	H	175	PRO	CB-CA-C	5.50	118.43	111.39
3	I	96	ASN	OD1-CG-ND2	5.50	128.10	122.60
3	J	141	GLU	N-CA-C	-5.50	106.62	113.38
1	f	123	TYR	CB-CG-CD2	5.50	129.05	120.80
2	l	95	SER	CB-CA-C	-5.50	101.51	110.85
3	J	282	LYS	CA-C-N	-5.50	115.97	123.12
3	J	282	LYS	C-N-CA	-5.50	115.97	123.12
1	g	27	ALA	CA-C-N	5.50	130.02	120.68
1	g	27	ALA	C-N-CA	5.50	130.02	120.68
3	M	305	ARG	N-CA-C	-5.50	100.95	109.14
1	A	96	ALA	CB-CA-C	-5.49	101.51	110.85
1	b	172	THR	N-CA-CB	5.49	117.98	110.01
1	e	111	GLU	CA-C-N	5.49	127.58	120.44
1	e	111	GLU	C-N-CA	5.49	127.58	120.44
1	e	151	ASP	CA-C-N	5.49	125.58	119.87
1	e	151	ASP	C-N-CA	5.49	125.58	119.87
2	h	126	ASP	N-CA-C	-5.49	102.15	110.50
2	j	76	LEU	CA-C-N	5.49	127.58	120.44
2	j	76	LEU	C-N-CA	5.49	127.58	120.44
2	6	106	TYR	N-CA-C	-5.49	99.10	110.80
2	m	30	ARG	N-CA-C	-5.49	100.72	109.23
2	n	55	THR	N-CA-C	-5.49	100.82	109.50
3	I	202	THR	CA-C-N	5.49	129.98	122.84
3	I	202	THR	C-N-CA	5.49	129.98	122.84
1	B	133	GLY	N-CA-C	-5.49	106.51	115.46
2	3	186	ILE	O-C-N	-5.49	117.33	123.26
3	H	375	PHE	CA-CB-CG	-5.49	108.31	113.80
1	E	91	ARG	CA-C-O	-5.49	114.60	120.42
1	f	139	ALA	O-C-N	-5.49	116.90	123.27
2	4	62	ASP	CA-C-N	5.49	127.64	120.28
2	4	62	ASP	C-N-CA	5.49	127.64	120.28
3	J	169	GLU	N-CA-CB	5.49	118.28	110.16
1	C	81	LEU	N-CA-CB	5.49	118.11	109.83
2	6	118	GLU	N-CA-CB	5.49	118.61	110.49
3	M	211	PHE	CA-CB-CG	-5.49	108.31	113.80
1	G	212	GLY	O-C-N	-5.49	118.83	123.60
2	k	212	ARG	N-CA-C	-5.49	106.63	113.38
2	h	64	GLN	N-CA-CB	5.48	118.28	110.16
2	i	26	ALA	O-C-N	5.48	129.50	123.25
2	k	99	ASN	OD1-CG-ND2	-5.48	117.12	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	200	ILE	CA-CB-CG2	-5.48	101.18	110.50
2	i	204	VAL	CA-C-N	5.48	128.18	120.28
2	i	204	VAL	C-N-CA	5.48	128.18	120.28
1	A	212	GLY	N-CA-C	-5.48	102.79	110.96
1	b	86	ARG	N-CA-C	-5.48	105.31	111.28
1	d	122	GLN	OE1-CD-NE2	5.48	128.08	122.60
2	m	69	ILE	CB-CA-C	-5.48	104.66	112.22
3	J	90	ASN	CB-CG-OD1	-5.48	109.84	120.80
3	J	210	GLU	CA-C-N	5.48	128.55	120.82
3	J	210	GLU	C-N-CA	5.48	128.55	120.82
1	B	120	LYS	CB-CA-C	-5.48	100.15	110.67
1	b	82	VAL	N-CA-C	-5.48	104.24	111.09
1	C	16	SER	CA-C-O	-5.48	114.75	120.88
1	G	71	ASP	CA-C-O	5.48	124.13	120.19
3	K	36	PHE	CB-CA-C	-5.48	101.54	110.85
3	M	309	VAL	N-CA-CB	5.48	117.28	111.20
2	j	24	VAL	N-CA-C	-5.47	100.45	108.11
2	k	171	ALA	CA-C-N	5.47	129.62	120.64
2	k	171	ALA	C-N-CA	5.47	129.62	120.64
1	a	236	ALA	CA-C-N	5.47	128.16	120.28
1	a	236	ALA	C-N-CA	5.47	128.16	120.28
1	C	31	VAL	CA-C-O	-5.47	115.26	120.95
2	i	23	VAL	N-CA-C	-5.47	101.13	108.35
2	n	145	LEU	CA-C-O	-5.47	114.62	120.42
3	K	397	PHE	O-C-N	5.47	130.58	122.81
3	J	18	GLU	CA-C-N	5.47	127.61	120.28
3	J	18	GLU	C-N-CA	5.47	127.61	120.28
2	k	38	ALA	N-CA-C	-5.47	101.09	109.41
3	I	41	ARG	CG-CD-NE	-5.47	99.96	112.00
3	L	146	LEU	O-C-N	-5.47	116.67	122.30
1	A	13	THR	CA-CB-OG1	5.47	117.81	109.60
2	3	166	GLU	CA-C-O	5.47	126.56	120.82
3	I	390	PRO	N-CD-CG	5.47	111.40	103.20
3	M	138	VAL	N-CA-CB	5.47	117.04	110.31
1	g	94	ILE	O-C-N	5.47	127.46	121.83
3	K	315	GLU	N-CA-CB	5.47	118.25	110.16
3	M	69	SER	N-CA-C	-5.47	106.28	113.12
1	D	17	PRO	CA-C-N	5.47	127.55	120.44
1	D	17	PRO	C-N-CA	5.47	127.55	120.44
1	F	72	GLU	N-CA-C	-5.47	106.81	112.93
2	m	72	ILE	CA-C-O	-5.47	114.57	120.47
2	7	22	GLY	CA-C-O	5.47	127.76	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	15	LYS	CA-C-N	5.47	128.05	120.29
3	J	15	LYS	C-N-CA	5.47	128.05	120.29
1	e	238	GLU	CA-C-O	5.46	126.56	120.82
1	G	93	ARG	NE-CZ-NH1	-5.46	116.03	121.50
2	4	109	GLN	N-CA-CB	5.46	119.15	110.57
1	D	51	ASP	CA-CB-CG	5.46	118.06	112.60
3	J	232	GLU	CB-CG-CD	-5.46	103.31	112.60
1	b	73	HIS	N-CA-C	-5.46	104.88	113.02
1	d	88	LEU	CA-C-O	-5.46	114.76	120.55
2	j	140	THR	O-C-N	-5.46	117.25	123.48
3	M	18	GLU	O-C-N	5.46	127.99	122.09
1	B	201	GLU	N-CA-C	-5.46	104.37	111.74
1	C	183	LEU	N-CA-C	-5.46	100.42	108.99
2	l	56	THR	CA-C-O	5.46	126.38	120.32
1	c	190	VAL	CA-C-N	5.46	127.60	120.28
1	c	190	VAL	C-N-CA	5.46	127.60	120.28
1	d	61	ALA	CA-C-O	5.46	125.93	121.02
2	h	202	GLU	CA-C-N	5.46	128.61	120.31
2	h	202	GLU	C-N-CA	5.46	128.61	120.31
3	H	93	GLN	N-CA-CB	5.46	119.71	110.49
3	L	14	LYS	N-CA-C	5.46	117.31	111.36
3	M	361	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	86	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	f	58	LEU	CA-C-N	5.46	129.50	120.94
1	f	58	LEU	C-N-CA	5.46	129.50	120.94
2	k	192	THR	CA-C-N	5.46	132.33	123.93
2	k	192	THR	C-N-CA	5.46	132.33	123.93
3	K	269	LEU	O-C-N	-5.46	115.33	122.59
1	D	217	ASP	N-CA-CB	5.46	118.14	110.12
2	1	72	ILE	CA-C-N	5.45	128.03	120.29
2	1	72	ILE	C-N-CA	5.45	128.03	120.29
2	4	43	LYS	N-CA-C	5.45	118.71	110.64
2	l	208	LEU	N-CA-C	-5.45	106.21	112.92
2	m	198	GLN	CA-C-O	-5.45	114.67	120.40
1	a	12	ILE	O-C-N	-5.45	117.01	122.62
2	i	187	ASP	CA-C-O	5.45	126.59	120.70
2	3	32	THR	CA-C-N	5.45	131.95	121.54
2	3	32	THR	C-N-CA	5.45	131.95	121.54
2	3	82	GLU	N-CA-C	-5.45	104.62	111.92
2	7	30	ARG	NE-CZ-NH1	-5.45	116.05	121.50
3	K	62	PRO	N-CA-CB	5.45	108.60	102.60
3	J	227	PHE	CA-C-N	5.45	128.03	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	227	PHE	C-N-CA	5.45	128.03	120.29
3	H	99	GLU	N-CA-CB	5.45	118.56	110.49
3	K	230	ALA	CA-C-N	5.45	128.03	120.29
3	K	230	ALA	C-N-CA	5.45	128.03	120.29
1	b	130	ARG	CA-C-O	-5.45	115.05	120.66
2	6	132	ILE	CA-C-O	-5.45	116.11	121.67
2	k	66	LEU	CA-C-O	-5.45	113.36	119.79
3	I	324	HIS	CA-C-N	5.45	127.58	120.28
3	I	324	HIS	C-N-CA	5.45	127.58	120.28
3	I	333	ASP	CA-CB-CG	-5.45	107.15	112.60
3	K	105	ARG	N-CA-CB	5.45	117.97	109.97
3	L	227	PHE	N-CA-CB	5.45	118.12	110.12
3	J	251	THR	CA-CB-CG2	5.45	119.76	110.50
1	E	244	LEU	N-CA-C	-5.44	105.95	112.59
1	f	151	ASP	N-CA-CB	5.44	117.29	109.78
2	h	33	MET	N-CA-C	-5.44	100.44	108.99
2	n	178	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	f	134	VAL	N-CA-C	-5.44	99.99	108.81
3	H	147	ASP	CA-CB-CG	-5.44	107.16	112.60
3	L	48	VAL	CA-CB-CG1	5.44	119.65	110.40
3	L	294	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	42	CYS	N-CA-C	-5.44	101.21	108.34
2	l	16	GLY	N-CA-C	-5.44	100.29	113.18
2	6	134	GLU	CA-C-N	5.44	127.51	120.44
2	6	134	GLU	C-N-CA	5.44	127.51	120.44
3	L	315	GLU	CA-C-N	5.44	126.02	119.98
3	L	315	GLU	C-N-CA	5.44	126.02	119.98
3	J	305	ARG	O-C-N	-5.44	115.94	123.01
1	F	73	HIS	CA-C-O	5.44	124.47	118.65
1	F	149	GLU	CB-CG-CD	-5.44	103.36	112.60
2	2	148	TYR	N-CA-CB	5.44	118.21	110.16
3	H	280	ASP	N-CA-C	-5.44	99.22	110.80
1	G	122	GLN	N-CA-C	-5.44	105.43	111.36
2	m	170	ARG	CA-CB-CG	-5.44	103.23	114.10
3	L	169	GLU	N-CA-C	5.44	117.20	111.28
1	b	188	ALA	CA-C-N	5.43	127.51	120.44
1	b	188	ALA	C-N-CA	5.43	127.51	120.44
1	d	67	ILE	N-CA-CB	5.43	118.31	111.46
3	L	364	ARG	CA-CB-CG	-5.43	103.23	114.10
1	b	141	VAL	CA-C-O	5.43	126.04	120.39
1	D	141	VAL	N-CA-C	-5.43	98.64	107.28
2	1	72	ILE	N-CA-C	-5.43	105.08	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	309	VAL	O-C-N	5.43	127.29	121.10
2	1	71	LYS	CA-C-N	5.43	127.90	120.46
2	1	71	LYS	C-N-CA	5.43	127.90	120.46
1	f	26	TYR	N-CA-C	5.43	117.28	111.36
2	7	49	ALA	N-CA-C	-5.43	101.05	108.38
3	M	204	ILE	N-CA-C	-5.43	100.24	108.17
3	J	21	TYR	CA-C-N	5.43	128.00	120.29
3	J	21	TYR	C-N-CA	5.43	128.00	120.29
2	3	48	ILE	N-CA-C	-5.43	106.51	111.67
1	C	210	GLU	N-CA-C	-5.43	100.56	109.40
1	c	100	ARG	O-C-N	-5.43	115.87	122.22
1	d	242	GLU	CA-C-N	5.43	128.00	120.29
1	d	242	GLU	C-N-CA	5.43	128.00	120.29
2	m	68	ARG	CA-C-N	5.43	128.13	120.42
2	m	68	ARG	C-N-CA	5.43	128.13	120.42
2	m	112	ILE	N-CA-CB	5.43	118.90	111.41
1	e	46	VAL	CA-C-O	5.42	126.34	120.43
1	f	159	TYR	CD1-CG-CD2	5.42	126.24	118.10
1	f	204	LEU	O-C-N	5.42	129.48	122.81
2	j	92	THR	CA-C-N	5.42	127.99	120.29
2	j	92	THR	C-N-CA	5.42	127.99	120.29
2	m	99	ASN	N-CA-CB	5.42	117.88	110.01
3	K	36	PHE	N-CA-CB	5.42	118.19	110.16
1	e	240	ILE	N-CA-C	-5.42	105.09	110.62
2	n	96	ASN	CA-C-N	5.42	127.49	120.44
2	n	96	ASN	C-N-CA	5.42	127.49	120.44
1	A	57	LYS	N-CA-C	-5.42	106.17	112.89
1	b	240	ILE	O-C-N	5.42	127.22	121.91
1	D	71	ASP	O-C-N	5.42	129.80	122.59
2	3	46	TYR	N-CA-C	-5.42	100.07	108.90
2	7	193	GLU	N-CA-CB	5.42	119.65	110.49
3	L	279	GLY	CA-C-O	5.42	126.22	119.88
3	L	283	VAL	O-C-N	-5.42	117.49	123.18
3	J	53	SER	CA-C-O	-5.42	114.81	120.55
1	A	129	VAL	CA-C-O	5.42	126.69	120.90
1	C	128	GLY	N-CA-C	-5.42	106.63	115.46
1	F	232	TYR	CA-C-N	5.42	128.11	120.42
1	F	232	TYR	C-N-CA	5.42	128.11	120.42
1	g	62	ASP	N-CA-CB	5.42	121.61	111.43
2	2	182	SER	N-CA-CB	5.42	119.65	110.49
2	m	21	ASP	O-C-N	-5.42	115.69	122.35
3	I	22	LYS	CA-C-N	5.42	127.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	22	LYS	C-N-CA	5.42	127.54	120.28
3	I	254	ASP	CA-C-N	5.42	131.45	121.70
3	I	254	ASP	C-N-CA	5.42	131.45	121.70
3	K	325	THR	CA-C-O	5.42	126.22	120.10
3	K	391	ASP	CA-C-N	5.42	131.89	121.54
3	K	391	ASP	C-N-CA	5.42	131.89	121.54
1	c	188	ALA	CA-C-O	5.42	126.29	120.55
3	K	203	PHE	N-CA-C	-5.42	98.94	108.20
3	K	331	ALA	N-CA-C	-5.42	101.75	110.14
1	a	212	GLY	O-C-N	-5.41	118.49	123.42
2	m	51	ARG	CA-C-O	-5.41	113.88	119.51
3	L	105	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	172	THR	CA-C-N	5.41	127.53	120.28
1	A	172	THR	C-N-CA	5.41	127.53	120.28
1	a	93	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
1	E	151	ASP	O-C-N	-5.41	115.85	120.99
2	4	156	THR	N-CA-C	-5.41	92.47	107.84
2	l	148	TYR	CA-C-N	5.41	125.95	119.94
2	l	148	TYR	C-N-CA	5.41	125.95	119.94
3	K	209	SER	N-CA-C	-5.41	106.45	113.16
3	M	359	GLY	CA-C-N	5.41	127.97	120.29
3	M	359	GLY	C-N-CA	5.41	127.97	120.29
2	4	28	GLU	CA-C-O	-5.41	115.05	121.16
3	H	384	LYS	CA-C-O	-5.41	114.82	120.55
1	f	24	VAL	O-C-N	-5.41	116.62	121.87
3	L	140	TYR	N-CA-C	-5.41	106.66	113.20
3	L	163	LYS	N-CA-C	-5.41	97.47	108.12
1	e	177	LYS	N-CA-C	-5.41	104.72	112.13
3	J	202	THR	O-C-N	5.41	129.46	122.43
1	e	35	ALA	CA-C-O	-5.40	115.23	121.07
1	F	12	ILE	O-C-N	-5.40	116.79	122.25
3	K	16	LEU	CA-C-N	5.40	128.06	120.28
3	K	16	LEU	C-N-CA	5.40	128.06	120.28
3	K	113	LEU	CA-C-N	5.40	131.51	121.62
3	K	113	LEU	C-N-CA	5.40	131.51	121.62
3	M	188	LYS	CA-C-N	5.40	127.52	120.28
3	M	188	LYS	C-N-CA	5.40	127.52	120.28
1	d	55	GLY	N-CA-C	-5.40	103.04	112.55
1	g	198	LEU	CA-C-N	5.40	127.52	120.28
1	g	198	LEU	C-N-CA	5.40	127.52	120.28
3	J	392	LEU	N-CA-CB	5.40	119.68	110.50
1	B	31	VAL	N-CA-C	-5.40	105.27	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	83	ALA	O-C-N	5.40	127.63	122.07
3	L	34	LYS	CB-CA-C	-5.40	100.31	110.67
1	C	197	GLY	CA-C-O	-5.40	115.19	120.75
1	D	180	ARG	NE-CZ-NH2	5.40	124.06	119.20
3	H	224	ARG	CA-C-N	5.40	127.51	120.28
3	H	224	ARG	C-N-CA	5.40	127.51	120.28
3	H	291	ASP	CA-CB-CG	5.40	118.00	112.60
3	K	308	GLU	N-CA-C	-5.40	102.49	110.48
1	d	53	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	b	25	GLU	CA-C-N	5.39	128.51	120.31
1	b	25	GLU	C-N-CA	5.39	128.51	120.31
1	C	122	GLN	CB-CG-CD	-5.39	103.43	112.60
1	f	126	TYR	CB-CG-CD1	5.39	128.89	120.80
1	G	176	GLU	N-CA-C	-5.39	105.51	111.71
2	4	142	SER	CA-C-O	5.39	125.07	119.14
2	4	208	LEU	N-CA-CB	5.39	118.57	110.53
3	K	370	VAL	N-CA-C	-5.39	100.67	108.71
3	L	243	LEU	N-CA-C	-5.39	106.55	113.02
3	M	228	GLN	CB-CA-C	-5.39	102.41	110.88
1	b	67	ILE	N-CA-CB	5.39	119.39	111.52
1	E	32	LYS	N-CA-C	5.39	119.12	112.54
2	1	184	ASP	N-CA-C	-5.39	100.87	109.07
2	3	47	GLN	N-CA-CB	5.39	118.31	109.95
3	K	112	THR	N-CA-C	-5.39	99.89	109.06
3	K	158	GLU	CB-CG-CD	-5.39	103.44	112.60
1	B	112	LEU	N-CA-CB	5.39	118.14	110.16
1	c	216	VAL	CA-CB-CG1	5.39	119.56	110.40
1	d	120	LYS	CG-CD-CE	5.39	123.69	111.30
1	E	184	SER	CA-C-N	5.39	127.94	120.29
1	E	184	SER	C-N-CA	5.39	127.94	120.29
1	f	42	CYS	N-CA-CB	5.39	120.35	111.62
2	7	148	TYR	O-C-N	5.39	128.53	122.22
2	n	188	VAL	CA-C-N	5.39	130.43	122.94
2	n	188	VAL	C-N-CA	5.39	130.43	122.94
1	E	81	LEU	CB-CA-C	-5.39	101.50	109.90
3	H	382	VAL	N-CA-C	5.39	115.59	110.42
1	B	222	LYS	N-CA-C	-5.39	100.88	109.23
1	F	42	CYS	N-CA-C	-5.39	101.22	109.41
2	3	15	VAL	N-CA-C	-5.39	100.94	108.80
1	c	35	ALA	CA-C-N	5.38	128.36	120.71
1	c	35	ALA	C-N-CA	5.38	128.36	120.71
2	l	133	GLU	CB-CG-CD	-5.38	103.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	55	THR	N-CA-C	-5.38	100.92	109.59
2	6	194	ASP	N-CA-C	-5.38	107.97	114.75
3	L	93	GLN	N-CA-C	-5.38	106.56	113.02
2	h	73	GLU	CB-CG-CD	-5.38	103.45	112.60
2	l	142	SER	CB-CA-C	-5.38	100.28	109.65
1	c	165	GLY	N-CA-C	-5.38	100.43	113.18
2	7	169	VAL	CA-C-O	5.38	126.56	120.85
3	J	361	PHE	N-CA-CB	5.38	118.62	110.28
3	I	100	LEU	CA-C-O	5.38	127.19	121.16
3	L	101	LYS	CA-C-N	5.38	126.56	119.84
3	L	101	LYS	C-N-CA	5.38	126.56	119.84
3	M	77	VAL	CA-C-N	5.38	129.09	122.37
3	M	77	VAL	C-N-CA	5.38	129.09	122.37
2	4	100	SER	N-CA-CB	5.38	117.87	110.07
3	L	154	ARG	CA-CB-CG	5.38	124.86	114.10
1	a	95	GLU	O-C-N	5.38	127.82	122.12
2	5	158	GLU	N-CA-C	-5.38	106.31	112.92
3	L	27	TYR	CA-C-O	-5.38	114.72	120.42
3	L	173	GLU	CA-CB-CG	5.38	124.85	114.10
1	a	59	LEU	N-CA-CB	5.38	117.87	109.97
2	i	61	GLY	O-C-N	5.38	127.45	122.13
2	4	193	GLU	N-CA-CB	5.38	119.57	110.49
2	n	49	ALA	CA-C-O	5.38	127.72	121.49
3	H	26	LEU	N-CA-C	-5.38	105.32	111.07
1	C	81	LEU	CA-C-N	5.37	127.82	120.46
1	C	81	LEU	C-N-CA	5.37	127.82	120.46
1	D	216	VAL	CA-C-N	5.37	127.48	120.28
1	D	216	VAL	C-N-CA	5.37	127.48	120.28
1	g	163	ALA	CA-C-O	5.37	126.77	120.43
2	h	206	GLN	N-CA-CB	5.37	118.82	110.44
2	7	147	ALA	CB-CA-C	-5.37	101.87	110.79
3	I	110	GLN	CB-CG-CD	-5.37	103.46	112.60
3	J	336	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	207	GLU	CB-CG-CD	-5.37	103.47	112.60
1	F	115	LYS	CA-CB-CG	-5.37	103.36	114.10
2	1	160	GLY	O-C-N	5.37	127.98	122.88
2	h	129	GLY	O-C-N	5.37	128.10	122.51
3	I	207	VAL	N-CA-C	-5.37	100.11	108.81
1	B	158	GLU	CA-CB-CG	5.37	124.84	114.10
2	2	154	ARG	NE-CZ-NH2	5.37	124.03	119.20
3	L	306	ILE	N-CA-C	-5.37	100.59	108.54
1	A	184	SER	O-C-N	5.37	128.96	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	ILE	CB-CA-C	-5.37	104.89	112.14
1	c	70	ILE	CA-C-O	5.37	125.35	120.30
1	E	36	THR	CA-C-N	5.37	131.23	121.89
1	E	36	THR	C-N-CA	5.37	131.23	121.89
3	L	392	LEU	N-CA-C	-5.37	95.97	111.00
2	n	172	ILE	CB-CA-C	5.37	120.95	112.26
3	M	355	CYS	CA-C-N	5.37	127.42	120.44
3	M	355	CYS	C-N-CA	5.37	127.42	120.44
2	h	151	LEU	N-CA-C	5.37	117.13	111.28
2	k	60	VAL	CA-C-N	5.37	126.05	119.99
2	k	60	VAL	C-N-CA	5.37	126.05	119.99
3	L	300	PRO	N-CD-CG	5.37	111.25	103.20
1	e	211	VAL	CA-C-N	5.36	126.19	121.58
1	e	211	VAL	C-N-CA	5.36	126.19	121.58
2	k	64	GLN	O-C-N	-5.36	115.14	122.33
2	k	179	ASP	CB-CA-C	-5.36	101.96	110.81
3	K	44	TYR	CA-C-N	5.36	127.47	120.28
3	K	44	TYR	C-N-CA	5.36	127.47	120.28
1	D	150	THR	N-CA-CB	5.36	119.32	110.69
2	j	115	ILE	N-CA-C	-5.36	100.74	108.89
2	i	44	LYS	CA-C-N	5.36	130.23	123.10
2	i	44	LYS	C-N-CA	5.36	130.23	123.10
3	M	324	HIS	ND1-CE1-NE2	5.36	113.76	108.40
1	g	238	GLU	CA-C-N	5.36	128.46	120.31
1	g	238	GLU	C-N-CA	5.36	128.46	120.31
2	l	86	THR	CB-CA-C	5.36	119.40	109.54
2	l	104	PHE	O-C-N	-5.36	116.57	121.34
1	C	14	VAL	O-C-N	-5.36	117.83	123.03
1	D	67	ILE	CA-C-N	5.36	130.02	122.09
1	D	67	ILE	C-N-CA	5.36	130.02	122.09
1	d	191	LEU	CA-C-N	5.36	125.89	120.00
1	d	191	LEU	C-N-CA	5.36	125.89	120.00
2	k	140	THR	N-CA-CB	5.36	120.61	111.50
3	K	56	GLU	N-CA-CB	5.36	118.09	110.16
3	J	76	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	G	10	ARG	NE-CZ-NH1	-5.36	116.14	121.50
3	L	321	PHE	CA-C-N	5.35	127.45	120.28
3	L	321	PHE	C-N-CA	5.35	127.45	120.28
1	A	106	PRO	CA-N-CD	-5.35	104.51	112.00
1	A	178	GLU	CA-C-O	-5.35	114.82	120.55
1	F	96	ALA	O-C-N	5.35	128.25	122.15
1	g	73	HIS	ND1-CE1-NE2	5.35	113.75	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	47	GLN	CB-CG-CD	5.35	121.70	112.60
3	J	386	THR	CA-C-O	5.35	128.16	120.51
1	e	33	ARG	CA-C-N	5.35	126.76	120.71
1	e	33	ARG	C-N-CA	5.35	126.76	120.71
1	F	31	VAL	N-CA-C	-5.35	105.17	110.62
1	g	161	ALA	CA-C-O	-5.35	114.12	120.43
2	m	21	ASP	CB-CA-C	-5.35	100.56	109.55
3	K	180	LEU	N-CA-C	-5.35	100.68	109.40
3	K	395	VAL	CA-C-O	-5.35	114.99	120.71
1	E	130	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
1	E	182	ASP	CA-C-N	5.35	129.73	122.19
1	E	182	ASP	C-N-CA	5.35	129.73	122.19
1	G	22	PHE	CA-C-O	-5.35	113.82	119.97
1	G	63	THR	CB-CA-C	5.35	118.24	109.90
2	h	198	GLN	N-CA-C	-5.35	98.66	108.02
1	c	192	GLY	CA-C-O	5.35	125.81	120.09
1	C	197	GLY	CA-C-N	5.34	127.44	120.28
1	C	197	GLY	C-N-CA	5.34	127.44	120.28
2	2	176	MET	O-C-N	5.34	128.24	122.15
2	i	192	THR	O-C-N	5.34	129.42	122.42
2	5	21	ASP	CB-CA-C	5.34	121.67	110.45
2	l	135	LYS	N-CA-C	-5.34	104.34	112.04
1	D	10	ARG	N-CA-C	-5.34	104.34	111.87
1	e	10	ARG	NE-CZ-NH1	-5.34	116.16	121.50
2	h	47	GLN	CA-C-O	-5.34	114.74	120.46
2	3	81	ARG	N-CA-C	-5.34	106.89	113.41
1	a	120	LYS	O-C-N	5.34	129.17	122.23
1	E	36	THR	N-CA-CB	5.34	119.51	110.49
2	1	128	ILE	CA-CB-CG1	5.34	119.48	110.40
1	a	201	GLU	N-CA-C	-5.34	103.87	111.24
2	i	44	LYS	CA-C-O	5.34	124.39	118.52
2	m	138	VAL	CA-C-O	-5.34	115.94	120.96
2	m	210	LYS	CA-C-O	5.34	125.06	119.51
3	L	151	GLU	CA-C-O	-5.34	114.89	120.55
1	a	59	LEU	CB-CA-C	-5.34	100.52	109.65
1	f	220	THR	N-CA-C	-5.34	100.33	109.24
2	3	95	SER	CA-C-O	-5.34	114.89	120.55
2	n	21	ASP	N-CA-CB	5.34	118.02	110.98
3	H	345	GLY	N-CA-C	-5.34	107.85	115.64
3	H	386	THR	CA-C-N	5.34	127.81	120.39
3	H	386	THR	C-N-CA	5.34	127.81	120.39
1	b	162	THR	N-CA-C	-5.33	100.81	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	95	GLU	CA-C-N	5.33	127.86	120.29
1	c	95	GLU	C-N-CA	5.33	127.86	120.29
3	H	108	LEU	N-CA-C	-5.33	101.42	109.85
1	b	84	ASP	CA-C-N	5.33	127.42	120.28
1	b	84	ASP	C-N-CA	5.33	127.42	120.28
1	e	57	LYS	CA-C-N	5.33	127.86	120.29
1	e	57	LYS	C-N-CA	5.33	127.86	120.29
1	F	142	ASP	N-CA-CB	5.33	119.81	110.27
2	2	46	TYR	CA-C-N	5.33	129.51	122.42
2	2	46	TYR	C-N-CA	5.33	129.51	122.42
2	m	188	VAL	CA-C-O	5.33	126.64	120.67
2	n	148	TYR	CB-CA-C	-5.33	101.79	110.85
3	L	133	GLU	O-C-N	-5.33	115.37	122.20
3	M	80	LYS	N-CA-C	-5.33	99.08	108.20
1	c	203	GLU	O-C-N	-5.33	116.98	123.16
1	a	125	GLN	CA-C-N	5.33	128.28	120.71
1	a	125	GLN	C-N-CA	5.33	128.28	120.71
1	e	25	GLU	CB-CA-C	-5.33	101.79	110.85
1	g	62	ASP	CA-CB-CG	-5.33	107.27	112.60
3	H	54	GLU	N-CA-C	5.33	118.00	111.82
1	b	115	LYS	O-C-N	-5.33	116.34	122.09
1	G	132	PHE	CA-CB-CG	-5.33	108.47	113.80
2	2	194	ASP	N-CA-CB	5.33	119.49	110.49
1	e	73	HIS	N-CA-C	-5.33	104.42	112.99
2	4	144	SER	CA-C-N	5.33	127.42	120.28
2	4	144	SER	C-N-CA	5.33	127.42	120.28
2	5	70	ILE	CA-CB-CG1	5.33	119.45	110.40
2	m	67	ALA	N-CA-C	5.33	117.08	111.28
3	H	44	TYR	CB-CG-CD1	-5.33	112.81	120.80
3	H	368	ALA	CB-CA-C	-5.33	100.87	110.35
2	1	88	ARG	NE-CZ-NH1	-5.32	116.18	121.50
2	1	195	GLU	O-C-N	-5.32	115.65	122.94
2	k	32	THR	N-CA-C	-5.32	101.09	109.50
2	k	166	GLU	CB-CA-C	-5.32	101.80	110.85
3	I	158	GLU	CA-CB-CG	-5.32	103.45	114.10
3	I	372	MET	CA-C-N	5.32	128.40	120.31
3	I	372	MET	C-N-CA	5.32	128.40	120.31
3	K	122	SER	N-CA-C	5.32	117.59	110.35
3	K	334	VAL	N-CA-C	-5.32	100.72	108.17
3	M	173	GLU	N-CA-C	-5.32	103.33	109.93
1	a	200	ILE	CA-C-N	5.32	130.50	122.68
1	a	200	ILE	C-N-CA	5.32	130.50	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	148	TYR	CA-CB-CG	-5.32	104.32	113.90
2	1	44	LYS	CA-C-N	5.32	130.11	123.14
2	1	44	LYS	C-N-CA	5.32	130.11	123.14
2	7	51	ARG	NE-CZ-NH1	-5.32	116.18	121.50
3	M	123	LYS	CA-C-N	5.32	128.65	121.20
3	M	123	LYS	C-N-CA	5.32	128.65	121.20
3	M	310	PRO	CA-C-N	5.32	131.02	121.76
3	M	310	PRO	C-N-CA	5.32	131.02	121.76
2	h	104	PHE	CA-C-O	-5.32	115.81	120.60
2	m	40	LYS	CB-CG-CD	5.32	123.54	111.30
2	7	150	VAL	CB-CA-C	-5.32	104.88	112.22
3	I	154	ARG	O-C-N	5.32	127.76	122.12
3	J	349	ALA	CA-C-O	-5.32	113.85	119.97
1	c	224	VAL	O-C-N	5.32	128.71	122.81
1	F	185	PHE	CA-C-O	-5.32	114.91	120.55
3	K	129	GLY	N-CA-C	-5.32	108.06	114.66
1	g	159	TYR	CB-CG-CD2	-5.32	112.82	120.80
3	K	191	LEU	CA-C-N	5.32	127.84	120.29
3	K	191	LEU	C-N-CA	5.32	127.84	120.29
3	M	91	THR	O-C-N	5.32	129.66	122.59
1	a	88	LEU	N-CA-CB	5.32	117.93	110.12
1	D	52	LYS	CA-C-O	-5.32	116.24	121.02
1	D	91	ARG	CA-C-O	-5.32	114.92	120.55
1	f	77	ALA	N-CA-C	-5.32	101.33	109.41
2	h	91	ALA	CB-CA-C	-5.32	101.81	110.85
2	2	13	THR	CA-C-N	5.32	130.93	122.59
2	2	13	THR	C-N-CA	5.32	130.93	122.59
2	k	77	TYR	CA-C-N	5.32	127.40	120.28
2	k	77	TYR	C-N-CA	5.32	127.40	120.28
1	a	96	ALA	N-CA-CB	-5.31	102.30	110.01
1	B	151	ASP	CA-CB-CG	-5.31	107.29	112.60
1	D	112	LEU	N-CA-CB	5.31	118.03	110.16
1	C	193	LEU	CA-C-N	5.31	127.25	120.56
1	C	193	LEU	C-N-CA	5.31	127.25	120.56
1	D	218	ASP	N-CA-C	-5.31	104.92	111.40
3	H	242	GLU	N-CA-C	-5.31	99.48	110.80
1	a	98	ILE	CB-CG1-CD1	5.31	124.95	113.80
2	1	89	ALA	O-C-N	-5.31	116.60	122.07
3	H	41	ARG	CA-C-N	5.31	127.74	120.46
3	H	41	ARG	C-N-CA	5.31	127.74	120.46
1	B	85	ALA	N-CA-CB	5.31	117.92	110.12
1	g	84	ASP	CA-CB-CG	-5.31	107.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	VAL	CA-C-N	5.31	127.92	120.28
1	A	190	VAL	C-N-CA	5.31	127.92	120.28
1	D	197	GLY	N-CA-C	-5.31	106.34	112.50
2	2	111	LEU	N-CA-C	-5.31	100.25	108.90
2	m	197	TYR	CA-CB-CG	-5.31	104.34	113.90
3	I	387	THR	CA-C-O	-5.31	114.50	119.91
3	L	24	ARG	CA-C-N	5.31	127.39	120.28
3	L	24	ARG	C-N-CA	5.31	127.39	120.28
1	A	26	TYR	CB-CG-CD2	5.31	128.76	120.80
3	M	321	PHE	CA-C-N	5.31	127.92	120.28
3	M	321	PHE	C-N-CA	5.31	127.92	120.28
1	c	98	ILE	CA-C-O	-5.30	115.43	120.95
1	E	98	ILE	CB-CA-C	-5.30	104.98	112.14
2	h	54	MET	CA-C-N	5.30	130.90	122.94
2	h	54	MET	C-N-CA	5.30	130.90	122.94
3	H	13	LEU	CB-CA-C	-5.30	101.83	110.85
1	D	134	VAL	CB-CA-C	5.30	119.26	110.30
3	I	97	GLU	N-CA-C	-5.30	106.49	113.17
3	L	263	ARG	N-CA-C	-5.30	105.58	111.36
2	k	135	LYS	N-CA-C	-5.30	99.51	110.80
2	5	44	LYS	O-C-N	5.30	128.01	122.23
3	H	272	LEU	CA-C-O	5.30	126.17	120.55
1	a	14	VAL	CA-C-N	5.30	128.40	120.87
1	a	14	VAL	C-N-CA	5.30	128.40	120.87
1	F	102	THR	CA-C-O	-5.30	113.15	119.35
2	h	68	ARG	N-CA-C	-5.30	105.67	111.82
2	2	72	ILE	CA-CB-CG2	5.30	119.51	110.50
2	k	43	LYS	CB-CG-CD	5.30	123.49	111.30
2	m	102	ARG	N-CA-CB	5.30	118.78	110.46
2	7	123	TYR	CA-C-N	5.30	130.54	122.65
2	7	123	TYR	C-N-CA	5.30	130.54	122.65
3	H	351	ILE	CA-C-O	-5.30	115.44	120.95
1	B	73	HIS	CG-CD2-NE2	5.30	112.50	107.20
3	M	129	GLY	CA-C-N	5.30	129.21	121.31
3	M	129	GLY	C-N-CA	5.30	129.21	121.31
1	A	160	LYS	O-C-N	-5.30	115.89	122.25
1	E	68	TYR	N-CA-C	-5.30	102.21	110.42
1	g	226	PRO	N-CA-C	5.30	121.64	113.75
1	a	145	PRO	CB-CA-C	-5.29	104.17	111.21
1	E	193	LEU	N-CA-C	-5.29	105.59	111.36
3	I	75	GLY	N-CA-C	-5.29	107.33	116.01
1	b	167	GLY	CA-C-N	5.29	127.64	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	167	GLY	C-N-CA	5.29	127.64	120.44
2	h	61	GLY	CA-C-N	5.29	128.35	120.31
2	h	61	GLY	C-N-CA	5.29	128.35	120.31
2	i	48	ILE	N-CA-C	-5.29	104.89	112.35
2	5	124	SER	CA-C-O	5.29	126.15	120.38
2	l	80	ARG	NE-CZ-NH1	-5.29	116.21	121.50
3	H	200	ARG	NE-CZ-NH2	-5.29	114.44	119.20
3	H	235	PRO	CA-C-N	5.29	131.93	122.09
3	H	235	PRO	C-N-CA	5.29	131.93	122.09
3	I	29	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	F	86	ARG	N-CA-C	5.29	117.95	111.82
2	h	51	ARG	NE-CZ-NH1	-5.29	116.21	121.50
2	m	45	ILE	O-C-N	-5.29	117.49	123.20
2	m	107	LEU	CB-CA-C	-5.29	101.62	110.29
2	n	147	ALA	CA-C-O	-5.29	115.25	120.70
1	F	161	ALA	N-CA-CB	5.29	119.42	110.49
2	l	26	ALA	N-CA-C	-5.29	100.69	108.99
3	K	173	GLU	CA-C-O	-5.29	114.78	119.75
3	J	366	GLU	N-CA-CB	5.29	119.95	111.91
1	A	201	GLU	N-CA-C	-5.29	104.14	111.28
1	d	117	CYS	N-CA-CB	5.29	117.98	110.16
1	f	95	GLU	CA-C-O	-5.29	114.95	120.55
2	3	79	ILE	O-C-N	5.29	127.27	121.83
2	j	111	LEU	N-CA-CB	5.29	118.88	110.84
2	5	103	TYR	N-CA-C	-5.29	106.68	113.02
3	M	334	VAL	CA-CB-CG1	5.29	119.39	110.40
1	a	223	GLU	N-CA-C	-5.28	99.91	108.52
1	b	81	LEU	CA-C-N	5.28	128.96	120.30
1	b	81	LEU	C-N-CA	5.28	128.96	120.30
2	i	139	ALA	N-CA-CB	5.28	119.75	111.56
2	j	116	ASP	N-CA-C	-5.28	101.45	108.74
1	G	108	THR	O-C-N	-5.28	117.02	122.94
3	L	364	ARG	CA-C-N	5.28	128.34	120.31
3	L	364	ARG	C-N-CA	5.28	128.34	120.31
1	C	129	VAL	O-C-N	5.28	128.26	123.19
1	F	48	LEU	N-CA-C	-5.28	99.83	108.76
2	2	170	ARG	CA-C-N	5.28	127.79	120.29
2	2	170	ARG	C-N-CA	5.28	127.79	120.29
3	H	46	ARG	O-C-N	5.28	128.17	122.15
1	C	72	GLU	N-CA-C	-5.28	106.70	112.72
2	n	92	THR	CA-C-N	5.28	127.79	120.29
2	n	92	THR	C-N-CA	5.28	127.79	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	208	ASN	CA-CB-CG	5.28	117.88	112.60
2	j	81	ARG	CD-NE-CZ	-5.28	117.01	124.40
2	6	63	ALA	O-C-N	5.28	127.79	122.09
3	J	361	PHE	O-C-N	-5.28	115.78	122.27
1	c	240	ILE	O-C-N	5.28	126.99	121.87
2	h	97	LEU	CA-C-N	5.28	128.33	120.31
2	h	97	LEU	C-N-CA	5.28	128.33	120.31
2	2	86	THR	N-CA-CB	5.28	118.47	110.45
2	k	104	PHE	N-CA-C	-5.28	102.55	110.73
2	m	79	ILE	CB-CA-C	-5.28	105.22	111.97
3	K	333	ASP	N-CA-C	-5.28	106.61	112.57
1	E	14	VAL	CA-C-N	5.27	131.02	122.53
1	E	14	VAL	C-N-CA	5.27	131.02	122.53
1	F	82	VAL	CA-C-N	5.27	127.61	120.44
1	F	82	VAL	C-N-CA	5.27	127.61	120.44
1	G	221	PHE	N-CA-C	5.27	122.03	110.80
2	h	70	ILE	CA-C-N	5.27	127.30	120.44
2	h	70	ILE	C-N-CA	5.27	127.30	120.44
1	a	18	ASP	N-CA-C	-5.27	105.61	111.36
1	c	56	SER	N-CA-CB	5.27	118.83	110.55
2	j	94	THR	CA-C-N	5.27	127.34	120.28
2	j	94	THR	C-N-CA	5.27	127.34	120.28
2	l	179	ASP	N-CA-C	-5.27	101.40	109.41
3	H	109	ASN	CA-CB-CG	-5.27	107.33	112.60
3	M	211	PHE	N-CA-CB	5.27	118.07	109.69
1	C	102	THR	CA-CB-OG1	5.27	117.51	109.60
2	2	150	VAL	CB-CA-C	-5.27	105.03	112.14
3	I	370	VAL	CB-CA-C	5.27	117.44	110.91
1	e	218	ASP	CA-CB-CG	-5.27	107.33	112.60
2	2	203	GLU	N-CA-CB	5.27	117.96	110.16
1	b	166	MET	N-CA-C	-5.27	105.54	111.28
1	D	58	LEU	CA-C-N	5.27	128.70	120.75
1	D	58	LEU	C-N-CA	5.27	128.70	120.75
2	2	137	ILE	CB-CA-C	-5.27	103.32	110.90
3	I	64	LEU	CA-C-N	5.27	128.93	121.66
3	I	64	LEU	C-N-CA	5.27	128.93	121.66
3	L	324	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	A	122	GLN	CA-C-N	5.26	131.91	122.38
1	A	122	GLN	C-N-CA	5.26	131.91	122.38
1	b	131	PRO	N-CA-CB	5.26	109.18	103.23
1	e	188	ALA	O-C-N	5.26	128.74	122.27
2	4	97	LEU	N-CA-CB	5.26	117.64	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASN	CB-CG-ND2	-5.26	108.51	116.40
1	d	98	ILE	N-CA-CB	5.26	117.70	110.54
1	G	70	ILE	N-CA-C	-5.26	107.70	112.96
2	h	91	ALA	N-CA-C	5.26	117.10	111.36
2	7	69	ILE	N-CA-CB	5.26	116.71	110.55
1	A	120	LYS	CA-CB-CG	-5.26	103.58	114.10
1	a	29	GLU	CB-CA-C	-5.26	102.06	110.79
1	b	242	GLU	CA-C-O	5.26	126.34	120.82
1	E	150	THR	N-CA-C	-5.26	100.66	109.24
1	f	228	GLU	N-CA-C	-5.26	107.03	113.50
1	g	180	ARG	N-CA-C	-5.26	101.30	109.24
3	H	30	LEU	N-CA-C	-5.26	105.63	111.36
3	I	49	ARG	CB-CA-C	-5.26	101.91	110.85
3	I	218	GLU	CA-C-O	-5.26	114.84	120.42
3	K	66	GLY	O-C-N	-5.26	119.90	123.95
3	L	240	ILE	CA-C-N	5.26	131.07	122.07
3	L	240	ILE	C-N-CA	5.26	131.07	122.07
3	J	28	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	A	15	PHE	CA-C-O	-5.26	115.24	121.66
1	b	136	LEU	N-CA-C	-5.26	101.19	109.50
2	6	192	THR	CA-CB-OG1	5.26	117.49	109.60
1	F	203	GLU	CB-CG-CD	-5.26	103.66	112.60
2	2	123	TYR	CB-CG-CD1	-5.26	112.91	120.80
2	n	44	LYS	CA-C-N	5.26	130.45	122.98
2	n	44	LYS	C-N-CA	5.26	130.45	122.98
1	B	142	ASP	N-CA-C	-5.26	105.22	111.69
1	d	150	THR	O-C-N	5.26	130.02	123.19
2	l	116	ASP	CA-C-O	-5.26	115.79	121.36
2	n	203	GLU	CA-C-N	5.26	127.88	120.42
2	n	203	GLU	C-N-CA	5.26	127.88	120.42
3	L	239	PHE	CA-CB-CG	5.26	119.06	113.80
3	M	302	ARG	NH1-CZ-NH2	5.26	126.13	119.30
1	g	138	ILE	O-C-N	-5.25	117.63	123.20
2	i	81	ARG	NE-CZ-NH2	-5.25	114.47	119.20
3	M	84	GLY	CA-C-N	5.25	125.25	119.89
3	M	84	GLY	C-N-CA	5.25	125.25	119.89
1	b	40	ILE	CA-C-O	-5.25	114.79	120.36
1	b	128	GLY	N-CA-C	-5.25	108.15	114.66
1	b	212	GLY	N-CA-C	-5.25	103.34	112.06
1	E	21	LEU	N-CA-C	-5.25	98.83	108.02
1	F	238	GLU	O-C-N	-5.25	116.55	122.12
1	f	180	ARG	N-CA-C	-5.25	101.38	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	138	VAL	N-CA-C	-5.25	100.29	107.75
1	b	113	ALA	N-CA-CB	5.25	117.93	110.16
1	D	8	TYR	N-CA-C	-5.25	105.58	112.41
1	E	23	GLN	CA-C-N	5.25	129.32	120.29
1	E	23	GLN	C-N-CA	5.25	129.32	120.29
1	e	189	MET	CG-SD-CE	5.25	112.45	100.90
2	k	140	THR	CA-CB-OG1	5.25	117.48	109.60
2	k	148	TYR	N-CA-CB	5.25	117.84	110.12
3	M	171	GLY	N-CA-C	-5.25	107.87	115.27
1	d	135	SER	O-C-N	-5.25	116.33	123.15
2	l	130	GLY	N-CA-C	-5.25	100.74	113.18
1	E	31	VAL	N-CA-CB	5.25	117.68	110.54
1	E	221	PHE	CA-C-N	5.25	130.71	122.21
1	E	221	PHE	C-N-CA	5.25	130.71	122.21
2	m	38	ALA	CA-C-O	5.25	126.11	120.70
3	M	18	GLU	CA-C-O	-5.25	115.29	120.70
3	J	223	VAL	N-CA-C	5.25	115.97	110.62
2	5	84	LYS	CA-C-N	5.25	125.45	120.31
2	5	84	LYS	C-N-CA	5.25	125.45	120.31
2	l	72	ILE	CA-CB-CG2	5.25	119.42	110.50
3	H	312	PRO	CA-C-N	5.25	130.92	121.06
3	H	312	PRO	C-N-CA	5.25	130.92	121.06
3	I	198	GLN	CB-CG-CD	-5.25	103.68	112.60
3	J	26	LEU	CA-C-O	5.25	126.33	120.82
1	B	91	ARG	N-CA-C	5.25	117.00	111.28
1	e	162	THR	CA-C-O	5.25	126.84	121.23
2	h	156	THR	O-C-N	-5.25	117.29	121.80
1	b	186	ASP	CA-C-N	5.24	127.31	120.28
1	b	186	ASP	C-N-CA	5.24	127.31	120.28
2	2	180	SER	N-CA-CB	5.24	117.92	110.16
2	3	204	VAL	O-C-N	5.24	127.23	121.83
2	j	18	VAL	CA-CB-CG1	5.24	119.32	110.40
2	n	203	GLU	N-CA-CB	5.24	117.61	110.01
1	b	151	ASP	CA-C-O	-5.24	115.26	120.66
1	c	36	THR	CA-C-O	-5.24	115.42	121.19
2	2	39	SER	CB-CA-C	-5.24	101.47	110.22
2	n	24	VAL	O-C-N	-5.24	117.54	123.20
3	K	168	ALA	N-CA-C	5.24	116.68	111.07
2	i	107	LEU	N-CA-C	-5.24	98.85	108.02
2	i	206	GLN	CB-CA-C	5.24	121.26	110.31
2	4	127	PRO	N-CA-C	-5.24	107.31	113.86
2	5	104	PHE	CA-C-N	5.24	125.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	104	PHE	C-N-CA	5.24	125.25	119.90
3	I	48	VAL	N-CA-CB	5.24	116.68	110.55
3	K	51	LEU	N-CA-CB	5.24	118.40	110.28
1	E	235	ARG	O-C-N	5.24	127.67	122.12
2	7	132	ILE	CA-C-N	5.24	131.54	121.54
2	7	132	ILE	C-N-CA	5.24	131.54	121.54
2	n	165	VAL	CA-C-N	5.24	127.73	120.29
2	n	165	VAL	C-N-CA	5.24	127.73	120.29
1	E	14	VAL	O-C-N	-5.24	117.24	123.00
1	G	31	VAL	CB-CA-C	-5.24	104.99	112.22
1	C	164	ILE	N-CA-C	-5.24	100.33	108.44
2	k	63	ALA	N-CA-C	5.24	117.07	111.36
2	6	85	PRO	N-CA-CB	5.24	108.16	103.19
2	m	70	ILE	CA-C-N	5.24	127.25	120.44
2	m	70	ILE	C-N-CA	5.24	127.25	120.44
2	7	106	TYR	CB-CA-C	-5.24	102.31	110.74
3	I	210	GLU	N-CA-C	-5.24	106.94	113.38
3	M	221	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	c	187	ASP	CA-C-O	5.23	125.97	120.42
1	D	140	GLY	CA-C-O	5.23	126.68	121.29
1	D	180	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	F	220	THR	CA-C-N	5.23	131.54	121.54
1	F	220	THR	C-N-CA	5.23	131.54	121.54
1	B	73	HIS	ND1-CE1-NE2	5.23	113.63	108.40
2	h	211	PHE	N-CA-CB	5.23	118.23	110.49
3	K	142	ASP	CA-CB-CG	-5.23	107.37	112.60
1	C	141	VAL	CB-CA-C	-5.23	103.36	110.42
2	5	127	PRO	N-CA-C	-5.23	106.91	114.18
3	L	33	GLU	N-CA-CB	5.23	118.28	110.22
3	M	95	ILE	N-CA-C	-5.23	100.67	108.46
1	f	101	LEU	N-CA-CB	5.23	117.99	110.20
2	h	203	GLU	CA-C-N	5.23	128.88	120.30
2	h	203	GLU	C-N-CA	5.23	128.88	120.30
3	J	21	TYR	CB-CA-C	-5.23	102.11	110.79
1	B	25	GLU	N-CA-C	-5.23	106.86	113.18
2	2	86	THR	CA-CB-OG1	5.23	117.44	109.60
3	L	330	LEU	N-CA-CB	5.23	119.32	110.49
3	M	233	LYS	N-CA-C	-5.23	104.57	112.99
3	J	18	GLU	N-CA-C	5.23	116.98	111.28
3	J	102	PRO	CA-C-N	5.23	130.82	122.25
3	J	102	PRO	C-N-CA	5.23	130.82	122.25
2	3	160	GLY	N-CA-C	-5.23	104.19	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	98	ILE	N-CA-C	-5.22	105.44	110.72
1	G	171	VAL	CB-CA-C	-5.22	105.09	112.14
2	k	14	THR	CA-C-O	-5.22	114.33	120.60
1	B	65	GLU	CB-CA-C	5.22	120.02	110.10
1	B	91	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	m	107	LEU	CA-C-N	5.22	128.96	121.96
2	m	107	LEU	C-N-CA	5.22	128.96	121.96
3	K	246	ILE	O-C-N	5.22	129.10	122.57
3	M	226	VAL	CB-CA-C	-5.22	103.80	112.26
1	a	162	THR	CA-CB-CG2	5.22	119.38	110.50
1	C	10	ARG	N-CA-C	-5.22	106.14	112.88
2	h	191	ILE	N-CA-C	-5.22	98.48	109.34
3	H	94	TYR	N-CA-CB	5.22	117.64	110.07
3	L	237	ILE	N-CA-C	-5.22	100.80	108.11
1	E	174	PHE	CB-CA-C	-5.22	102.69	110.88
1	F	20	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	g	125	GLN	CB-CG-CD	5.22	121.47	112.60
2	7	18	VAL	N-CA-C	-5.22	100.23	107.80
3	H	240	ILE	N-CA-C	-5.22	100.55	108.17
3	J	112	THR	CA-CB-OG1	5.22	117.43	109.60
2	k	47	GLN	O-C-N	5.22	129.19	122.93
2	l	96	ASN	N-CA-C	-5.22	105.67	111.36
1	B	25	GLU	CA-C-O	-5.22	112.43	119.11
1	G	82	VAL	O-C-N	-5.22	117.40	122.09
2	j	121	SER	CA-C-O	-5.22	114.66	120.66
1	e	99	ASN	CA-C-N	5.21	127.79	120.28
1	e	99	ASN	C-N-CA	5.21	127.79	120.28
1	G	202	SER	CA-C-N	5.21	128.11	120.71
1	G	202	SER	C-N-CA	5.21	128.11	120.71
2	j	50	ASP	CB-CA-C	-5.21	100.34	110.46
2	j	116	ASP	CA-C-N	5.21	128.24	120.31
2	j	116	ASP	C-N-CA	5.21	128.24	120.31
3	I	270	ALA	N-CA-C	5.21	121.90	110.80
1	F	164	ILE	CA-CB-CG1	5.21	119.26	110.40
2	1	152	GLU	CB-CG-CD	-5.21	103.74	112.60
2	3	49	ALA	CA-C-N	5.21	127.78	120.28
2	3	49	ALA	C-N-CA	5.21	127.78	120.28
2	3	188	VAL	CA-C-O	-5.21	116.20	121.67
2	m	212	ARG	NE-CZ-NH2	-5.21	114.51	119.20
2	n	150	VAL	CA-C-N	5.21	127.22	120.44
2	n	150	VAL	C-N-CA	5.21	127.22	120.44
3	M	265	MET	CA-C-O	-5.21	114.90	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	146	THR	CA-C-O	-5.21	114.90	120.42
2	6	134	GLU	CB-CG-CD	-5.21	103.74	112.60
3	I	152	GLU	N-CA-C	-5.21	105.68	111.36
1	A	196	MET	CA-C-N	5.21	125.73	120.00
1	A	196	MET	C-N-CA	5.21	125.73	120.00
1	D	200	ILE	O-C-N	5.21	128.16	122.12
1	G	164	ILE	N-CA-C	-5.21	100.78	108.23
3	H	382	VAL	CA-C-N	5.21	127.26	120.28
3	H	382	VAL	C-N-CA	5.21	127.26	120.28
3	L	61	PRO	N-CA-C	5.21	115.47	110.47
3	J	36	PHE	CA-C-N	5.21	127.60	120.46
3	J	36	PHE	C-N-CA	5.21	127.60	120.46
1	c	45	GLY	CA-C-O	-5.21	116.93	121.04
1	e	176	GLU	CA-CB-CG	-5.21	103.69	114.10
2	k	164	ALA	O-C-N	-5.21	114.63	122.28
3	I	276	ASP	CA-C-O	-5.21	115.05	120.88
3	I	352	LYS	O-C-N	5.21	128.09	122.15
2	1	153	ASP	N-CA-CB	5.21	117.56	110.01
2	3	13	THR	N-CA-C	-5.21	101.16	109.23
1	C	217	ASP	CA-CB-CG	5.20	117.80	112.60
2	i	100	SER	O-C-N	5.20	127.64	122.12
3	K	34	LYS	CA-CB-CG	-5.20	103.69	114.10
3	K	229	LEU	CA-C-O	-5.20	114.47	120.24
1	D	12	ILE	N-CA-CB	-5.20	105.36	112.28
1	e	237	ASN	CA-C-N	5.20	127.20	120.44
1	e	237	ASN	C-N-CA	5.20	127.20	120.44
3	H	29	ARG	CA-C-O	-5.20	114.91	120.42
1	c	219	ARG	CA-C-N	5.20	130.10	122.77
1	c	219	ARG	C-N-CA	5.20	130.10	122.77
1	f	137	LEU	O-C-N	5.20	129.99	123.12
2	l	48	ILE	N-CA-C	-5.20	105.02	112.35
3	H	213	GLN	N-CA-C	-5.20	101.53	108.86
3	K	187	GLY	CA-C-N	5.20	127.25	120.28
3	K	187	GLY	C-N-CA	5.20	127.25	120.28
3	M	118	VAL	N-CA-CB	5.20	116.20	110.53
3	M	130	PHE	CA-C-O	-5.20	115.45	121.07
1	e	106	PRO	CA-C-O	-5.20	115.53	121.56
1	f	223	GLU	N-CA-C	-5.20	100.56	109.24
2	i	148	TYR	CB-CA-C	-5.20	102.16	110.79
2	k	122	ILE	CA-C-O	-5.20	115.04	120.76
2	m	64	GLN	N-CA-CB	5.20	117.61	110.07
3	H	327	LYS	CA-C-N	5.20	128.60	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	327	LYS	C-N-CA	5.20	128.60	120.75
3	M	97	GLU	N-CA-C	-5.20	106.91	113.20
1	B	156	LEU	N-CA-C	-5.20	100.77	109.24
3	J	370	VAL	CA-CB-CG2	-5.20	101.57	110.40
1	E	100	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	e	126	TYR	N-CA-C	-5.20	102.50	110.14
1	F	94	ILE	CA-C-N	5.20	127.24	120.28
1	F	94	ILE	C-N-CA	5.20	127.24	120.28
1	G	195	ALA	CA-C-O	-5.20	114.91	120.42
3	H	114	ALA	CA-C-N	5.20	128.04	120.98
3	H	114	ALA	C-N-CA	5.20	128.04	120.98
1	d	14	VAL	CA-C-O	5.19	127.27	120.78
2	1	185	GLY	CA-C-N	5.19	130.40	122.25
2	1	185	GLY	C-N-CA	5.19	130.40	122.25
2	n	102	ARG	CA-C-N	5.19	127.67	120.29
2	n	102	ARG	C-N-CA	5.19	127.67	120.29
2	3	44	LYS	N-CA-C	-5.19	106.86	114.39
3	L	319	GLN	CA-C-N	5.19	127.79	120.42
3	L	319	GLN	C-N-CA	5.19	127.79	120.42
1	d	73	HIS	ND1-CE1-NE2	5.19	113.59	108.40
1	G	186	ASP	CA-C-N	5.19	127.19	120.44
1	G	186	ASP	C-N-CA	5.19	127.19	120.44
2	j	65	PHE	O-C-N	5.19	128.07	122.15
2	k	209	ALA	N-CA-CB	5.19	117.93	110.20
3	I	159	LEU	CA-C-O	-5.19	113.64	118.73
1	A	108	THR	CA-C-O	-5.19	115.48	121.19
1	A	191	LEU	CA-C-N	5.19	125.71	120.00
1	A	191	LEU	C-N-CA	5.19	125.71	120.00
1	g	32	LYS	CA-C-N	5.19	128.20	120.31
1	g	32	LYS	C-N-CA	5.19	128.20	120.31
2	3	139	ALA	N-CA-C	-5.19	99.75	110.80
2	4	88	ARG	CD-NE-CZ	-5.19	117.14	124.40
3	I	139	SER	N-CA-C	-5.19	99.75	110.80
1	a	181	ASP	CA-C-N	5.19	130.53	122.49
1	a	181	ASP	C-N-CA	5.19	130.53	122.49
1	c	80	GLY	N-CA-C	-5.19	104.34	111.76
2	k	46	TYR	O-C-N	-5.19	117.24	123.31
2	7	35	ASN	CB-CG-ND2	-5.19	108.62	116.40
3	M	78	VAL	N-CA-C	-5.19	100.29	108.23
1	B	157	LEU	N-CA-CB	5.18	120.51	111.13
1	b	33	ARG	NH1-CZ-NH2	5.18	126.04	119.30
2	5	181	ALA	CA-C-N	5.18	129.58	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	181	ALA	C-N-CA	5.18	129.58	121.08
3	H	226	VAL	O-C-N	5.18	126.90	121.87
3	K	116	VAL	CA-CB-CG1	-5.18	101.59	110.40
1	C	216	VAL	CA-C-O	-5.18	115.56	120.95
1	d	241	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	E	87	VAL	N-CA-C	-5.18	105.48	110.72
1	f	174	PHE	O-C-N	5.18	127.61	122.12
2	3	97	LEU	CB-CA-C	5.18	119.10	110.81
2	n	14	THR	N-CA-CB	5.18	121.16	111.52
3	K	103	GLY	N-CA-C	-5.18	107.64	114.95
3	M	276	ASP	N-CA-C	-5.18	103.42	110.36
2	i	90	ILE	CA-C-N	5.18	127.17	120.44
2	i	90	ILE	C-N-CA	5.18	127.17	120.44
2	3	54	MET	CA-C-N	5.18	130.44	122.93
2	3	54	MET	C-N-CA	5.18	130.44	122.93
2	n	96	ASN	CB-CA-C	-5.18	102.04	110.85
3	K	199	THR	CA-CB-OG1	5.18	117.37	109.60
3	J	185	GLY	CA-C-O	5.18	124.75	119.10
1	D	205	VAL	CA-C-N	5.18	124.84	119.56
1	D	205	VAL	C-N-CA	5.18	124.84	119.56
2	h	210	LYS	O-C-N	5.18	129.35	122.26
2	5	138	VAL	N-CA-C	5.18	120.11	109.34
2	l	107	LEU	N-CA-CB	5.18	118.10	110.49
2	l	210	LYS	N-CA-C	-5.18	106.64	113.17
3	K	267	GLN	CA-C-N	5.18	127.64	120.29
3	K	267	GLN	C-N-CA	5.18	127.64	120.29
2	1	144	SER	N-CA-CB	5.18	117.73	110.12
1	D	83	ALA	N-CA-C	5.18	116.92	111.28
1	D	241	ARG	N-CA-C	5.18	116.92	111.28
1	e	227	GLU	N-CA-C	5.18	116.92	111.28
2	h	64	GLN	CB-CA-C	-5.18	102.05	110.85
2	4	165	VAL	N-CA-CB	5.18	117.58	110.54
1	b	205	VAL	CA-C-N	5.17	124.79	119.56
1	b	205	VAL	C-N-CA	5.17	124.79	119.56
1	G	93	ARG	NH1-CZ-NH2	5.17	126.03	119.30
3	H	257	GLY	N-CA-C	5.17	118.75	112.49
3	L	194	ALA	CA-C-N	5.17	127.55	120.46
3	L	194	ALA	C-N-CA	5.17	127.55	120.46
3	J	96	ASN	N-CA-C	-5.17	102.12	110.14
1	b	155	ALA	N-CA-CB	5.17	118.63	110.56
2	4	55	THR	CA-CB-OG1	5.17	117.36	109.60
2	l	162	ASP	CA-C-O	5.17	126.03	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	367	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	30	ALA	N-CA-CB	5.17	118.83	110.40
1	d	66	LYS	CB-CA-C	5.17	117.41	109.03
2	2	113	GLY	O-C-N	-5.17	119.10	123.60
2	3	23	VAL	N-CA-C	-5.17	100.80	108.45
2	j	163	GLU	N-CA-C	-5.17	106.13	112.90
3	J	328	MET	CB-CA-C	-5.17	103.26	111.17
1	C	39	GLY	O-C-N	-5.17	119.35	123.49
1	a	21	LEU	O-C-N	5.17	128.74	122.85
1	b	175	PHE	CA-C-O	-5.17	112.50	119.11
1	E	104	ASP	CA-C-O	5.17	127.43	121.28
2	3	63	ALA	CA-C-N	5.17	127.47	120.44
2	3	63	ALA	C-N-CA	5.17	127.47	120.44
3	I	155	GLU	CB-CG-CD	-5.17	103.81	112.60
3	L	168	ALA	CB-CA-C	-5.17	102.21	110.79
3	M	105	ARG	CB-CG-CD	5.17	123.19	111.30
3	M	312	PRO	N-CD-CG	5.17	110.95	103.20
3	J	394	GLY	CA-C-O	5.17	129.56	120.57
1	f	214	VAL	O-C-N	5.17	128.65	123.07
2	j	19	CYS	N-CA-C	-5.17	101.90	109.81
1	a	88	LEU	O-C-N	-5.17	116.64	122.12
2	j	126	ASP	CA-C-O	-5.17	115.90	121.27
2	m	60	VAL	CA-C-O	-5.17	115.32	121.05
1	a	10	ARG	CB-CG-CD	5.16	123.17	111.30
1	F	149	GLU	CA-C-N	5.16	130.34	122.65
1	F	149	GLU	C-N-CA	5.16	130.34	122.65
1	G	166	MET	CB-CA-C	-5.16	102.07	110.85
1	A	110	LYS	N-CA-C	5.16	116.59	111.07
1	D	82	VAL	CB-CA-C	-5.16	103.75	112.16
1	f	190	VAL	CA-C-N	5.16	127.20	120.28
1	f	190	VAL	C-N-CA	5.16	127.20	120.28
2	m	192	THR	N-CA-C	-5.16	106.76	113.16
3	M	309	VAL	CA-C-O	-5.16	116.23	119.12
1	c	98	ILE	N-CA-C	-5.16	105.36	110.62
1	G	121	GLN	CG-CD-NE2	5.16	124.14	116.40
2	h	147	ALA	CA-C-N	5.16	127.46	120.44
2	h	147	ALA	C-N-CA	5.16	127.46	120.44
2	2	67	ALA	CB-CA-C	-5.16	102.22	110.79
2	k	94	THR	CA-C-N	5.16	127.19	120.28
2	k	94	THR	C-N-CA	5.16	127.19	120.28
3	I	364	ARG	CA-C-N	5.16	131.44	122.56
3	I	364	ARG	C-N-CA	5.16	131.44	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	207	VAL	CB-CA-C	-5.16	105.91	111.59
1	C	234	GLU	CB-CA-C	-5.16	102.95	110.95
2	j	199	TYR	CD1-CG-CD2	5.16	125.84	118.10
2	k	78	GLU	O-C-N	5.16	127.59	122.12
3	K	358	ALA	CA-C-O	-5.16	115.08	120.55
3	L	78	VAL	CA-CB-CG2	-5.16	101.63	110.40
1	g	72	GLU	N-CA-C	-5.16	107.16	112.93
3	H	105	ARG	CA-C-O	-5.16	115.38	121.16
1	a	153	SER	N-CA-C	-5.16	106.84	113.23
2	n	115	ILE	O-C-N	-5.16	117.61	123.18
1	C	109	VAL	CA-C-O	-5.15	115.59	120.95
1	e	149	GLU	CA-C-O	5.15	126.04	120.32
2	4	146	THR	N-CA-CB	5.15	117.54	110.07
2	l	188	VAL	N-CA-C	-5.15	101.05	108.42
2	m	132	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	a	213	TYR	CB-CG-CD1	-5.15	113.08	120.80
1	c	166	MET	CG-SD-CE	-5.15	89.57	100.90
1	e	84	ASP	CA-C-N	5.15	127.18	120.28
1	e	84	ASP	C-N-CA	5.15	127.18	120.28
2	h	63	ALA	CB-CA-C	-5.15	102.76	110.90
3	M	56	GLU	CB-CA-C	-5.15	100.78	110.67
2	7	151	LEU	O-C-N	5.15	128.02	122.15
1	C	62	ASP	N-CA-CB	5.15	118.26	110.28
1	G	202	SER	N-CA-C	-5.15	100.91	108.79
3	H	313	THR	N-CA-C	-5.15	104.08	110.41
1	C	14	VAL	CA-C-O	5.15	125.35	120.31
1	d	176	GLU	CB-CG-CD	-5.14	103.86	112.60
1	E	201	GLU	CA-C-O	-5.14	115.16	121.28
2	1	53	ALA	N-CA-CB	-5.14	103.25	111.43
2	3	37	ILE	CA-C-O	5.14	125.81	120.36
2	j	57	ALA	N-CA-C	-5.14	100.65	109.24
2	n	61	GLY	CA-C-N	5.14	129.38	120.58
2	n	61	GLY	C-N-CA	5.14	129.38	120.58
3	K	277	PRO	CB-CA-C	5.14	117.97	111.39
3	L	210	GLU	N-CA-CB	5.14	118.47	110.44
3	L	241	ASP	CA-C-N	5.14	131.36	121.54
3	L	241	ASP	C-N-CA	5.14	131.36	121.54
1	C	100	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	g	53	ARG	N-CA-C	-5.14	102.03	109.59
2	5	212	ARG	N-CA-CB	5.14	119.18	110.49
2	6	131	ALA	N-CA-CB	5.14	119.25	110.71
3	M	88	VAL	N-CA-CB	5.14	118.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	194	ALA	CA-C-N	5.14	127.04	120.56
3	K	194	ALA	C-N-CA	5.14	127.04	120.56
1	a	16	SER	CB-CA-C	-5.14	101.71	109.26
1	B	151	ASP	N-CA-C	-5.14	104.14	110.31
1	B	223	GLU	CA-C-O	-5.14	115.10	120.80
1	G	154	GLY	CA-C-O	5.14	124.43	118.98
2	m	27	THR	N-CA-C	-5.14	101.48	109.14
2	7	94	THR	O-C-N	5.14	128.01	122.15
3	H	217	GLY	CA-C-O	5.14	126.10	119.68
3	K	71	ILE	N-CA-C	-5.14	100.97	108.99
3	K	158	GLU	N-CA-CB	5.14	117.46	110.01
3	L	397	PHE	N-CA-C	-5.14	107.04	113.72
2	h	211	PHE	N-CA-C	-5.14	106.70	113.17
2	4	33	MET	N-CA-C	-5.14	99.86	110.80
3	L	126	MET	N-CA-C	5.14	117.78	111.82
1	a	22	PHE	N-CA-C	-5.13	105.68	111.28
1	F	9	ASP	CA-C-O	5.13	127.85	120.51
2	2	146	THR	CA-C-N	5.13	127.16	120.28
2	2	146	THR	C-N-CA	5.13	127.16	120.28
1	A	13	THR	CA-CB-CG2	-5.13	101.78	110.50
1	B	191	LEU	CA-C-O	5.13	125.99	120.55
1	b	122	GLN	N-CA-CB	5.13	117.75	110.16
1	E	204	LEU	CA-C-O	5.13	126.50	120.80
1	G	172	THR	N-CA-CB	5.13	117.45	110.01
2	2	182	SER	N-CA-C	-5.13	99.87	110.80
2	i	171	ALA	CA-C-N	5.13	127.71	120.42
2	i	171	ALA	C-N-CA	5.13	127.71	120.42
2	l	75	ASN	CA-C-N	5.13	127.16	120.28
2	l	75	ASN	C-N-CA	5.13	127.16	120.28
1	D	108	THR	CB-CA-C	5.13	118.90	109.46
2	j	69	ILE	CA-C-N	5.13	127.49	120.46
2	j	69	ILE	C-N-CA	5.13	127.49	120.46
2	6	37	ILE	CB-CG1-CD1	5.13	124.57	113.80
3	K	112	THR	CA-CB-OG1	5.13	117.29	109.60
1	A	215	LYS	CA-C-N	5.13	128.75	120.55
1	A	215	LYS	C-N-CA	5.13	128.75	120.55
1	g	25	GLU	CB-CA-C	-5.13	102.13	110.85
1	g	240	ILE	O-C-N	5.13	126.94	121.91
2	k	85	PRO	N-CA-C	5.13	118.66	111.33
2	m	32	THR	N-CA-CB	5.13	121.06	111.53
3	M	36	PHE	N-CA-C	5.13	116.95	111.36
3	M	95	ILE	O-C-N	-5.13	117.61	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	263	ARG	N-CA-C	-5.13	105.87	111.82
2	3	137	ILE	O-C-N	-5.12	116.67	122.72
1	A	137	LEU	N-CA-C	-5.12	101.34	109.59
1	a	88	LEU	CA-C-O	5.12	125.98	120.55
1	e	129	VAL	CA-C-O	5.12	124.78	120.22
2	h	50	ASP	CB-CA-C	-5.12	103.33	111.17
2	3	64	GLN	OE1-CD-NE2	5.12	127.72	122.60
2	l	46	TYR	CA-CB-CG	-5.12	104.68	113.90
3	K	121	THR	N-CA-C	5.12	117.76	111.82
3	L	120	PRO	O-C-N	5.12	128.84	123.10
3	M	259	ARG	CB-CA-C	-5.12	102.29	110.79
1	a	17	PRO	N-CA-C	-5.12	106.74	113.65
1	c	219	ARG	N-CA-CB	5.12	119.86	112.13
2	n	206	GLN	N-CA-C	-5.12	106.98	113.18
3	H	316	GLY	CA-C-N	5.12	127.10	120.44
3	H	316	GLY	C-N-CA	5.12	127.10	120.44
3	J	264	THR	N-CA-CB	5.12	118.22	110.28
1	c	225	SER	CA-C-N	5.12	125.41	119.47
1	c	225	SER	C-N-CA	5.12	125.41	119.47
2	4	34	GLY	N-CA-C	-5.12	107.74	115.32
2	n	71	LYS	N-CA-CB	5.12	117.65	110.12
3	J	352	LYS	CA-C-N	5.12	127.56	120.29
3	J	352	LYS	C-N-CA	5.12	127.56	120.29
1	g	172	THR	CB-CA-C	5.12	119.28	110.79
2	h	81	ARG	N-CA-C	-5.12	107.20	113.50
1	d	73	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
2	5	32	THR	CB-CA-C	-5.12	102.59	110.78
3	H	23	LEU	N-CA-C	-5.12	105.78	112.23
1	E	204	LEU	O-C-N	-5.12	117.21	123.19
2	n	116	ASP	CA-C-O	5.12	126.78	121.31
3	M	222	LEU	CB-CA-C	-5.12	99.30	109.99
2	1	154	ARG	NE-CZ-NH1	-5.11	116.39	121.50
3	I	214	LYS	N-CA-C	5.11	118.62	112.38
1	B	168	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	c	132	PHE	CA-C-O	-5.11	116.25	121.87
1	e	67	ILE	N-CA-CB	5.11	117.90	111.46
2	4	153	ASP	CA-CB-CG	-5.11	107.49	112.60
3	H	197	ASN	CA-CB-CG	5.11	117.71	112.60
3	I	210	GLU	N-CA-CB	-5.11	102.91	110.53
3	I	382	VAL	CA-C-N	5.11	127.64	120.28
3	I	382	VAL	C-N-CA	5.11	127.64	120.28
3	L	388	PRO	N-CA-C	-5.11	101.94	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	345	GLY	CA-C-O	5.11	125.49	119.46
1	c	220	THR	CA-C-N	5.11	128.02	120.82
1	c	220	THR	C-N-CA	5.11	128.02	120.82
2	2	46	TYR	O-C-N	-5.11	116.72	123.21
3	L	348	GLY	CA-C-N	5.11	127.64	120.28
3	L	348	GLY	C-N-CA	5.11	127.64	120.28
3	J	223	VAL	O-C-N	5.11	126.83	121.87
3	J	381	LYS	CA-C-N	5.11	127.19	120.60
3	J	381	LYS	C-N-CA	5.11	127.19	120.60
1	a	36	THR	CA-CB-CG2	5.11	119.18	110.50
1	b	65	GLU	CB-CG-CD	-5.11	103.92	112.60
1	c	181	ASP	CA-CB-CG	-5.11	107.49	112.60
1	g	176	GLU	N-CA-CB	5.11	118.08	110.22
2	3	93	LEU	CA-C-N	5.11	127.54	120.29
2	3	93	LEU	C-N-CA	5.11	127.54	120.29
2	3	201	PRO	N-CD-CG	5.11	110.86	103.20
3	J	319	GLN	CG-CD-OE1	5.11	131.01	120.80
1	D	148	TYR	CA-C-O	5.10	127.41	121.44
1	a	38	ILE	N-CA-C	-5.10	100.54	108.86
1	a	109	VAL	CB-CA-C	-5.10	105.25	112.14
1	A	197	GLY	CA-C-N	5.10	127.62	120.28
1	A	197	GLY	C-N-CA	5.10	127.62	120.28
1	b	99	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	D	118	ASP	CB-CA-C	-5.10	102.18	110.85
1	e	224	VAL	CA-C-N	5.10	130.74	122.48
1	e	224	VAL	C-N-CA	5.10	130.74	122.48
2	3	99	ASN	CA-CB-CG	-5.10	107.50	112.60
3	K	126	MET	CA-C-O	-5.10	116.43	121.02
3	M	125	PRO	CB-CA-C	-5.10	104.27	110.95
1	A	108	THR	N-CA-CB	5.10	117.53	109.83
1	E	130	ARG	N-CA-C	5.10	116.11	109.64
1	E	237	ASN	CA-CB-CG	5.10	117.70	112.60
1	G	179	TYR	N-CA-C	5.10	117.62	110.23
2	j	62	ASP	CA-CB-CG	-5.10	107.50	112.60
2	k	22	GLY	CA-C-O	-5.10	116.41	120.79
3	H	117	ASN	N-CA-CB	5.10	119.31	111.46
1	B	30	ALA	CA-C-N	5.10	127.66	120.42
1	B	30	ALA	C-N-CA	5.10	127.66	120.42
3	K	143	ILE	CB-CA-C	5.10	118.91	110.30
1	D	196	MET	N-CA-C	5.09	117.57	111.71
1	F	132	PHE	N-CA-CB	5.09	118.03	110.29
1	f	119	PHE	CA-C-N	5.09	127.37	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	119	PHE	C-N-CA	5.09	127.37	120.44
1	g	34	GLY	O-C-N	-5.09	116.29	122.71
2	j	21	ASP	N-CA-C	-5.09	106.62	114.16
1	C	177	LYS	N-CA-CB	5.09	119.39	110.27
1	E	45	GLY	O-C-N	-5.09	118.92	123.96
2	1	93	LEU	O-C-N	-5.09	116.82	122.07
3	I	74	ASP	N-CA-C	-5.09	107.02	113.18
2	4	186	ILE	N-CA-C	-5.09	100.91	108.45
2	k	209	ALA	N-CA-C	-5.09	105.43	111.69
3	H	190	LEU	CA-C-O	-5.09	115.02	120.42
1	B	124	THR	N-CA-C	-5.09	104.71	112.04
1	B	195	ALA	CA-C-O	-5.09	115.03	120.42
2	k	86	THR	CA-C-N	5.09	127.65	120.42
2	k	86	THR	C-N-CA	5.09	127.65	120.42
3	H	116	VAL	CA-CB-CG2	5.09	119.05	110.40
3	H	193	LYS	CB-CA-C	-5.09	102.20	110.85
3	I	124	ASP	CA-C-N	5.09	125.12	119.32
3	I	124	ASP	C-N-CA	5.09	125.12	119.32
3	K	275	PHE	CA-CB-CG	5.09	118.89	113.80
3	J	9	LEU	CB-CA-C	-5.09	100.43	110.10
1	F	91	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	k	44	LYS	CA-C-O	5.09	124.54	118.69
1	c	27	ALA	CA-C-N	5.09	127.61	120.28
1	c	27	ALA	C-N-CA	5.09	127.61	120.28
1	d	169	ASN	OD1-CG-ND2	5.09	127.69	122.60
2	j	31	ALA	CA-C-O	5.09	126.70	120.60
3	L	29	ARG	CA-C-O	5.09	125.94	120.55
1	g	39	GLY	N-CA-C	-5.08	101.13	113.18
3	H	167	PHE	CA-CB-CG	-5.08	108.72	113.80
1	a	158	GLU	CA-C-N	5.08	131.36	122.82
1	a	158	GLU	C-N-CA	5.08	131.36	122.82
1	G	157	LEU	N-CA-C	-5.08	99.69	108.69
3	L	262	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	D	10	ARG	O-C-N	-5.08	115.39	122.20
2	4	68	ARG	N-CA-C	5.08	116.90	111.36
3	H	238	ILE	N-CA-C	-5.08	100.25	107.77
1	c	15	PHE	N-CA-CB	5.08	118.05	109.92
3	L	344	GLU	CA-C-N	5.08	129.23	121.51
3	L	344	GLU	C-N-CA	5.08	129.23	121.51
1	D	93	ARG	CA-C-N	5.08	127.06	120.56
1	D	93	ARG	C-N-CA	5.08	127.06	120.56
1	e	89	ILE	N-CA-C	-5.08	105.59	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	104	PHE	N-CA-CB	5.08	119.64	110.10
1	b	98	ILE	CA-C-N	5.08	127.50	120.29
1	b	98	ILE	C-N-CA	5.08	127.50	120.29
1	C	54	VAL	N-CA-CB	5.08	118.04	111.19
1	E	156	LEU	CD1-CG-CD2	-5.08	99.63	110.80
2	1	13	THR	CA-C-O	-5.08	115.80	121.23
1	a	117	CYS	CB-CA-C	-5.07	102.92	110.88
1	b	86	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	c	84	ASP	CA-CB-CG	-5.07	107.53	112.60
1	g	191	LEU	N-CA-C	5.07	116.89	111.36
2	1	76	LEU	CA-C-N	5.07	127.04	120.44
2	1	76	LEU	C-N-CA	5.07	127.04	120.44
2	l	149	GLY	CA-C-N	5.07	127.62	120.42
2	l	149	GLY	C-N-CA	5.07	127.62	120.42
3	H	231	LYS	CA-C-O	-5.07	115.17	120.55
3	K	269	LEU	N-CA-C	5.07	121.61	110.80
1	A	18	ASP	CA-CB-CG	-5.07	107.53	112.60
1	c	131	PRO	CA-C-N	5.07	129.44	120.87
1	c	131	PRO	C-N-CA	5.07	129.44	120.87
1	f	169	ASN	CA-C-N	5.07	127.08	120.28
1	f	169	ASN	C-N-CA	5.07	127.08	120.28
2	3	14	THR	N-CA-C	-5.07	100.77	109.24
1	B	159	TYR	N-CA-C	-5.07	101.59	109.14
1	d	103	TYR	CA-C-N	5.07	129.75	122.35
1	d	103	TYR	C-N-CA	5.07	129.75	122.35
3	J	276	ASP	N-CA-C	-5.07	103.15	110.40
1	E	151	ASP	CA-C-N	5.07	124.68	119.56
1	E	151	ASP	C-N-CA	5.07	124.68	119.56
2	1	78	GLU	CA-C-N	5.07	127.05	120.56
2	1	78	GLU	C-N-CA	5.07	127.05	120.56
2	6	33	MET	N-CA-C	-5.07	99.85	108.26
3	H	25	GLU	O-C-N	5.07	127.93	122.15
1	E	13	THR	N-CA-C	-5.07	106.69	112.92
2	i	102	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	H	16	LEU	O-C-N	-5.07	116.38	122.15
3	H	215	TYR	N-CA-C	-5.07	101.72	108.86
3	I	301	GLY	N-CA-C	-5.07	101.18	113.18
3	K	57	ARG	NE-CZ-NH1	-5.07	116.44	121.50
1	B	23	GLN	O-C-N	-5.06	116.38	122.15
1	d	148	TYR	N-CA-C	-5.06	101.67	109.52
1	e	151	ASP	CA-C-O	-5.06	115.25	120.87
1	f	51	ASP	CA-CB-CG	5.06	117.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	153	ASP	N-CA-CB	5.06	117.30	109.91
3	M	38	GLU	CA-C-N	5.06	127.07	120.28
3	M	38	GLU	C-N-CA	5.06	127.07	120.28
1	g	85	ALA	CB-CA-C	-5.06	102.39	110.79
2	2	204	VAL	CA-C-N	5.06	127.77	120.38
2	2	204	VAL	C-N-CA	5.06	127.77	120.38
2	j	48	ILE	O-C-N	-5.06	116.64	121.90
2	j	198	GLN	CB-CA-C	-5.06	102.98	110.62
2	4	21	ASP	CA-CB-CG	-5.06	107.54	112.60
3	J	341	ARG	O-C-N	-5.06	116.75	122.12
1	G	189	MET	CA-C-N	5.06	127.61	120.42
1	G	189	MET	C-N-CA	5.06	127.61	120.42
2	k	103	TYR	CA-C-N	5.06	127.44	122.28
2	k	103	TYR	C-N-CA	5.06	127.44	122.28
3	H	260	GLU	N-CA-CB	5.06	117.65	110.16
1	c	60	GLU	N-CA-C	-5.06	101.72	109.76
1	F	61	ALA	CA-C-N	5.06	128.41	120.82
1	F	61	ALA	C-N-CA	5.06	128.41	120.82
1	F	70	ILE	O-C-N	-5.06	116.25	122.57
2	3	197	TYR	N-CA-C	-5.06	101.00	109.24
2	6	81	ARG	CA-C-O	5.06	124.61	119.05
3	I	10	LEU	CA-C-N	5.06	127.32	120.44
3	I	10	LEU	C-N-CA	5.06	127.32	120.44
3	L	115	ILE	O-C-N	-5.06	116.50	122.77
1	C	121	GLN	OE1-CD-NE2	5.06	127.66	122.60
2	4	125	ILE	N-CA-CB	5.06	118.39	111.41
1	B	90	ASP	CA-C-N	5.05	127.05	120.28
1	B	90	ASP	C-N-CA	5.05	127.05	120.28
1	C	137	LEU	CD1-CG-CD2	-5.05	99.68	110.80
1	F	62	ASP	CB-CA-C	-5.05	102.35	110.74
1	G	66	LYS	N-CA-C	-5.05	105.91	113.89
3	L	136	PRO	CA-C-N	5.05	129.99	121.14
3	L	136	PRO	C-N-CA	5.05	129.99	121.14
1	g	144	VAL	CA-C-O	-5.05	115.94	119.38
2	4	122	ILE	N-CA-C	-5.05	100.79	108.17
3	J	152	GLU	CB-CG-CD	-5.05	104.01	112.60
2	i	84	LYS	N-CA-CB	5.05	118.77	109.73
2	i	98	LEU	CA-C-O	-5.05	115.06	120.42
2	7	159	ILE	N-CA-CB	5.05	116.23	110.72
3	H	226	VAL	CB-CA-C	5.05	118.96	112.14
3	M	173	GLU	CB-CA-C	5.05	116.69	109.26
3	M	193	LYS	N-CA-C	-5.05	105.85	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	236	ALA	CA-C-N	5.05	127.55	120.28
1	e	236	ALA	C-N-CA	5.05	127.55	120.28
1	g	72	GLU	N-CA-CB	5.05	117.53	110.56
2	h	210	LYS	N-CA-C	-5.05	105.43	112.30
3	I	366	GLU	N-CA-C	-5.05	104.46	111.28
3	L	164	PRO	N-CD-CG	5.05	110.77	103.20
1	A	130	ARG	CA-C-O	-5.05	115.20	120.70
2	h	88	ARG	CA-C-N	5.05	127.00	120.44
2	h	88	ARG	C-N-CA	5.05	127.00	120.44
2	7	30	ARG	N-CA-CB	5.05	117.41	109.69
1	f	77	ALA	CA-C-N	5.05	130.51	122.59
1	f	77	ALA	C-N-CA	5.05	130.51	122.59
3	I	317	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	G	214	VAL	N-CA-C	-5.04	100.38	107.75
1	d	81	LEU	N-CA-CB	5.04	116.96	109.19
2	h	196	PHE	CB-CG-CD2	-5.04	112.13	120.70
2	n	189	VAL	CA-CB-CG2	-5.04	101.83	110.40
3	I	100	LEU	N-CA-CB	5.04	117.39	109.97
1	a	115	LYS	N-CA-C	5.04	116.78	111.28
1	B	58	LEU	N-CA-C	-5.04	106.72	112.92
1	D	132	PHE	CA-CB-CG	-5.04	108.76	113.80
1	g	159	TYR	CG-CD1-CE1	-5.04	113.64	121.20
3	H	15	LYS	CA-C-N	5.04	127.45	120.29
3	H	15	LYS	C-N-CA	5.04	127.45	120.29
3	K	350	ASP	N-CA-CB	5.04	117.53	110.12
3	K	376	THR	O-C-N	5.04	128.47	122.27
1	c	101	LEU	N-CA-C	-5.04	105.49	111.69
2	l	188	VAL	N-CA-C	-5.04	101.22	108.53
2	m	150	VAL	CA-C-N	5.04	127.03	120.28
2	m	150	VAL	C-N-CA	5.04	127.03	120.28
1	B	150	THR	O-C-N	-5.04	117.31	123.30
1	c	121	GLN	CB-CG-CD	5.04	121.17	112.60
1	E	8	TYR	CA-C-O	5.04	125.42	119.48
2	m	153	ASP	O-C-N	5.04	127.53	122.09
3	K	388	PRO	N-CA-CB	5.04	105.74	102.92
1	d	205	VAL	N-CA-C	-5.04	98.00	108.88
1	F	118	ASP	N-CA-C	-5.04	106.64	112.89
3	I	382	VAL	CA-C-O	-5.04	114.97	120.96
1	b	100	ARG	N-CA-C	5.04	117.50	111.71
1	e	91	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	i	42	ALA	N-CA-C	-5.04	101.42	109.07
2	k	132	ILE	N-CA-CB	5.04	118.36	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	63	ALA	CA-C-O	-5.04	115.51	120.70
3	H	184	PRO	CA-C-O	-5.04	115.85	122.19
3	K	279	GLY	O-C-N	5.04	129.25	122.70
3	J	259	ARG	CA-C-N	5.04	127.03	120.28
3	J	259	ARG	C-N-CA	5.04	127.03	120.28
3	J	397	PHE	N-CA-C	-5.04	101.03	109.24
1	a	46	VAL	CA-CB-CG2	5.03	118.96	110.40
1	c	206	PRO	N-CA-C	-5.03	106.19	114.75
1	D	60	GLU	CB-CG-CD	-5.03	104.04	112.60
1	f	93	ARG	CB-CA-C	-5.03	102.29	110.85
2	h	166	GLU	CB-CG-CD	5.03	121.16	112.60
2	7	153	ASP	N-CA-C	5.03	116.77	111.28
2	n	44	LYS	CA-CB-CG	5.03	124.17	114.10
3	I	376	THR	N-CA-CB	5.03	117.52	110.12
1	e	119	PHE	CA-CB-CG	5.03	118.83	113.80
2	3	194	ASP	N-CA-C	-5.03	106.56	113.30
2	6	128	ILE	CA-C-O	5.03	127.07	120.78
1	c	94	ILE	O-C-N	5.03	127.01	121.83
2	6	68	ARG	CA-C-N	5.03	126.99	120.70
2	6	68	ARG	C-N-CA	5.03	126.99	120.70
1	C	191	LEU	CB-CA-C	-5.03	102.44	110.79
1	f	61	ALA	N-CA-C	-5.03	106.83	113.17
1	g	57	LYS	N-CA-C	5.03	116.76	111.28
3	M	147	ASP	CA-CB-CG	-5.03	107.57	112.60
3	M	225	GLU	CB-CG-CD	-5.03	104.05	112.60
1	g	158	GLU	N-CA-C	-5.03	101.04	109.24
2	j	78	GLU	CA-C-N	5.03	127.35	120.46
2	j	78	GLU	C-N-CA	5.03	127.35	120.46
2	k	139	ALA	O-C-N	-5.03	117.26	123.44
2	5	104	PHE	N-CA-CB	5.03	116.39	110.71
3	I	193	LYS	CA-C-N	5.03	126.98	120.44
3	I	193	LYS	C-N-CA	5.03	126.98	120.44
3	I	382	VAL	O-C-N	5.03	128.44	121.90
1	A	235	ARG	N-CA-C	-5.03	106.41	112.54
1	b	91	ARG	CB-CG-CD	5.03	122.86	111.30
1	E	20	ARG	O-C-N	-5.03	117.31	122.94
2	4	156	THR	O-C-N	-5.03	116.93	122.06
2	7	44	LYS	CA-C-N	5.03	129.78	123.10
2	7	44	LYS	C-N-CA	5.03	129.78	123.10
2	7	122	ILE	N-CA-C	-5.03	100.97	108.46
3	I	250	ARG	CB-CG-CD	5.03	122.86	111.30
1	C	196	MET	CA-C-O	5.02	125.87	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	110	LYS	N-CA-CB	5.02	117.50	110.12
2	n	134	GLU	N-CA-CB	5.02	119.57	110.83
3	K	277	PRO	N-CA-CB	5.02	107.54	103.32
3	J	303	PHE	N-CA-C	-5.02	101.11	108.79
2	m	44	LYS	CA-C-O	5.02	126.63	120.15
3	H	124	ASP	CA-C-O	-5.02	115.72	120.34
3	J	76	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	f	118	ASP	CB-CA-C	-5.02	102.32	110.85
2	h	19	CYS	CA-C-N	5.02	131.13	121.54
2	h	19	CYS	C-N-CA	5.02	131.13	121.54
2	i	186	ILE	N-CA-C	-5.02	101.72	108.35
3	L	318	ILE	CA-C-O	-5.02	115.85	121.17
3	J	226	VAL	CA-C-N	5.02	127.01	120.28
3	J	226	VAL	C-N-CA	5.02	127.01	120.28
1	b	66	LYS	N-CA-CB	5.02	118.97	110.49
1	C	134	VAL	CA-C-O	5.02	126.99	121.67
2	h	52	MET	N-CA-CB	5.02	120.08	111.00
2	j	161	VAL	N-CA-CB	5.02	118.11	110.58
3	L	317	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	e	130	ARG	NH1-CZ-NH2	-5.02	112.78	119.30
1	g	69	LYS	N-CA-C	-5.02	100.98	108.96
1	d	204	LEU	CA-C-N	5.01	131.41	122.13
1	d	204	LEU	C-N-CA	5.01	131.41	122.13
2	6	160	GLY	N-CA-C	-5.01	103.92	112.64
2	n	84	LYS	CA-C-N	5.01	125.80	120.13
2	n	84	LYS	C-N-CA	5.01	125.80	120.13
3	H	203	PHE	CA-CB-CG	-5.01	108.79	113.80
1	b	42	CYS	N-CA-CB	5.01	119.68	111.31
1	d	93	ARG	N-CA-C	5.01	116.82	111.36
1	f	71	ASP	CA-C-O	5.01	126.67	121.36
1	G	59	LEU	N-CA-CB	5.01	117.11	110.29
1	B	9	ASP	O-C-N	-5.01	116.10	122.26
1	D	95	GLU	CB-CA-C	-5.01	101.05	110.67
1	g	84	ASP	CA-C-N	5.01	126.99	120.28
1	g	84	ASP	C-N-CA	5.01	126.99	120.28
2	j	90	ILE	N-CA-C	-5.01	104.73	111.44
2	k	36	PHE	CA-CB-CG	5.01	118.81	113.80
2	m	62	ASP	CA-C-N	5.01	126.95	120.44
2	m	62	ASP	C-N-CA	5.01	126.95	120.44
2	n	121	SER	N-CA-C	-5.01	100.13	110.80
3	J	238	ILE	O-C-N	5.01	128.35	122.99
1	D	227	GLU	CA-CB-CG	5.01	124.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	91	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	3	102	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	k	116	ASP	CA-C-O	-5.01	116.05	121.36
3	J	154	ARG	CA-C-N	5.01	126.99	120.28
3	J	154	ARG	C-N-CA	5.01	126.99	120.28
1	a	190	VAL	CA-C-N	5.01	126.99	120.28
1	a	190	VAL	C-N-CA	5.01	126.99	120.28
1	F	124	THR	CA-C-O	-5.01	113.72	119.78
1	f	179	TYR	N-CA-C	-5.01	100.13	110.80
1	G	215	LYS	O-C-N	-5.01	117.33	122.94
2	h	172	ILE	N-CA-C	5.01	117.35	111.09
2	k	191	ILE	CA-C-N	5.01	129.80	121.99
2	k	191	ILE	C-N-CA	5.01	129.80	121.99
3	M	144	GLY	N-CA-C	-5.01	104.31	111.42
1	B	63	THR	CA-C-N	5.00	130.98	121.97
1	B	63	THR	C-N-CA	5.00	130.98	121.97
2	3	123	TYR	CA-C-O	5.00	126.36	120.80
2	k	166	GLU	CA-C-N	5.00	126.95	120.44
2	k	166	GLU	C-N-CA	5.00	126.95	120.44
2	5	156	THR	N-CA-C	-5.00	100.74	108.55
3	H	281	VAL	N-CA-CB	5.00	118.15	111.64
1	a	18	ASP	CB-CA-C	-5.00	102.34	110.85
1	e	148	TYR	N-CA-CB	5.00	120.25	111.55
1	e	209	ILE	CA-CB-CG2	-5.00	101.99	110.50
1	F	105	GLU	N-CA-C	-5.00	97.24	107.95
1	G	98	ILE	CB-CA-C	-5.00	104.16	112.26
1	g	57	LYS	CB-CA-C	-5.00	102.48	110.79
2	1	148	TYR	CB-CA-C	-5.00	103.03	110.88
1	D	142	ASP	N-CA-C	-5.00	105.30	111.40
1	e	108	THR	CA-CB-CG2	-5.00	102.00	110.50
2	1	55	THR	N-CA-C	-5.00	100.31	108.76
2	1	109	GLN	N-CA-C	-5.00	100.37	108.52
2	2	77	TYR	CA-C-O	5.00	125.85	120.55
2	2	77	TYR	N-CA-C	5.00	116.73	111.28
2	4	180	SER	N-CA-C	-5.00	104.66	111.56
2	6	168	ALA	CB-CA-C	-5.00	102.35	110.85
2	m	178	ARG	N-CA-C	-5.00	107.23	113.38
2	7	174	SER	CA-C-N	5.00	126.98	120.28
2	7	174	SER	C-N-CA	5.00	126.98	120.28
3	H	66	GLY	N-CA-C	-5.00	103.80	111.10

There are no chirality outliers.

All (286) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	123	TYR	Sidechain
2	1	178	ARG	Sidechain
2	1	51	ARG	Sidechain
2	1	83	ARG	Sidechain
2	2	102	ARG	Sidechain
2	2	103	TYR	Sidechain
2	2	139	ALA	Mainchain,Peptide
2	2	154	ARG	Sidechain
2	2	170	ARG	Sidechain
2	3	106	TYR	Sidechain
2	3	170	ARG	Sidechain
2	3	199	TYR	Sidechain
2	3	46	TYR	Sidechain
2	4	102	ARG	Sidechain
2	4	139	ALA	Peptide
2	4	148	TYR	Sidechain
2	4	211	PHE	Sidechain
2	4	68	ARG	Sidechain
2	4	83	ARG	Sidechain
2	5	101	TYR	Sidechain
2	5	106	TYR	Sidechain
2	5	132	ILE	Peptide
2	5	155	PHE	Sidechain
2	5	170	ARG	Sidechain
2	5	197	TYR	Sidechain
2	5	211	PHE	Sidechain
2	6	101	TYR	Sidechain
2	6	106	TYR	Sidechain
2	6	148	TYR	Sidechain
2	6	154	ARG	Sidechain
2	6	170	ARG	Sidechain
2	6	197	TYR	Sidechain
2	6	46	TYR	Sidechain
2	6	81	ARG	Sidechain
2	7	106	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	178	ARG	Sidechain
2	7	196	PHE	Sidechain
2	7	68	ARG	Sidechain
1	A	174	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	A	26	TYR	Sidechain
1	A	65	GLU	Peptide
1	A	66	LYS	Peptide
1	A	91	ARG	Sidechain
1	B	14	VAL	Mainchain
1	B	159	TYR	Sidechain
1	B	175	PHE	Sidechain
1	B	20	ARG	Sidechain
1	B	213	TYR	Sidechain
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain
1	B	235	ARG	Sidechain
1	B	26	TYR	Sidechain
1	B	66	LYS	Peptide
1	B	93	ARG	Sidechain
1	C	100	ARG	Sidechain
1	C	123	TYR	Sidechain
1	C	126	TYR	Sidechain
1	C	168	ARG	Sidechain
1	C	220	THR	Peptide
1	C	26	TYR	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	D	10	ARG	Sidechain
1	D	123	TYR	Sidechain
1	D	15	PHE	Sidechain
1	D	175	PHE	Sidechain
1	D	179	TYR	Sidechain
1	D	180	ARG	Sidechain
1	D	185	PHE	Sidechain
1	D	20	ARG	Sidechain
1	D	220	THR	Peptide
1	D	8	TYR	Sidechain
1	D	91	ARG	Sidechain
1	E	10	ARG	Sidechain
1	E	100	ARG	Sidechain
1	E	126	TYR	Sidechain
1	E	159	TYR	Sidechain
1	E	213	TYR	Sidechain
1	E	22	PHE	Sidechain
1	E	220	THR	Peptide

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Mol	Chain	Res	Type	Group
1	E	235	ARG	Sidechain
1	E	86	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	10	ARG	Sidechain
1	F	103	TYR	Sidechain
1	F	123	TYR	Sidechain
1	F	15	PHE	Sidechain
1	F	175	PHE	Sidechain
1	F	179	TYR	Sidechain
1	F	180	ARG	Sidechain
1	F	220	THR	Peptide
1	F	235	ARG	Sidechain
1	F	28	ARG	Sidechain
1	F	53	ARG	Sidechain
1	F	68	TYR	Sidechain
1	F	86	ARG	Sidechain
1	G	103	TYR	Sidechain
1	G	126	TYR	Sidechain
1	G	15	PHE	Sidechain
1	G	179	TYR	Sidechain
1	G	220	THR	Peptide
1	G	241	ARG	Sidechain
1	G	28	ARG	Sidechain
1	G	33	ARG	Sidechain
1	G	5	GLN	Peptide
1	G	86	ARG	Sidechain
3	H	130	PHE	Sidechain
3	H	140	TYR	Sidechain
3	H	205	ARG	Sidechain
3	H	215	TYR	Peptide
3	H	218	GLU	Peptide
3	H	221	ARG	Sidechain
3	H	224	ARG	Sidechain
3	H	236	SER	Peptide
3	H	240	ILE	Peptide
3	H	254	ASP	Peptide
3	H	263	ARG	Sidechain
3	H	276	ASP	Peptide
3	H	278	ARG	Sidechain
3	H	305	ARG	Sidechain
3	H	311	LEU	Peptide
3	H	336	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	H	36	PHE	Sidechain
3	H	387	THR	Peptide
3	H	50	ARG	Sidechain
3	H	76	ARG	Sidechain
3	I	154	ARG	Sidechain
3	I	181	TYR	Mainchain,Peptide
3	I	215	TYR	Sidechain
3	I	220	ALA	Peptide
3	I	224	ARG	Sidechain
3	I	254	ASP	Peptide
3	I	269	LEU	Peptide
3	I	289	ARG	Sidechain
3	I	303	PHE	Peptide
3	I	44	TYR	Sidechain
3	I	46	ARG	Sidechain
3	I	49	ARG	Sidechain
3	J	186	THR	Peptide
3	J	190	LEU	Peptide
3	J	207	VAL	Peptide
3	J	215	TYR	Sidechain
3	J	299	ARG	Sidechain
3	J	317	ARG	Sidechain
3	J	36	PHE	Sidechain
3	J	367	ARG	Sidechain
3	J	46	ARG	Sidechain
3	K	128	TYR	Sidechain
3	K	181	TYR	Sidechain
3	K	201	ALA	Peptide
3	K	203	PHE	Sidechain
3	K	213	GLN	Peptide
3	K	215	TYR	Sidechain
3	K	259	ARG	Sidechain
3	K	269	LEU	Mainchain,Peptide
3	K	277	PRO	Peptide
3	K	299	ARG	Sidechain
3	K	317	ARG	Sidechain
3	K	364	ARG	Sidechain
3	K	43	ARG	Sidechain
3	K	44	TYR	Sidechain
3	K	50	ARG	Sidechain
3	K	57	ARG	Sidechain
3	L	140	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	L	24	ARG	Sidechain
3	L	249	ARG	Sidechain
3	L	305	ARG	Sidechain
3	L	341	ARG	Sidechain
3	L	385	LYS	Peptide
3	L	52	ARG	Sidechain
3	L	57	ARG	Sidechain
3	L	76	ARG	Sidechain
3	L	94	TYR	Sidechain
3	M	21	TYR	Sidechain
3	M	215	TYR	Sidechain,Peptide
3	M	254	ASP	Peptide
3	M	27	TYR	Sidechain
3	M	28	ARG	Sidechain
3	M	314	PHE	Sidechain
3	M	341	ARG	Sidechain
3	M	371	THR	Peptide
3	M	385	LYS	Peptide
3	M	44	TYR	Sidechain
3	M	52	ARG	Sidechain
3	M	57	ARG	Sidechain
3	M	94	TYR	Sidechain
1	a	126	TYR	Sidechain
1	a	148	TYR	Sidechain
1	a	220	THR	Peptide
1	a	241	ARG	Sidechain
1	a	46	VAL	Mainchain
1	a	91	ARG	Sidechain
1	b	126	TYR	Sidechain
1	b	179	TYR	Sidechain
1	b	220	THR	Peptide
1	b	28	ARG	Sidechain
1	c	123	TYR	Sidechain
1	c	126	TYR	Sidechain
1	c	159	TYR	Sidechain
1	c	175	PHE	Sidechain
1	c	219	ARG	Sidechain
1	c	53	ARG	Sidechain
1	c	68	TYR	Sidechain
1	d	10	ARG	Sidechain
1	d	123	TYR	Sidechain
1	d	159	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	d	179	TYR	Sidechain
1	d	220	THR	Peptide
1	d	239	ARG	Sidechain
1	d	241	ARG	Sidechain
1	d	26	TYR	Sidechain
1	d	91	ARG	Sidechain
1	e	100	ARG	Sidechain
1	e	103	TYR	Sidechain
1	e	123	TYR	Sidechain
1	e	168	ARG	Sidechain
1	e	180	ARG	Sidechain
1	e	213	TYR	Sidechain
1	e	220	THR	Peptide
1	e	239	ARG	Sidechain
1	e	68	TYR	Sidechain
1	f	100	ARG	Sidechain
1	f	123	TYR	Sidechain
1	f	126	TYR	Sidechain
1	f	220	THR	Peptide
1	f	68	TYR	Sidechain
1	f	86	ARG	Sidechain
1	g	103	TYR	Sidechain
1	g	159	TYR	Sidechain
1	g	213	TYR	Sidechain
1	g	219	ARG	Sidechain
1	g	220	THR	Peptide
1	g	28	ARG	Sidechain
1	g	53	ARG	Sidechain
1	g	68	TYR	Sidechain
2	h	101	TYR	Sidechain
2	h	102	ARG	Sidechain
2	h	103	TYR	Sidechain
2	h	123	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	154	ARG	Sidechain
2	h	155	PHE	Sidechain
2	h	173	TYR	Sidechain
2	h	196	PHE	Sidechain
2	h	199	TYR	Sidechain
2	h	30	ARG	Sidechain
2	h	51	ARG	Sidechain
2	i	104	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	i	106	TYR	Sidechain
2	i	139	ALA	Peptide
2	i	178	ARG	Sidechain
2	i	197	TYR	Sidechain
2	i	83	ARG	Sidechain
2	j	101	TYR	Sidechain
2	j	139	ALA	Peptide
2	j	77	TYR	Sidechain
2	k	103	TYR	Sidechain
2	k	123	TYR	Sidechain
2	k	196	PHE	Sidechain
2	k	199	TYR	Sidechain
2	k	36	PHE	Sidechain
2	k	46	TYR	Sidechain
2	l	103	TYR	Sidechain
2	l	106	TYR	Sidechain
2	l	148	TYR	Sidechain
2	l	51	ARG	Sidechain
2	l	77	TYR	Sidechain
2	l	81	ARG	Sidechain
2	l	88	ARG	Sidechain
2	m	212	ARG	Sidechain
2	m	65	PHE	Sidechain
2	n	101	TYR	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	170	ARG	Sidechain
2	n	173	TYR	Sidechain
2	n	178	ARG	Sidechain
2	n	77	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1941	12	0
1	B	1907	0	1941	7	0
1	C	1907	0	1941	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1907	0	1941	5	0
1	E	1907	0	1941	5	0
1	F	1907	0	1941	3	0
1	G	1907	0	1941	7	0
1	a	1866	0	1908	5	0
1	b	1866	0	1908	7	0
1	c	1866	0	1908	9	0
1	d	1866	0	1908	9	0
1	e	1866	0	1908	3	0
1	f	1866	0	1908	4	0
1	g	1866	0	1908	5	0
2	1	1553	0	1580	5	0
2	2	1553	0	1580	4	0
2	3	1553	0	1580	1	0
2	4	1553	0	1580	5	0
2	5	1553	0	1580	29	0
2	6	1553	0	1580	5	0
2	7	1553	0	1580	6	0
2	h	1553	0	1580	3	0
2	i	1553	0	1580	2	0
2	j	1553	0	1580	6	0
2	k	1553	0	1580	6	0
2	l	1553	0	1580	30	0
2	m	1553	0	1580	9	0
2	n	1553	0	1580	4	0
3	H	3100	0	3220	41	0
3	I	3100	0	3220	24	0
3	J	3100	0	3220	45	0
3	K	3100	0	3220	22	0
3	L	3100	0	3220	37	0
3	M	3100	0	3220	23	0
4	H	31	0	11	0	0
4	I	31	0	12	0	0
4	J	31	0	12	0	0
4	K	31	0	12	2	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	L	27	0	12	0	0
All	All	66909	0	68442	359	0

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

All (359) 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)
2:5:211:PHE:CE2	2:5:211:PHE:CD2	1.99	1.51
2:1:211:PHE:CE1	2:1:211:PHE:CD1	1.98	1.49
2:1:211:PHE:CE2	2:1:211:PHE:CD2	2.02	1.47
2:5:211:PHE:CD1	2:5:211:PHE:CG	2.05	1.45
2:5:211:PHE:CE2	2:5:211:PHE:CZ	2.05	1.43
2:1:211:PHE:CE2	2:1:211:PHE:CZ	2.04	1.43
2:1:211:PHE:CD1	2:1:211:PHE:CG	2.05	1.42
2:1:211:PHE:CE1	2:1:211:PHE:CZ	2.07	1.42
2:5:211:PHE:CD2	2:5:211:PHE:CG	2.09	1.40
2:5:211:PHE:CD1	2:5:211:PHE:CE1	2.11	1.39
2:5:211:PHE:CZ	2:5:211:PHE:CE1	2.10	1.38
2:1:211:PHE:CD2	2:1:211:PHE:CG	2.12	1.37
3:H:216:ILE:CG2	3:H:263:ARG:HH22	1.38	1.36
3:L:320:ILE:HG22	3:L:351:ILE:HG21	1.24	1.19
3:K:212:VAL:CG1	3:L:216:ILE:HG22	1.75	1.16
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.09	1.15
2:1:170:ARG:CZ	2:1:170:ARG:NH1	2.11	1.13
2:1:170:ARG:CZ	2:1:211:PHE:CE2	2.33	1.11
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.36	1.09
2:1:170:ARG:CZ	2:1:211:PHE:CD1	2.36	1.08
3:H:216:ILE:HG22	3:H:263:ARG:HH22	1.13	1.08
2:1:170:ARG:NH1	2:1:211:PHE:CE1	2.22	1.08
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.37	1.07
2:1:170:ARG:CZ	2:1:211:PHE:CG	2.38	1.07
3:L:320:ILE:CG2	3:L:351:ILE:HG21	1.83	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.22	1.07
2:1:170:ARG:CZ	2:1:211:PHE:CZ	2.38	1.07
2:1:170:ARG:NH1	2:1:211:PHE:CZ	2.22	1.07
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.37	1.06
2:5:170:ARG:NH1	2:5:211:PHE:CZ	2.23	1.06
2:1:170:ARG:NH1	2:1:211:PHE:CD1	2.23	1.06
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.38	1.06
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.22	1.06
2:1:170:ARG:NH1	2:1:211:PHE:CE2	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.24	1.04
2:1:170:ARG:CZ	2:1:211:PHE:CD2	2.40	1.04
2:1:170:ARG:NH1	2:1:211:PHE:CG	2.25	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:216:ILE:CG2	3:H:263:ARG:NH2	2.18	1.04
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.25	1.04
2:l:170:ARG:NH1	2:l:211:PHE:CD2	2.25	1.03
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.26	1.02
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.43	1.02
2:l:170:ARG:CZ	2:l:211:PHE:CE1	2.42	1.01
3:L:320:ILE:HG22	3:L:351:ILE:CG2	1.91	1.00
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.45	0.98
3:K:212:VAL:HG11	3:L:216:ILE:HG22	1.42	0.97
3:J:240:ILE:CG2	3:J:243:LEU:HB3	1.94	0.97
3:J:240:ILE:HG21	3:J:243:LEU:HB3	1.51	0.92
3:H:216:ILE:HG23	3:H:263:ARG:NH2	1.84	0.89
3:K:212:VAL:HG11	3:L:216:ILE:CG2	2.05	0.86
3:H:216:ILE:HG23	3:H:263:ARG:HH22	1.33	0.85
3:J:153:ILE:HG21	3:J:195:VAL:HG21	1.56	0.84
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.44	0.84
3:J:240:ILE:CG2	3:J:243:LEU:CB	2.54	0.83
3:L:320:ILE:CG2	3:L:351:ILE:CG2	2.55	0.83
2:l:170:ARG:NE	2:l:211:PHE:CZ	2.48	0.80
3:K:212:VAL:CG1	3:L:216:ILE:CG2	2.59	0.80
2:l:170:ARG:NE	2:l:211:PHE:CE1	2.48	0.80
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.48	0.80
3:H:216:ILE:HG22	3:H:263:ARG:NH2	1.91	0.79
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.50	0.79
2:l:170:ARG:NH2	2:l:211:PHE:CD2	2.51	0.79
3:I:398:VAL:HG22	3:I:398:VAL:OXT	1.83	0.78
3:M:342:ILE:CG2	3:M:379:ILE:HG21	2.12	0.77
2:l:170:ARG:NH2	2:l:211:PHE:CG	2.52	0.77
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.54	0.76
3:M:342:ILE:HG21	3:M:379:ILE:HG21	1.69	0.74
3:J:240:ILE:HG22	3:J:243:LEU:HB3	1.69	0.73
3:M:212:VAL:HG13	3:M:246:ILE:HG22	1.69	0.73
3:M:320:ILE:HG22	3:M:351:ILE:HG21	1.70	0.73
3:H:168:ALA:HA	3:H:278:ARG:HE	1.55	0.72
3:J:240:ILE:HG22	3:J:243:LEU:CB	2.19	0.71
3:K:212:VAL:HG12	3:L:216:ILE:HG22	1.73	0.70
3:I:398:VAL:OXT	3:I:398:VAL:CG2	2.38	0.70
1:B:125:GLN:HE22	1:C:87:VAL:HG11	1.58	0.69
3:J:342:ILE:CG2	3:J:379:ILE:HG21	2.23	0.68
3:J:238:ILE:HG22	3:J:240:ILE:HD11	1.77	0.67
3:H:201:ALA:HB3	3:H:237:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:172:ILE:HG21	3:M:359:GLY:HA3	1.78	0.65
1:D:82:VAL:HG22	3:I:398:VAL:HB	1.79	0.65
1:A:65:GLU:H	1:A:66:LYS:HA	1.61	0.64
3:I:230:ALA:CB	3:I:238:ILE:HD11	2.27	0.64
3:I:319:GLN:O	3:I:323:ILE:HG12	1.97	0.64
3:J:240:ILE:HG21	3:J:243:LEU:CB	2.24	0.64
3:K:251:THR:CG2	3:J:292:ILE:HD12	2.29	0.63
3:H:82:SER:HB2	3:I:86:LYS:H	1.63	0.63
2:L:24:VAL:HG21	2:L:164:ALA:HB3	1.81	0.62
3:I:320:ILE:HG22	3:I:351:ILE:HG21	1.81	0.62
1:d:21:LEU:HD22	1:d:21:LEU:H	1.66	0.61
3:J:398:VAL:HG22	3:J:398:VAL:OXT	1.99	0.61
3:M:342:ILE:HG22	3:M:379:ILE:HG21	1.81	0.61
3:L:157:VAL:HG21	3:L:284:ILE:HD11	1.83	0.60
3:M:211:PHE:CB	3:M:246:ILE:HG21	2.31	0.60
3:L:342:ILE:HG22	3:L:383:LEU:CD1	2.32	0.60
3:L:181:TYR:CG	3:L:290:ILE:HD13	2.36	0.60
2:k:136:ASP:O	2:k:137:ILE:HD13	2.01	0.60
3:H:398:VAL:HG22	3:H:398:VAL:OXT	2.02	0.59
3:J:109:ASN:HD21	3:J:111:GLN:HE21	1.49	0.59
3:J:204:ILE:HB	3:J:238:ILE:HD13	1.84	0.58
3:J:153:ILE:CG2	3:J:195:VAL:HG21	2.31	0.58
2:7:14:THR:HG22	2:7:27:THR:HG22	1.85	0.58
3:H:236:SER:C	3:H:237:ILE:HG12	2.29	0.58
3:M:247:ALA:HA	3:M:265:MET:HE2	1.86	0.57
3:J:240:ILE:CG2	3:J:243:LEU:HB2	2.32	0.57
3:J:342:ILE:HG21	3:J:379:ILE:HG21	1.84	0.57
3:H:206:VAL:O	3:H:240:ILE:HD12	2.04	0.57
3:L:398:VAL:HG22	3:L:398:VAL:OXT	2.05	0.57
3:J:238:ILE:HG22	3:J:240:ILE:CD1	2.35	0.56
3:I:230:ALA:HB2	3:I:238:ILE:HD11	1.86	0.56
3:L:281:VAL:CG1	3:L:283:VAL:HG13	2.35	0.56
3:K:206:VAL:HG22	3:K:207:VAL:H	1.70	0.56
3:L:283:VAL:HA	3:L:284:ILE:HB	1.88	0.56
1:e:155:ALA:HB1	1:f:82:VAL:HB	1.87	0.55
3:L:321:PHE:CE2	3:L:351:ILE:HD12	2.41	0.55
3:H:354:ILE:HD13	3:H:379:ILE:HG12	1.88	0.55
3:I:204:ILE:HD12	3:I:238:ILE:HG12	1.88	0.55
3:J:342:ILE:HG22	3:J:379:ILE:HG21	1.88	0.55
1:F:100:ARG:HB3	2:6:72:ILE:HD11	1.89	0.55
2:j:77:TYR:HA	2:j:80:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:240:ILE:CD1	3:J:283:VAL:HG13	2.38	0.54
3:I:356:THR:HA	3:J:172:ILE:HD12	1.88	0.54
2:l:27:THR:HG21	2:l:45:ILE:HB	1.90	0.54
2:m:86:THR:HG23	2:m:89:ALA:H	1.73	0.53
3:J:208:GLY:O	3:J:246:ILE:CD1	2.56	0.53
3:I:178:VAL:HB	3:I:284:ILE:HD12	1.89	0.53
1:e:204:LEU:HB2	1:e:233:VAL:HG13	1.90	0.53
3:K:251:THR:HG23	3:J:292:ILE:HD12	1.90	0.53
3:M:211:PHE:HB3	3:M:246:ILE:HG21	1.90	0.53
3:H:398:VAL:OXT	3:H:398:VAL:CG2	2.57	0.53
3:K:342:ILE:HG21	3:K:379:ILE:CG2	2.39	0.53
3:M:107:ALA:HB2	3:M:119:LEU:HD21	1.90	0.53
3:M:211:PHE:HB3	3:M:246:ILE:CG2	2.39	0.53
3:H:236:SER:HA	3:H:237:ILE:HB	1.90	0.52
3:I:207:VAL:HG12	3:I:209:SER:H	1.72	0.52
3:L:320:ILE:HG21	3:L:351:ILE:HB	1.90	0.52
3:J:240:ILE:HG21	3:J:243:LEU:HD23	1.90	0.52
1:E:211:VAL:HB	1:E:229:LEU:HD21	1.91	0.52
3:J:398:VAL:OXT	3:J:398:VAL:CG2	2.57	0.52
1:b:28:ARG:HH22	1:b:164:ILE:HG22	1.74	0.52
2:k:86:THR:HG23	2:k:89:ALA:H	1.75	0.52
2:m:169:VAL:HG22	2:m:204:VAL:HG13	1.92	0.52
2:7:156:THR:HG22	2:7:158:GLU:H	1.74	0.52
3:M:211:PHE:CD2	3:M:246:ILE:HD13	2.45	0.52
3:J:296:ALA:HA	3:J:299:ARG:HH11	1.75	0.51
2:n:94:THR:HG21	2:n:110:LEU:CD2	2.41	0.51
1:a:203:GLU:HA	1:a:240:ILE:HG21	1.93	0.51
3:J:152:GLU:OE2	3:J:307:ILE:HD12	2.11	0.51
1:A:36:THR:HG23	1:A:196:MET:HE2	1.92	0.51
3:H:236:SER:CA	3:H:237:ILE:HG12	2.41	0.51
3:L:95:ILE:HD12	3:L:118:VAL:HG23	1.93	0.51
1:g:73:HIS:CE1	1:g:106:PRO:HB3	2.46	0.50
3:J:389:ILE:HD12	3:J:391:ASP:HB2	1.92	0.50
3:J:351:ILE:HA	3:J:354:ILE:HD12	1.94	0.50
3:J:152:GLU:CD	3:J:307:ILE:HD12	2.37	0.50
2:k:139:ALA:HB1	2:k:144:SER:HA	1.94	0.50
1:D:50:ALA:HB1	1:D:66:LYS:HD2	1.94	0.50
1:G:147:LEU:HD21	1:G:162:THR:HG22	1.93	0.50
2:5:101:TYR:CD1	2:5:106:TYR:CE1	3.01	0.49
2:h:14:THR:HG22	2:h:27:THR:HG22	1.94	0.49
2:4:107:LEU:HD12	2:4:127:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:312:PRO:HB2	3:J:317:ARG:HG2	1.94	0.49
2:h:51:ARG:HB3	2:h:52:MET:HE3	1.94	0.49
2:j:23:VAL:HG12	2:j:25:MET:HG3	1.93	0.49
3:J:240:ILE:HG21	3:J:243:LEU:CD2	2.43	0.49
1:c:20:ARG:HE	1:c:25:GLU:HG2	1.77	0.49
1:E:36:THR:HG23	1:E:196:MET:HE2	1.95	0.49
3:H:213:GLN:HE21	3:I:221:ARG:HH12	1.61	0.49
3:K:216:ILE:HD12	3:J:212:VAL:HG21	1.94	0.49
3:M:109:ASN:HB2	3:M:116:VAL:HG11	1.95	0.49
3:K:398:VAL:OXT	3:K:398:VAL:HG22	2.13	0.48
1:c:21:LEU:HD12	1:c:21:LEU:H	1.77	0.48
1:c:52:LYS:HE2	1:c:210:GLU:HB2	1.94	0.48
1:F:70:ILE:HG21	1:F:112:LEU:HD21	1.95	0.48
2:k:33:MET:HE3	2:k:36:PHE:CE2	2.49	0.48
2:6:17:LEU:HD11	2:6:164:ALA:HB1	1.95	0.48
3:L:320:ILE:HG21	3:L:351:ILE:CG2	2.41	0.48
3:H:146:LEU:H	3:H:147:ASP:HA	1.79	0.48
3:H:208:GLY:CA	3:H:240:ILE:HD11	2.42	0.48
3:H:201:ALA:CB	3:H:237:ILE:HG13	2.43	0.48
3:I:263:ARG:HG2	3:I:263:ARG:HH11	1.79	0.48
2:7:33:MET:H	2:7:36:PHE:HB3	1.78	0.48
2:n:16:GLY:HA2	2:n:25:MET:HG2	1.96	0.48
3:I:323:ILE:HD13	3:I:326:ARG:NH2	2.29	0.48
3:M:181:TYR:CE2	3:M:306:ILE:HD12	2.49	0.47
3:H:238:ILE:O	3:H:238:ILE:HG23	2.14	0.47
1:C:59:LEU:HD12	1:C:59:LEU:H	1.80	0.47
1:C:68:TYR:HB3	1:C:93:ARG:HH21	1.79	0.47
3:H:318:ILE:HD13	3:H:337:LYS:HG2	1.96	0.47
1:A:69:LYS:O	2:1:79:ILE:HG23	2.14	0.47
2:1:204:VAL:HG12	2:1:204:VAL:O	2.14	0.47
2:l:68:ARG:CZ	2:m:92:THR:HG23	2.45	0.47
3:L:281:VAL:HG12	3:L:283:VAL:HG13	1.97	0.47
3:M:320:ILE:HG22	3:M:351:ILE:CG2	2.41	0.47
3:L:317:ARG:HH21	3:L:345:GLY:H	1.63	0.46
3:L:320:ILE:HG21	3:L:351:ILE:CB	2.44	0.46
1:c:93:ARG:HG2	2:j:79:ILE:HG21	1.97	0.46
2:5:56:THR:HG21	2:5:63:ALA:HB1	1.97	0.46
3:H:243:LEU:HD22	3:H:297:ILE:HG21	1.97	0.46
3:I:47:GLU:HG2	3:I:50:ARG:HH22	1.81	0.46
3:J:44:TYR:O	3:J:48:VAL:HG23	2.15	0.46
3:J:238:ILE:CG2	3:J:240:ILE:HD11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:LEU:HD22	1:E:134:VAL:HG13	1.97	0.46
2:l:211:PHE:CD2	2:l:211:PHE:HA	2.51	0.46
2:7:136:ASP:CG	2:7:137:ILE:H	2.23	0.46
3:M:49:ARG:HG2	3:M:52:ARG:HH21	1.80	0.46
1:D:82:VAL:HG22	3:I:398:VAL:CB	2.46	0.46
1:g:41:LYS:HA	1:g:46:VAL:HG23	1.97	0.46
3:K:143:ILE:HD11	4:K:401:ATP:N6	2.30	0.46
3:K:189:THR:HG22	3:K:193:LYS:HD2	1.97	0.46
2:k:17:LEU:HD21	2:k:151:LEU:HD22	1.98	0.46
3:L:178:VAL:HB	3:L:307:ILE:HD12	1.98	0.46
3:H:208:GLY:N	3:H:240:ILE:HD11	2.30	0.46
3:H:290:ILE:HG13	3:H:293:LEU:HD11	1.98	0.46
2:6:45:ILE:HD13	2:6:46:TYR:N	2.31	0.46
3:I:350:ASP:O	3:I:354:ILE:HG13	2.16	0.46
1:A:167:GLY:O	1:A:171:VAL:HG23	2.16	0.46
2:6:107:LEU:HD13	2:6:107:LEU:HA	1.83	0.45
3:J:209:SER:HB2	3:J:246:ILE:HD13	1.99	0.45
1:c:167:GLY:HA3	1:c:199:SER:HB3	1.98	0.45
2:1:68:ARG:HH22	2:2:131:ALA:H	1.63	0.45
3:M:230:ALA:HB2	3:M:238:ILE:HD11	1.98	0.45
1:A:102:THR:HG23	1:A:103:TYR:CD2	2.51	0.45
1:f:35:ALA:HB3	1:f:66:LYS:HE2	1.99	0.45
2:5:81:ARG:HH12	2:5:85:PRO:HA	1.81	0.45
3:H:220:ALA:HB1	3:H:267:GLN:HE22	1.82	0.45
2:5:12:THR:CG2	2:5:58:GLY:H	2.28	0.45
3:H:212:VAL:HB	3:I:216:ILE:HD12	1.98	0.45
3:L:339:LEU:H	3:L:339:LEU:HG	1.65	0.45
1:g:12:ILE:HD12	1:g:12:ILE:HA	1.88	0.45
2:1:66:LEU:HD11	2:1:97:LEU:HD23	1.97	0.45
2:j:22:GLY:HA2	2:j:115:ILE:HD11	1.99	0.45
3:H:70:ASP:CG	3:M:105:ARG:HH12	2.25	0.45
3:K:143:ILE:HD11	4:K:401:ATP:HN62	1.82	0.45
3:L:55:VAL:HG12	3:L:59:ARG:HE	1.81	0.45
3:L:178:VAL:HG11	3:L:307:ILE:CD1	2.47	0.44
1:D:19:GLY:HA3	1:E:30:ALA:HA	1.99	0.44
3:L:342:ILE:HG22	3:L:383:LEU:HD13	1.99	0.44
1:e:17:PRO:HA	1:f:26:TYR:CD1	2.52	0.44
2:3:19:CYS:SG	2:3:164:ALA:CB	3.06	0.44
3:M:181:TYR:CZ	3:M:306:ILE:HD12	2.53	0.44
2:m:30:ARG:HH11	2:m:40:LYS:HG2	1.82	0.44
3:L:317:ARG:NH2	3:L:345:GLY:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:70:ILE:HG13	2:1:94:THR:HG22	1.99	0.44
3:K:251:THR:HG21	3:J:292:ILE:HD12	2.00	0.44
3:L:339:LEU:HD22	3:L:379:ILE:CD1	2.47	0.44
3:H:236:SER:HA	3:H:237:ILE:CB	2.47	0.44
3:L:39:SER:HA	3:L:42:ILE:HD12	1.99	0.44
3:M:24:ARG:HH12	3:M:28:ARG:HD2	1.83	0.44
2:7:78:GLU:HB2	2:7:85:PRO:HD3	1.99	0.44
1:a:70:ILE:HA	1:a:93:ARG:HG2	2.00	0.44
1:d:204:LEU:HD13	1:d:209:ILE:HD13	1.98	0.44
1:b:116:ILE:HD11	1:b:138:ILE:HD11	1.99	0.44
2:k:18:VAL:HG21	2:k:135:LYS:HA	1.99	0.44
2:m:165:VAL:O	2:m:169:VAL:HG23	2.18	0.44
3:H:133:GLU:CD	3:H:133:GLU:H	2.26	0.44
3:H:236:SER:HA	3:H:237:ILE:HG12	2.00	0.44
1:B:155:ALA:HB1	1:C:82:VAL:HB	2.00	0.43
2:4:115:ILE:HG21	2:4:193:GLU:HG3	1.99	0.43
2:l:45:ILE:HD13	2:l:55:THR:HG22	2.00	0.43
2:m:151:LEU:HD23	2:m:167:LEU:HG	1.99	0.43
2:m:169:VAL:HG22	2:m:204:VAL:CG1	2.48	0.43
3:J:206:VAL:HG22	3:J:207:VAL:H	1.83	0.43
1:A:208:ASN:O	1:A:209:ILE:HG23	2.18	0.43
1:a:13:THR:O	1:a:21:LEU:HD12	2.19	0.43
1:G:74:ILE:CD1	1:G:109:VAL:HG22	2.48	0.43
3:J:153:ILE:HD11	3:J:191:LEU:HD23	2.00	0.43
1:b:108:THR:HB	1:b:111:GLU:H	1.83	0.43
1:g:214:VAL:HA	1:g:221:PHE:H	1.83	0.43
1:a:198:LEU:HD11	1:a:243:LEU:HD13	2.01	0.43
1:B:189:MET:O	1:B:193:LEU:HD13	2.18	0.43
1:b:84:ASP:HB2	1:b:134:VAL:HB	2.00	0.43
1:d:38:ILE:HD12	1:d:196:MET:HE3	2.00	0.43
1:F:114:LYS:HZ2	1:G:86:ARG:HH11	1.66	0.43
1:G:54:VAL:H	1:G:54:VAL:HG12	1.60	0.43
3:K:105:ARG:HB2	3:K:119:LEU:HB2	2.00	0.43
1:B:35:ALA:HA	1:B:166:MET:HE2	2.00	0.43
1:C:104:ASP:HB2	2:4:92:THR:HG21	2.01	0.43
1:c:110:LYS:HZ1	1:d:64:ILE:HG23	1.84	0.43
1:E:33:ARG:HB3	3:H:397:PHE:CE2	2.53	0.43
3:H:208:GLY:HA2	3:H:240:ILE:HD11	2.00	0.43
3:I:61:PRO:HA	3:I:62:PRO:C	2.44	0.43
3:I:281:VAL:HA	3:I:282:LYS:HB2	2.00	0.43
1:C:167:GLY:O	1:C:171:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:244:ASP:OD1	3:K:292:ILE:HD11	2.19	0.43
1:c:46:VAL:C	1:c:47:ILE:HD12	2.44	0.42
1:g:38:ILE:HD12	1:g:171:VAL:HG11	1.99	0.42
3:L:178:VAL:CB	3:L:307:ILE:HD12	2.49	0.42
1:A:104:ASP:HB2	2:2:92:THR:HG21	2.01	0.42
1:B:121:GLN:HG3	1:C:83:ALA:O	2.20	0.42
2:l:146:THR:HG21	2:l:175:ALA:HA	2.00	0.42
3:K:342:ILE:HG21	3:K:379:ILE:HG21	2.00	0.42
2:4:52:MET:HE2	2:4:52:MET:HB2	1.88	0.42
3:M:216:ILE:C	3:M:216:ILE:HD12	2.44	0.42
3:J:354:ILE:HG13	3:J:382:VAL:HG11	2.00	0.42
1:A:38:ILE:HG12	1:A:196:MET:HE3	2.02	0.42
1:A:17:PRO:HA	1:B:26:TYR:CD2	2.54	0.42
2:i:126:ASP:HA	2:i:127:PRO:HD3	1.90	0.42
3:I:87:PHE:CZ	3:I:113:LEU:HB3	2.54	0.42
2:4:45:ILE:HD12	2:4:189:VAL:HG22	2.01	0.42
2:5:14:THR:HG22	2:5:27:THR:HG23	2.00	0.42
1:A:159:TYR:CD2	1:A:162:THR:HB	2.54	0.42
1:B:19:GLY:O	1:C:30:ALA:HA	2.20	0.42
3:J:240:ILE:HG22	3:J:243:LEU:HB2	1.95	0.42
1:b:117:CYS:SG	1:b:150:THR:HG22	2.60	0.42
1:G:196:MET:HE2	1:G:209:ILE:HG22	2.02	0.42
3:J:202:THR:HG22	3:J:204:ILE:HD11	2.02	0.42
1:b:12:ILE:HD12	1:b:12:ILE:HA	1.90	0.41
1:b:204:LEU:HD22	1:b:209:ILE:HG21	2.02	0.41
1:d:164:ILE:HG22	1:d:168:ARG:HH21	1.83	0.41
1:f:59:LEU:HD12	1:f:60:GLU:H	1.85	0.41
1:G:64:ILE:HG23	1:G:65:GLU:HB3	2.01	0.41
1:G:64:ILE:HA	1:G:65:GLU:HA	1.87	0.41
3:H:318:ILE:CD1	3:H:337:LYS:HG2	2.50	0.41
3:K:292:ILE:HD12	3:L:262:GLN:HE22	1.85	0.41
1:A:143:GLU:HA	1:A:219:ARG:HH21	1.84	0.41
2:n:94:THR:HG21	2:n:110:LEU:HD21	2.01	0.41
1:A:174:PHE:CE1	1:A:178:GLU:HG3	2.56	0.41
1:d:53:ARG:HH21	1:d:60:GLU:HA	1.85	0.41
1:d:204:LEU:HD23	1:d:204:LEU:HA	1.94	0.41
2:2:27:THR:HG21	2:2:44:LYS:HG3	2.02	0.41
2:2:111:LEU:HD21	2:2:138:VAL:HG13	2.02	0.41
2:j:21:ASP:OD2	2:j:161:VAL:HG13	2.20	0.41
2:j:115:ILE:HD13	2:j:193:GLU:HB2	2.02	0.41
2:l:165:VAL:O	2:l:169:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:211:PHE:O	3:M:212:VAL:HG22	2.19	0.41
2:7:66:LEU:HD12	2:7:108:VAL:HG11	2.02	0.41
3:M:342:ILE:HG22	3:M:379:ILE:CG2	2.49	0.41
3:H:139:SER:O	3:H:143:ILE:HG13	2.20	0.41
1:C:76:ALA:HA	1:C:137:LEU:O	2.21	0.41
1:a:12:ILE:HD12	1:a:12:ILE:HA	1.88	0.41
1:C:239:ARG:HA	1:C:239:ARG:HH11	1.86	0.41
1:c:21:LEU:HD21	1:d:130:ARG:HE	1.85	0.41
2:i:15:VAL:HG22	2:i:26:ALA:HB3	2.03	0.41
2:m:77:TYR:CD1	2:m:77:TYR:C	2.98	0.41
3:H:386:THR:HG22	3:H:387:THR:H	1.85	0.41
3:K:275:PHE:HB2	3:J:205:ARG:HE	1.85	0.41
1:c:49:ILE:CD1	1:c:193:LEU:HD23	2.50	0.41
2:6:45:ILE:HD12	2:6:189:VAL:HG11	2.03	0.41
2:m:102:ARG:HD2	2:m:128:ILE:HG22	2.03	0.41
2:n:33:MET:HE2	2:n:38:ALA:HB2	2.02	0.41
3:H:330:LEU:HA	3:H:370:VAL:H	1.86	0.41
3:I:206:VAL:HG22	3:I:207:VAL:H	1.86	0.41
3:K:44:TYR:O	3:K:48:VAL:HG23	2.20	0.41
3:L:51:LEU:O	3:L:55:VAL:HG23	2.21	0.41
3:L:398:VAL:OXT	3:L:398:VAL:CG2	2.64	0.41
3:J:209:SER:HB2	3:J:246:ILE:CD1	2.50	0.41
3:J:281:VAL:HG12	3:J:283:VAL:HG23	2.03	0.41
1:C:81:LEU:H	1:C:81:LEU:HD12	1.86	0.41
3:I:249:ARG:HA	3:I:294:ASP:OD2	2.21	0.41
3:K:328:MET:HA	3:L:171:GLY:HA3	2.03	0.41
3:L:178:VAL:CG1	3:L:307:ILE:CD1	3.00	0.41
2:h:125:ILE:H	2:h:125:ILE:HD12	1.85	0.40
3:H:243:LEU:HD23	3:H:246:ILE:HG23	2.03	0.40
3:L:389:ILE:HB	3:L:390:PRO:HD3	2.02	0.40
1:D:103:TYR:O	2:5:89:ALA:HA	2.22	0.40
1:d:41:LYS:HA	1:d:46:VAL:HG23	2.03	0.40
3:H:236:SER:HA	3:H:237:ILE:CG1	2.51	0.40
3:H:168:ALA:CA	3:H:278:ARG:HE	2.30	0.40
3:J:342:ILE:HG22	3:J:379:ILE:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/242 (99%)	226 (94%)	12 (5%)	2 (1%)	16	54
1	B	240/242 (99%)	225 (94%)	9 (4%)	6 (2%)	4	26
1	C	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	5	30
1	D	240/242 (99%)	225 (94%)	11 (5%)	4 (2%)	7	36
1	E	240/242 (99%)	227 (95%)	11 (5%)	2 (1%)	16	54
1	F	240/242 (99%)	225 (94%)	12 (5%)	3 (1%)	9	42
1	G	240/242 (99%)	224 (93%)	13 (5%)	3 (1%)	9	42
1	a	235/242 (97%)	223 (95%)	9 (4%)	3 (1%)	9	42
1	b	235/242 (97%)	219 (93%)	14 (6%)	2 (1%)	14	50
1	c	235/242 (97%)	220 (94%)	13 (6%)	2 (1%)	14	50
1	d	235/242 (97%)	218 (93%)	12 (5%)	5 (2%)	5	30
1	e	235/242 (97%)	219 (93%)	12 (5%)	4 (2%)	7	36
1	f	235/242 (97%)	223 (95%)	10 (4%)	2 (1%)	14	50
1	g	235/242 (97%)	220 (94%)	8 (3%)	7 (3%)	3	22
2	1	200/202 (99%)	186 (93%)	11 (6%)	3 (2%)	8	39
2	2	200/202 (99%)	179 (90%)	15 (8%)	6 (3%)	3	22
2	3	200/202 (99%)	182 (91%)	13 (6%)	5 (2%)	4	26
2	4	200/202 (99%)	184 (92%)	10 (5%)	6 (3%)	3	22
2	5	200/202 (99%)	184 (92%)	10 (5%)	6 (3%)	3	22
2	6	200/202 (99%)	182 (91%)	12 (6%)	6 (3%)	3	22
2	7	200/202 (99%)	184 (92%)	12 (6%)	4 (2%)	6	31
2	h	200/202 (99%)	178 (89%)	14 (7%)	8 (4%)	2	18
2	i	200/202 (99%)	184 (92%)	12 (6%)	4 (2%)	6	31
2	j	200/202 (99%)	186 (93%)	10 (5%)	4 (2%)	6	31
2	k	200/202 (99%)	182 (91%)	13 (6%)	5 (2%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	200/202 (99%)	182 (91%)	12 (6%)	6 (3%)	3	22
2	m	200/202 (99%)	192 (96%)	6 (3%)	2 (1%)	12	48
2	n	200/202 (99%)	181 (90%)	8 (4%)	11 (6%)	1	14
3	H	388/390 (100%)	346 (89%)	25 (6%)	17 (4%)	2	17
3	I	388/390 (100%)	352 (91%)	20 (5%)	16 (4%)	2	17
3	J	388/390 (100%)	347 (89%)	27 (7%)	14 (4%)	2	20
3	K	388/390 (100%)	350 (90%)	28 (7%)	10 (3%)	4	25
3	L	388/390 (100%)	354 (91%)	21 (5%)	13 (3%)	3	20
3	M	388/390 (100%)	357 (92%)	25 (6%)	6 (2%)	8	39
All	All	8453/8556 (99%)	7792 (92%)	459 (5%)	202 (2%)	7	27

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	B	64	ILE
1	C	20	ARG
1	C	66	LYS
1	C	67	ILE
1	F	64	ILE
1	f	12	ILE
1	G	20	ARG
2	h	140	THR
2	2	41	ALA
2	2	182	SER
2	3	139	ALA
2	4	140	THR
2	l	128	ILE
2	6	139	ALA
2	n	131	ALA
2	n	139	ALA
3	H	237	ILE
3	I	247	ALA
3	I	255	THR
3	I	270	ALA
3	I	292	ILE
3	K	269	LEU
3	K	270	ALA
3	K	278	ARG

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Mol	Chain	Res	Type
3	J	128	TYR
3	J	190	LEU
3	J	191	LEU
3	J	280	ASP
1	a	161	ALA
1	b	143	GLU
1	C	221	PHE
1	c	179	TYR
1	D	65	GLU
1	D	161	ALA
1	d	143	GLU
1	d	161	ALA
1	d	221	PHE
1	E	221	PHE
1	e	161	ALA
1	f	179	TYR
1	G	143	GLU
1	G	221	PHE
1	g	143	GLU
2	1	39	SER
2	2	140	THR
2	i	41	ALA
2	3	212	ARG
2	j	136	ASP
2	j	212	ARG
2	4	33	MET
2	k	181	ALA
2	5	136	ASP
2	l	194	ASP
2	7	83	ARG
2	7	133	GLU
2	n	30	ARG
2	n	35	ASN
2	n	132	ILE
2	n	181	ALA
2	n	194	ASP
3	H	163	LYS
3	H	242	GLU
3	H	245	ALA
3	H	248	ALA
3	H	255	THR
3	H	280	ASP

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Mol	Chain	Res	Type
3	H	333	ASP
3	I	146	LEU
3	I	269	LEU
3	I	282	LYS
3	I	310	PRO
3	I	331	ALA
3	I	332	GLU
3	K	131	GLU
3	K	200	ARG
3	K	246	ILE
3	K	392	LEU
3	L	131	GLU
3	L	212	VAL
3	L	282	LYS
3	L	388	PRO
3	M	212	VAL
3	J	122	SER
3	J	134	GLU
3	J	282	LYS
3	J	292	ILE
1	B	65	GLU
1	B	73	HIS
1	B	143	GLU
1	B	221	PHE
1	b	66	LYS
1	D	143	GLU
1	d	12	ILE
1	E	73	HIS
1	F	221	PHE
1	g	66	LYS
1	g	73	HIS
1	g	218	ASP
2	1	136	ASP
2	h	20	LYS
2	h	41	ALA
2	2	106	TYR
2	3	181	ALA
2	j	193	GLU
2	4	136	ASP
2	4	211	PHE
2	k	135	LYS
2	5	191	ILE

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Mol	Chain	Res	Type
2	5	212	ARG
2	1	193	GLU
2	6	20	LYS
2	6	41	ALA
2	m	193	GLU
2	7	39	SER
3	H	310	PRO
3	H	366	GLU
3	I	212	VAL
3	I	221	ARG
3	K	212	VAL
3	K	391	ASP
3	L	183	PRO
3	L	273	ASP
3	L	395	VAL
3	J	273	ASP
3	J	301	GLY
3	J	331	ALA
1	A	64	ILE
1	B	60	GLU
1	C	143	GLU
1	d	14	VAL
1	e	14	VAL
1	e	62	ASP
1	e	104	ASP
1	g	217	ASP
1	g	221	PHE
2	h	21	ASP
2	h	35	ASN
2	2	139	ALA
2	i	140	THR
2	3	39	SER
2	k	41	ALA
2	5	193	GLU
2	l	40	LYS
2	6	136	ASP
2	6	193	GLU
2	7	193	GLU
2	n	137	ILE
2	n	140	THR
3	H	61	PRO
3	H	135	LYS

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Mol	Chain	Res	Type
3	H	296	ALA
3	I	330	LEU
3	I	393	LYS
3	K	125	PRO
3	L	135	LYS
3	L	242	GLU
3	L	335	ASP
3	M	91	THR
3	J	188	LYS
3	J	214	LYS
3	J	275	PHE
1	g	106	PRO
2	1	183	GLY
2	h	191	ILE
2	2	42	ALA
2	i	193	GLU
2	3	140	THR
2	4	107	LEU
2	4	193	GLU
2	5	35	ASN
2	5	200	SER
3	H	290	ILE
3	I	202	THR
3	L	284	ILE
3	M	385	LYS
1	F	9	ASP
2	h	137	ILE
2	k	30	ARG
2	l	30	ARG
2	m	200	SER
3	H	136	PRO
3	H	202	THR
3	H	246	ILE
3	I	275	PHE
3	L	253	SER
3	M	61	PRO
3	M	123	LYS
1	c	12	ILE
2	h	183	GLY
3	M	217	GLY
2	l	137	ILE
2	k	200	SER

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Mol	Chain	Res	Type
1	a	54	VAL
1	D	64	ILE
2	i	207	ILE
2	j	200	SER
2	6	128	ILE
2	n	200	SER
1	a	34	GLY
2	n	129	GLY
3	L	334	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	197 (97%)	6 (3%)	36	57
1	B	203/203 (100%)	197 (97%)	6 (3%)	36	57
1	C	203/203 (100%)	193 (95%)	10 (5%)	22	43
1	D	203/203 (100%)	194 (96%)	9 (4%)	25	47
1	E	203/203 (100%)	199 (98%)	4 (2%)	48	66
1	F	203/203 (100%)	195 (96%)	8 (4%)	28	49
1	G	203/203 (100%)	189 (93%)	14 (7%)	14	36
1	a	199/203 (98%)	191 (96%)	8 (4%)	28	49
1	b	199/203 (98%)	193 (97%)	6 (3%)	36	57
1	c	199/203 (98%)	186 (94%)	13 (6%)	15	37
1	d	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	e	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	f	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	g	199/203 (98%)	193 (97%)	6 (3%)	36	57
2	1	164/164 (100%)	152 (93%)	12 (7%)	13	34
2	2	164/164 (100%)	153 (93%)	11 (7%)	15	36
2	3	164/164 (100%)	156 (95%)	8 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	5	164/164 (100%)	152 (93%)	12 (7%)	13	34
2	6	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	7	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	h	164/164 (100%)	154 (94%)	10 (6%)	17	38
2	i	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	j	164/164 (100%)	159 (97%)	5 (3%)	36	57
2	k	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	l	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	m	164/164 (100%)	161 (98%)	3 (2%)	51	67
2	n	164/164 (100%)	156 (95%)	8 (5%)	22	43
3	H	338/338 (100%)	327 (97%)	11 (3%)	33	55
3	I	338/338 (100%)	330 (98%)	8 (2%)	43	63
3	J	338/338 (100%)	322 (95%)	16 (5%)	23	44
3	K	338/338 (100%)	324 (96%)	14 (4%)	27	48
3	L	338/338 (100%)	327 (97%)	11 (3%)	33	55
3	M	338/338 (100%)	320 (95%)	18 (5%)	20	41
All	All	7138/7166 (100%)	6826 (96%)	312 (4%)	27	47

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	86	ARG
1	A	87	VAL
1	A	108	THR
1	A	169	ASN
1	A	217	ASP
1	a	21	LEU
1	a	24	VAL
1	a	40	ILE
1	a	129	VAL
1	a	166	MET
1	a	169	ASN
1	a	213	TYR
1	a	234	GLU

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Mol	Chain	Res	Type
1	B	36	THR
1	B	48	LEU
1	B	178	GLU
1	B	210	GLU
1	B	216	VAL
1	B	229	LEU
1	b	31	VAL
1	b	54	VAL
1	b	87	VAL
1	b	108	THR
1	b	109	VAL
1	b	172	THR
1	C	24	VAL
1	C	46	VAL
1	C	56	SER
1	C	73	HIS
1	C	81	LEU
1	C	98	ILE
1	C	106	PRO
1	C	125	GLN
1	C	144	VAL
1	C	166	MET
1	c	14	VAL
1	c	18	ASP
1	c	22	PHE
1	c	24	VAL
1	c	46	VAL
1	c	102	THR
1	c	166	MET
1	c	173	GLU
1	c	178	GLU
1	c	180	ARG
1	c	213	TYR
1	c	216	VAL
1	c	222	LYS
1	D	12	ILE
1	D	14	VAL
1	D	22	PHE
1	D	82	VAL
1	D	121	GLN
1	D	147	LEU
1	D	213	TYR

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Mol	Chain	Res	Type
1	D	217	ASP
1	D	229	LEU
1	d	13	THR
1	d	21	LEU
1	d	24	VAL
1	d	40	ILE
1	d	49	ILE
1	d	54	VAL
1	d	89	ILE
1	d	134	VAL
1	d	158	GLU
1	E	42	CYS
1	E	43	LYS
1	E	213	TYR
1	E	224	VAL
1	e	21	LEU
1	e	31	VAL
1	e	40	ILE
1	e	81	LEU
1	e	116	ILE
1	e	129	VAL
1	e	142	ASP
1	e	180	ARG
1	e	181	ASP
1	F	97	GLN
1	F	125	GLN
1	F	129	VAL
1	F	144	VAL
1	F	205	VAL
1	F	206	PRO
1	F	209	ILE
1	F	226	PRO
1	f	10	ARG
1	f	21	LEU
1	f	43	LYS
1	f	46	VAL
1	f	54	VAL
1	f	64	ILE
1	f	129	VAL
1	f	134	VAL
1	f	220	THR
1	G	5	GLN

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Mol	Chain	Res	Type
1	G	24	VAL
1	G	54	VAL
1	G	57	LYS
1	G	58	LEU
1	G	78	THR
1	G	89	ILE
1	G	99	ASN
1	G	102	THR
1	G	121	GLN
1	G	164	ILE
1	G	209	ILE
1	G	220	THR
1	G	228	GLU
1	g	14	VAL
1	g	47	ILE
1	g	59	LEU
1	g	82	VAL
1	g	151	ASP
1	g	219	ARG
2	1	27	THR
2	1	45	ILE
2	1	55	THR
2	1	72	ILE
2	1	107	LEU
2	1	120	LYS
2	1	142	SER
2	1	159	ILE
2	1	186	ILE
2	1	189	VAL
2	1	202	GLU
2	1	208	LEU
2	h	52	MET
2	h	95	SER
2	h	107	LEU
2	h	116	ASP
2	h	121	SER
2	h	125	ILE
2	h	188	VAL
2	h	195	GLU
2	h	201	PRO
2	h	205	GLU
2	2	17	LEU

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Mol	Chain	Res	Type
2	2	27	THR
2	2	45	ILE
2	2	71	LYS
2	2	84	LYS
2	2	106	TYR
2	2	110	LEU
2	2	125	ILE
2	2	132	ILE
2	2	137	ILE
2	2	201	PRO
2	i	45	ILE
2	i	64	GLN
2	i	104	PHE
2	i	105	PRO
2	i	122	ILE
2	i	137	ILE
2	i	138	VAL
2	i	140	THR
2	i	211	PHE
2	3	45	ILE
2	3	69	ILE
2	3	72	ILE
2	3	90	ILE
2	3	110	LEU
2	3	132	ILE
2	3	140	THR
2	3	213	LYS
2	j	30	ARG
2	j	45	ILE
2	j	72	ILE
2	j	132	ILE
2	j	148	TYR
2	4	27	THR
2	4	32	THR
2	4	45	ILE
2	4	56	THR
2	4	136	ASP
2	4	140	THR
2	4	146	THR
2	4	154	ARG
2	4	188	VAL
2	k	60	VAL

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Mol	Chain	Res	Type
2	k	82	GLU
2	k	107	LEU
2	k	120	LYS
2	k	146	THR
2	k	188	VAL
2	k	190	LYS
2	5	13	THR
2	5	27	THR
2	5	28	GLU
2	5	33	MET
2	5	45	ILE
2	5	51	ARG
2	5	78	GLU
2	5	140	THR
2	5	145	LEU
2	5	186	ILE
2	5	190	LYS
2	5	205	GLU
2	1	17	LEU
2	1	28	GLU
2	1	72	ILE
2	1	121	SER
2	1	156	THR
2	1	186	ILE
2	1	199	TYR
2	6	17	LEU
2	6	21	ASP
2	6	40	LYS
2	6	45	ILE
2	6	55	THR
2	6	72	ILE
2	6	136	ASP
2	6	174	SER
2	6	202	GLU
2	m	27	THR
2	m	156	THR
2	m	201	PRO
2	7	45	ILE
2	7	64	GLN
2	7	110	LEU
2	7	115	ILE
2	7	132	ILE

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Mol	Chain	Res	Type
2	7	161	VAL
2	7	208	LEU
2	n	20	LYS
2	n	27	THR
2	n	87	VAL
2	n	103	TYR
2	n	115	ILE
2	n	116	ASP
2	n	166	GLU
2	n	200	SER
3	H	41	ARG
3	H	63	LEU
3	H	97	GLU
3	H	102	PRO
3	H	137	GLU
3	H	206	VAL
3	H	244	ASP
3	H	265	MET
3	H	293	LEU
3	H	311	LEU
3	H	330	LEU
3	I	118	VAL
3	I	170	VAL
3	I	175	PRO
3	I	250	ARG
3	I	299	ARG
3	I	370	VAL
3	I	393	LYS
3	I	398	VAL
3	K	12	LYS
3	K	14	LYS
3	K	22	LYS
3	K	79	VAL
3	K	132	VAL
3	K	136	PRO
3	K	159	LEU
3	K	165	GLU
3	K	189	THR
3	K	200	ARG
3	K	255	THR
3	K	282	LYS
3	K	298	LEU

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Mol	Chain	Res	Type
3	K	387	THR
3	L	113	LEU
3	L	136	PRO
3	L	160	PRO
3	L	183	PRO
3	L	214	LYS
3	L	269	LEU
3	L	283	VAL
3	L	291	ASP
3	L	319	GLN
3	L	352	LYS
3	L	370	VAL
3	M	61	PRO
3	M	80	LYS
3	M	85	PRO
3	M	89	VAL
3	M	113	LEU
3	M	118	VAL
3	M	120	PRO
3	M	158	GLU
3	M	181	TYR
3	M	183	PRO
3	M	190	LEU
3	M	206	VAL
3	M	214	LYS
3	M	223	VAL
3	M	275	PHE
3	M	312	PRO
3	M	327	LYS
3	M	387	THR
3	J	39	SER
3	J	92	SER
3	J	110	GLN
3	J	159	LEU
3	J	165	GLU
3	J	184	PRO
3	J	188	LYS
3	J	190	LEU
3	J	205	ARG
3	J	210	GLU
3	J	226	VAL
3	J	227	PHE

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Mol	Chain	Res	Type
3	J	250	ARG
3	J	265	MET
3	J	380	GLU
3	J	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	121	GLN
1	A	125	GLN
1	A	237	ASN
1	a	23	GLN
1	a	73	HIS
1	a	99	ASN
1	a	121	GLN
1	B	5	GLN
1	B	97	GLN
1	B	125	GLN
1	B	208	ASN
1	b	121	GLN
1	b	125	GLN
1	b	208	ASN
1	b	237	ASN
1	C	5	GLN
1	C	97	GLN
1	C	237	ASN
1	c	23	GLN
1	c	73	HIS
1	c	121	GLN
1	c	125	GLN
1	D	73	HIS
1	D	121	GLN
1	D	125	GLN
1	d	97	GLN
1	d	125	GLN
1	E	97	GLN
1	E	121	GLN
1	E	208	ASN
1	e	237	ASN
1	F	99	ASN
1	F	122	GLN

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Mol	Chain	Res	Type
1	f	73	HIS
1	f	97	GLN
1	f	99	ASN
1	f	121	GLN
1	f	125	GLN
1	G	99	ASN
1	G	125	GLN
1	g	23	GLN
1	g	73	HIS
1	g	208	ASN
2	1	109	GLN
2	h	198	GLN
2	2	35	ASN
2	2	64	GLN
2	i	47	GLN
2	i	64	GLN
2	3	64	GLN
2	3	75	ASN
2	3	109	GLN
2	j	75	ASN
2	j	99	ASN
2	k	96	ASN
2	5	35	ASN
2	5	109	GLN
2	5	198	GLN
2	l	96	ASN
2	6	96	ASN
2	m	35	ASN
2	m	64	GLN
2	m	75	ASN
2	7	109	GLN
2	n	75	ASN
3	H	109	ASN
3	H	197	ASN
3	H	198	GLN
3	H	213	GLN
3	H	252	ASN
3	H	319	GLN
3	I	267	GLN
3	K	111	GLN
3	K	213	GLN
3	K	288	ASN

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Mol	Chain	Res	Type
3	L	111	GLN
3	L	117	ASN
3	L	197	ASN
3	L	228	GLN
3	L	262	GLN
3	L	267	GLN
3	L	288	ASN
3	L	324	HIS
3	M	197	ASN
3	M	213	GLN
3	J	109	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
4	ATP	J	401	5	32,33,33	3.75	4 (12%)	48,52,52	1.45	6 (12%)
4	ATP	I	401	5	32,33,33	5.54	6 (18%)	48,52,52	1.10	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	K	401	5	32,33,33	4.76	5 (15%)	48,52,52	1.89	12 (25%)
4	ATP	H	401	5	32,33,33	4.27	11 (34%)	48,52,52	1.53	7 (14%)
6	ADP	L	401	5	28,29,29	2.42	4 (14%)	43,45,45	1.18	5 (11%)

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
4	ATP	J	401	5	-	2/22/38/38	0/3/3/3
4	ATP	I	401	5	-	5/22/38/38	0/3/3/3
4	ATP	K	401	5	-	5/22/38/38	0/3/3/3
4	ATP	H	401	5	-	6/22/38/38	0/3/3/3
6	ADP	L	401	5	-	6/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	401	ATP	PB-O3B	24.25	1.85	1.59
4	H	401	ATP	PB-O3A	20.50	1.81	1.59
4	J	401	ATP	PB-O3B	18.49	1.79	1.59
4	K	401	ATP	PB-O3B	17.92	1.78	1.59
4	I	401	ATP	PB-O3A	16.94	1.77	1.59
4	K	401	ATP	PB-O3A	16.68	1.77	1.59
6	L	401	ADP	PA-O3A	11.19	1.71	1.59
4	K	401	ATP	PA-O3A	9.50	1.69	1.59
4	J	401	ATP	PB-O3A	8.34	1.68	1.59
4	H	401	ATP	PB-O3B	8.11	1.68	1.59
4	I	401	ATP	PA-O3A	7.32	1.67	1.59
4	H	401	ATP	PA-O3A	4.58	1.64	1.59
4	I	401	ATP	C8-N9	4.06	1.44	1.37
4	J	401	ATP	PA-O3A	3.21	1.63	1.59
4	H	401	ATP	O4'-C1'	-3.19	1.34	1.42
4	J	401	ATP	O3'-C3'	3.06	1.50	1.43
4	H	401	ATP	C5'-C4'	2.83	1.60	1.51
4	H	401	ATP	C5-C4	2.66	1.43	1.39
4	H	401	ATP	O2'-C2'	-2.60	1.36	1.43
4	H	401	ATP	C6-N6	2.57	1.40	1.34
4	K	401	ATP	C5-N7	2.50	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	ATP	C2'-C1'	-2.45	1.45	1.53
6	L	401	ADP	C6-N6	2.45	1.40	1.34
4	H	401	ATP	C2-N1	2.29	1.38	1.33
6	L	401	ADP	C5-C4	2.28	1.43	1.39
6	L	401	ADP	C3'-C4'	2.25	1.58	1.53
4	H	401	ATP	PG-O1G	2.08	1.56	1.50
4	I	401	ATP	C2-N3	2.06	1.37	1.33
4	I	401	ATP	C5-C4	2.04	1.42	1.39
4	K	401	ATP	C8-N7	2.02	1.35	1.31

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	401	ATP	N6-C6-N1	6.25	132.31	118.38
4	H	401	ATP	N6-C6-N1	5.50	130.62	118.38
4	J	401	ATP	N6-C6-N1	4.07	127.45	118.38
4	K	401	ATP	C5-C4-N9	4.05	110.22	105.81
4	K	401	ATP	C4-C5-N7	-4.00	106.01	110.58
4	J	401	ATP	C6-C5-C4	3.95	122.57	117.18
4	K	401	ATP	C6-C5-C4	3.67	122.19	117.18
4	J	401	ATP	C4-N9-C8	-3.33	102.24	105.74
4	H	401	ATP	C5-C6-N6	-3.09	115.64	123.29
4	K	401	ATP	O3A-PA-O1A	-3.06	101.51	110.70
6	L	401	ADP	N3-C2-N1	3.05	133.20	128.58
6	L	401	ADP	N6-C6-N1	2.89	124.82	118.38
4	J	401	ATP	O3G-PG-O2G	2.84	118.44	107.80
4	K	401	ATP	C5-C6-N6	-2.83	116.29	123.29
4	K	401	ATP	N9-C8-N7	-2.79	109.98	113.94
4	K	401	ATP	C5-C6-N1	-2.79	110.44	117.51
4	H	401	ATP	O3B-PG-O1G	-2.67	97.01	111.04
4	I	401	ATP	O2B-PB-O3B	-2.57	100.33	107.27
4	K	401	ATP	C2-N1-C6	2.53	122.88	118.73
4	I	401	ATP	N9-C8-N7	-2.52	110.35	113.94
4	I	401	ATP	C5-N7-C8	2.46	107.32	103.45
6	L	401	ADP	O5'-C5'-C4'	2.45	117.34	108.99
6	L	401	ADP	C2-N3-C4	-2.41	105.94	111.83
4	H	401	ATP	C5-N7-C8	2.40	107.23	103.45
4	H	401	ATP	C6-C5-C4	2.39	120.45	117.18
4	J	401	ATP	C6-C5-N7	-2.39	127.48	132.09
4	H	401	ATP	C5'-C4'-C3'	-2.33	106.82	115.21
4	H	401	ATP	C4-C5-N7	-2.28	107.98	110.58
4	K	401	ATP	C5-N7-C8	2.24	106.98	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	401	ATP	C5-C6-N1	-2.15	112.05	117.51
4	K	401	ATP	O3B-PG-O1G	-2.11	99.92	111.04
6	L	401	ADP	C5-C4-N9	-2.06	103.56	105.81
4	K	401	ATP	O2B-PB-O3A	2.06	112.84	107.27

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	401	ATP	C5'-O5'-PA-O3A
4	I	401	ATP	C5'-O5'-PA-O2A
4	I	401	ATP	C5'-O5'-PA-O3A
4	K	401	ATP	C5'-O5'-PA-O3A
4	J	401	ATP	C5'-O5'-PA-O2A
4	J	401	ATP	C5'-O5'-PA-O3A
6	L	401	ADP	C5'-O5'-PA-O1A
6	L	401	ADP	C5'-O5'-PA-O2A
6	L	401	ADP	C5'-O5'-PA-O3A
4	I	401	ATP	PA-O3A-PB-O1B
4	H	401	ATP	PA-O3A-PB-O2B
4	K	401	ATP	PA-O3A-PB-O2B
6	L	401	ADP	PB-O3A-PA-O1A
4	K	401	ATP	C4'-C5'-O5'-PA
4	H	401	ATP	C5'-O5'-PA-O1A
4	I	401	ATP	C5'-O5'-PA-O1A
4	K	401	ATP	C5'-O5'-PA-O1A
4	I	401	ATP	PA-O3A-PB-O2B
6	L	401	ADP	C4'-C5'-O5'-PA
4	H	401	ATP	PG-O3B-PB-O2B
4	H	401	ATP	PA-O3A-PB-O1B
4	K	401	ATP	PA-O3A-PB-O1B
6	L	401	ADP	PB-O3A-PA-O2A
4	H	401	ATP	PG-O3B-PB-O1B

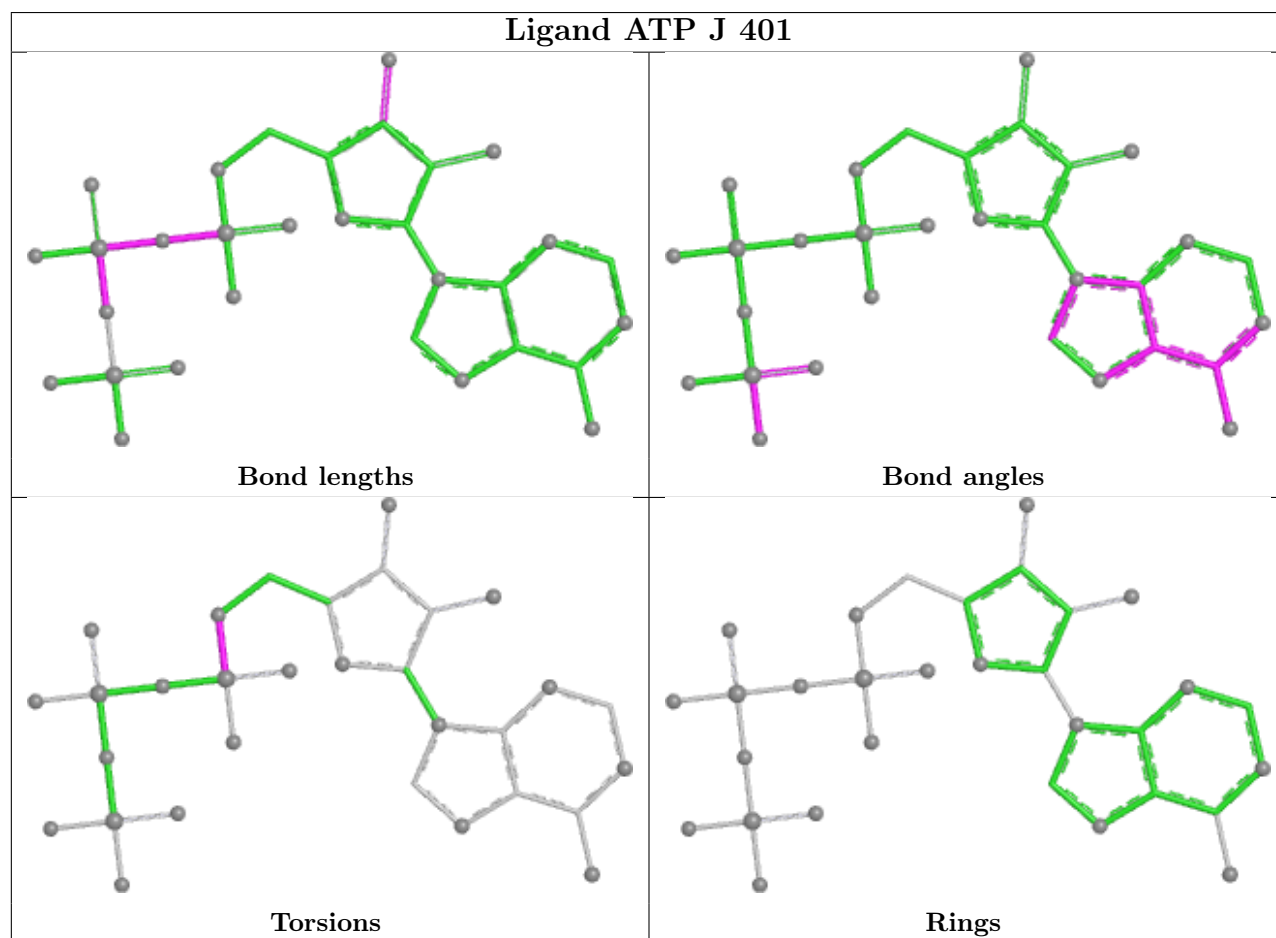
There are no ring outliers.

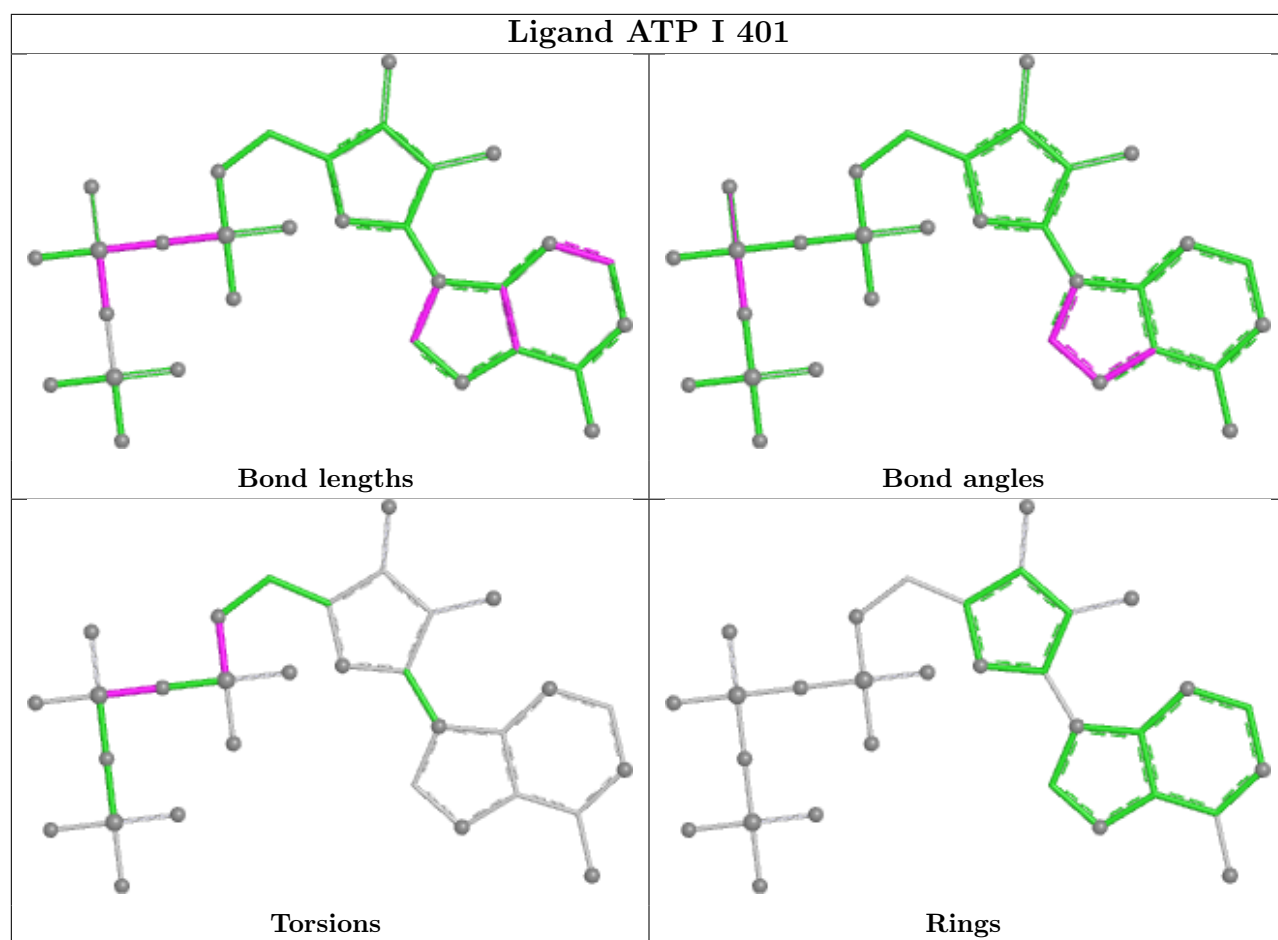
1 monomer is involved in 2 short contacts:

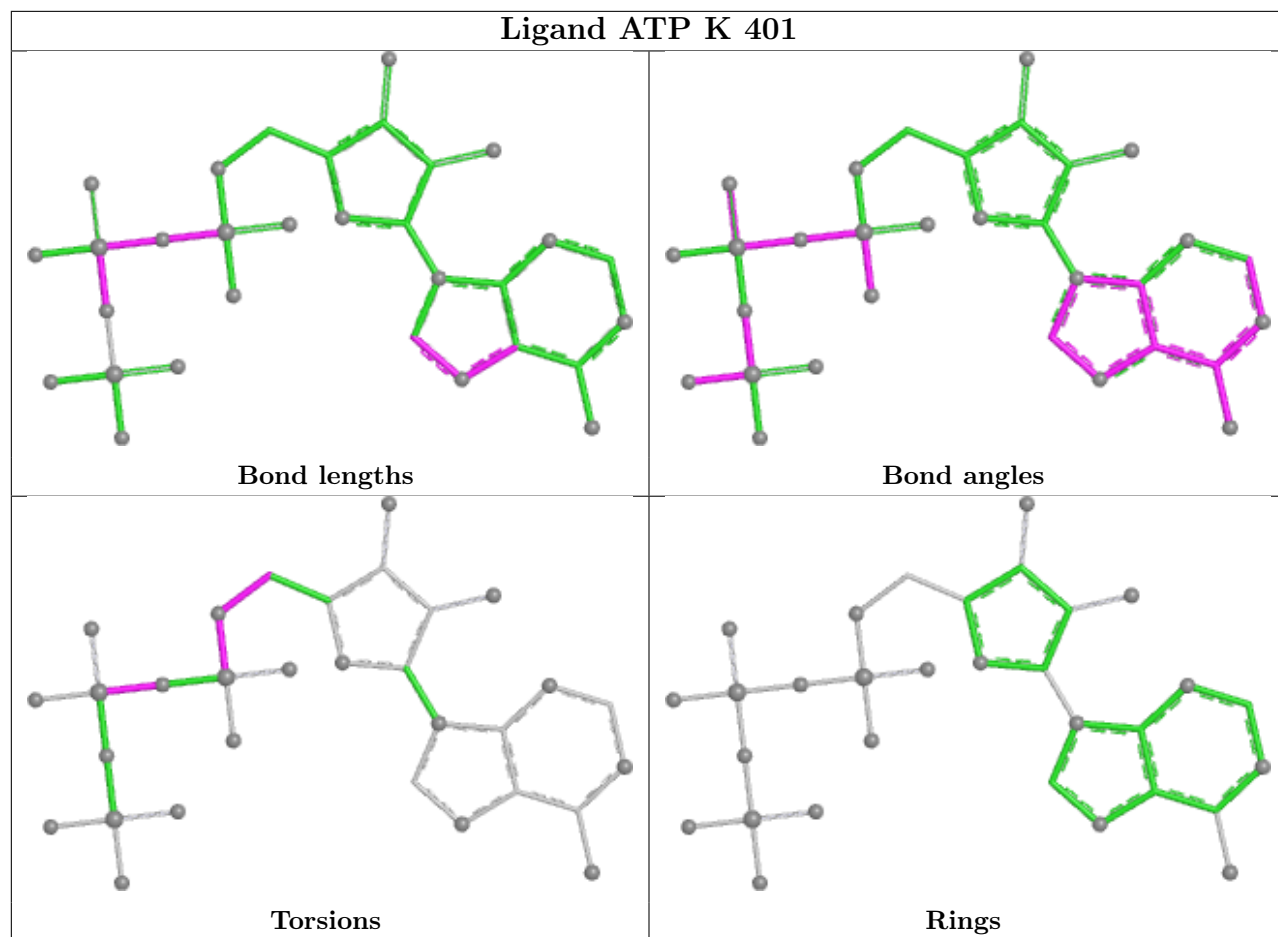
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	401	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

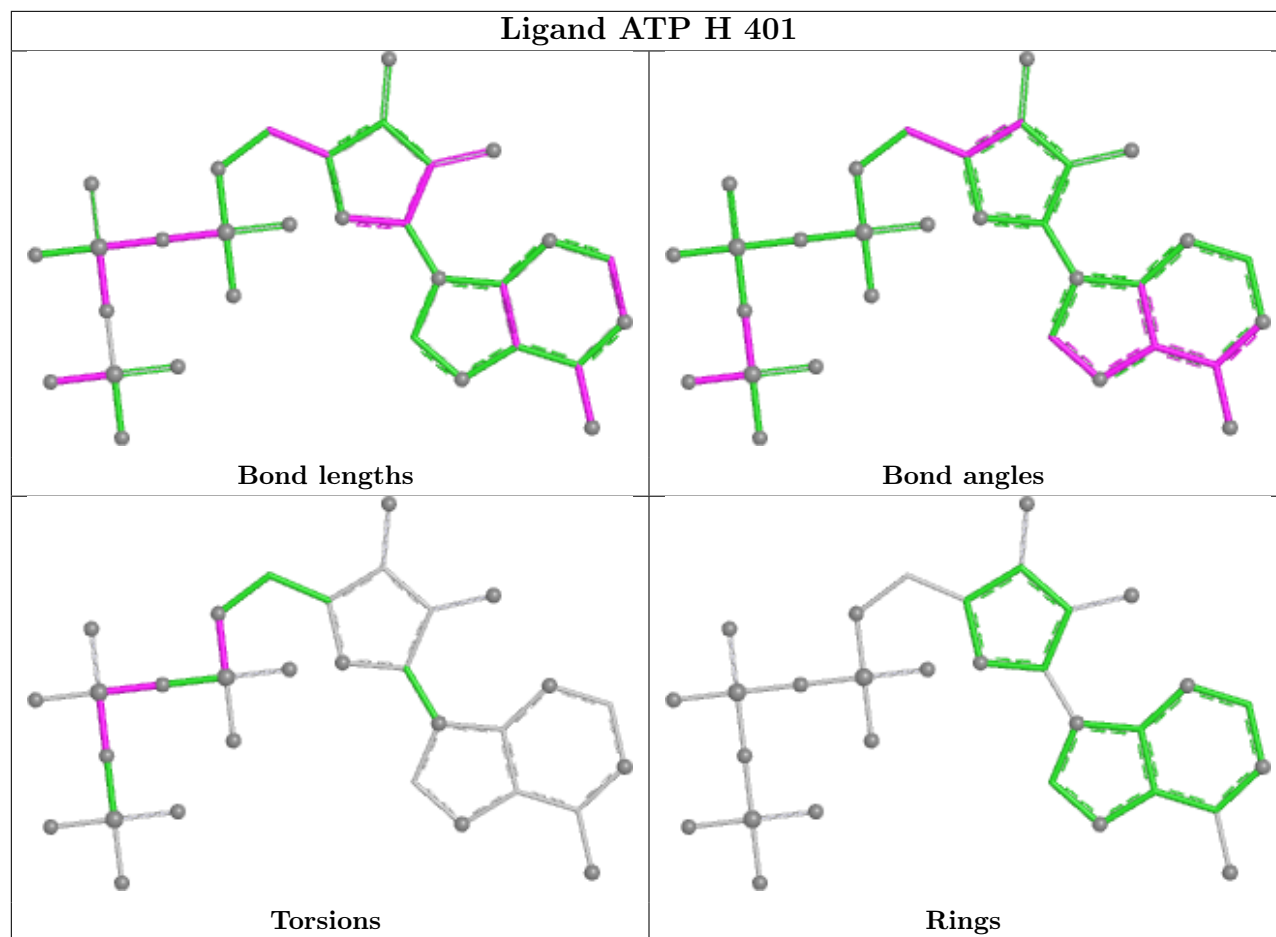
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



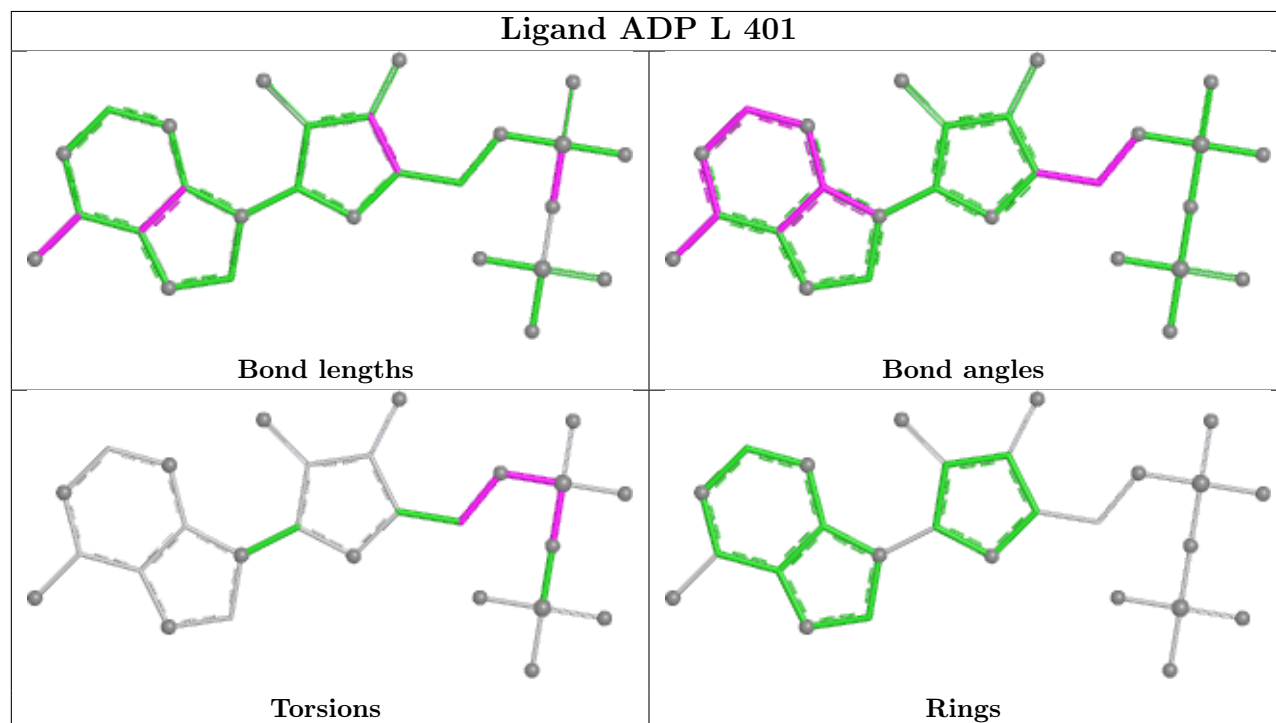




Ligand ATP H 401



Ligand ADP L 401



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0213. These allow visual inspection of the internal detail of the map and identification of artifacts.

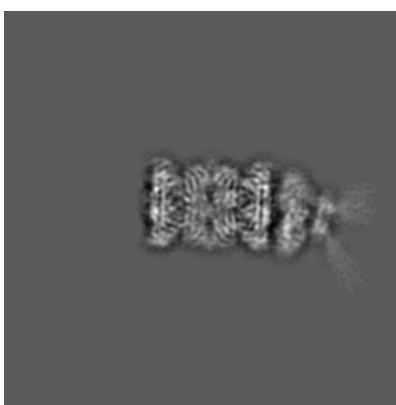
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

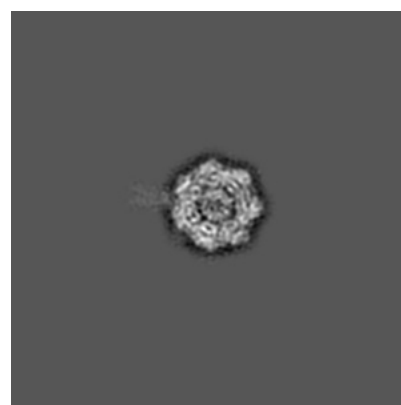
6.1.1 Primary map



X



Y

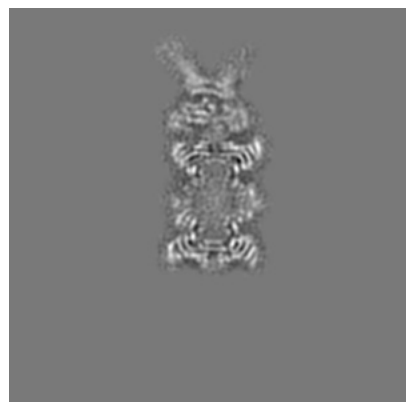


Z

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

6.2 Central slices [i](#)

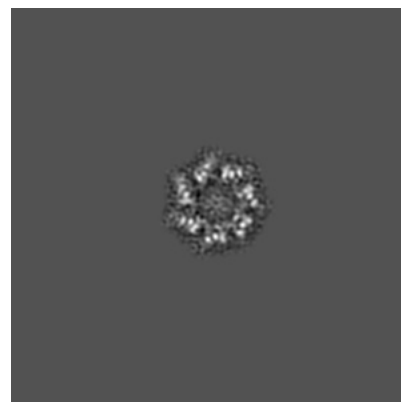
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

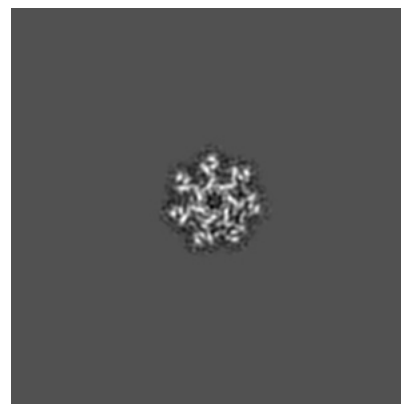
6.3.1 Primary map



X Index: 179



Y Index: 180

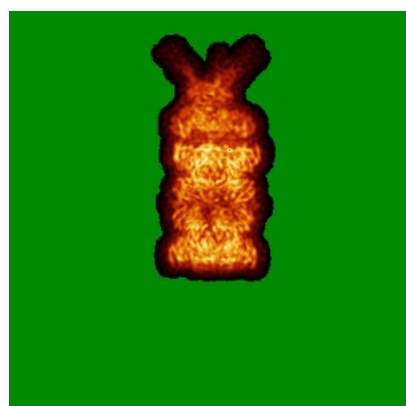


Z Index: 250

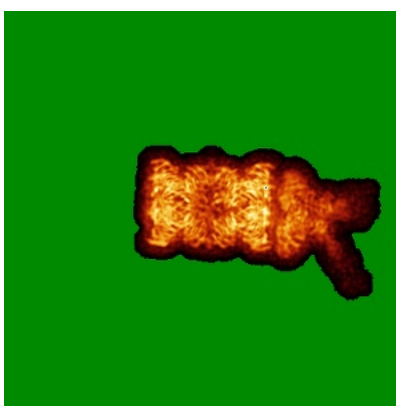
The images above show the largest variance slices of the map in three orthogonal directions.

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

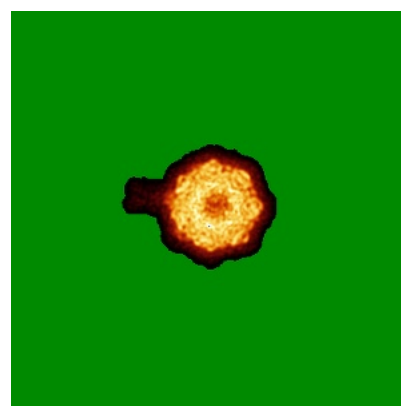
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

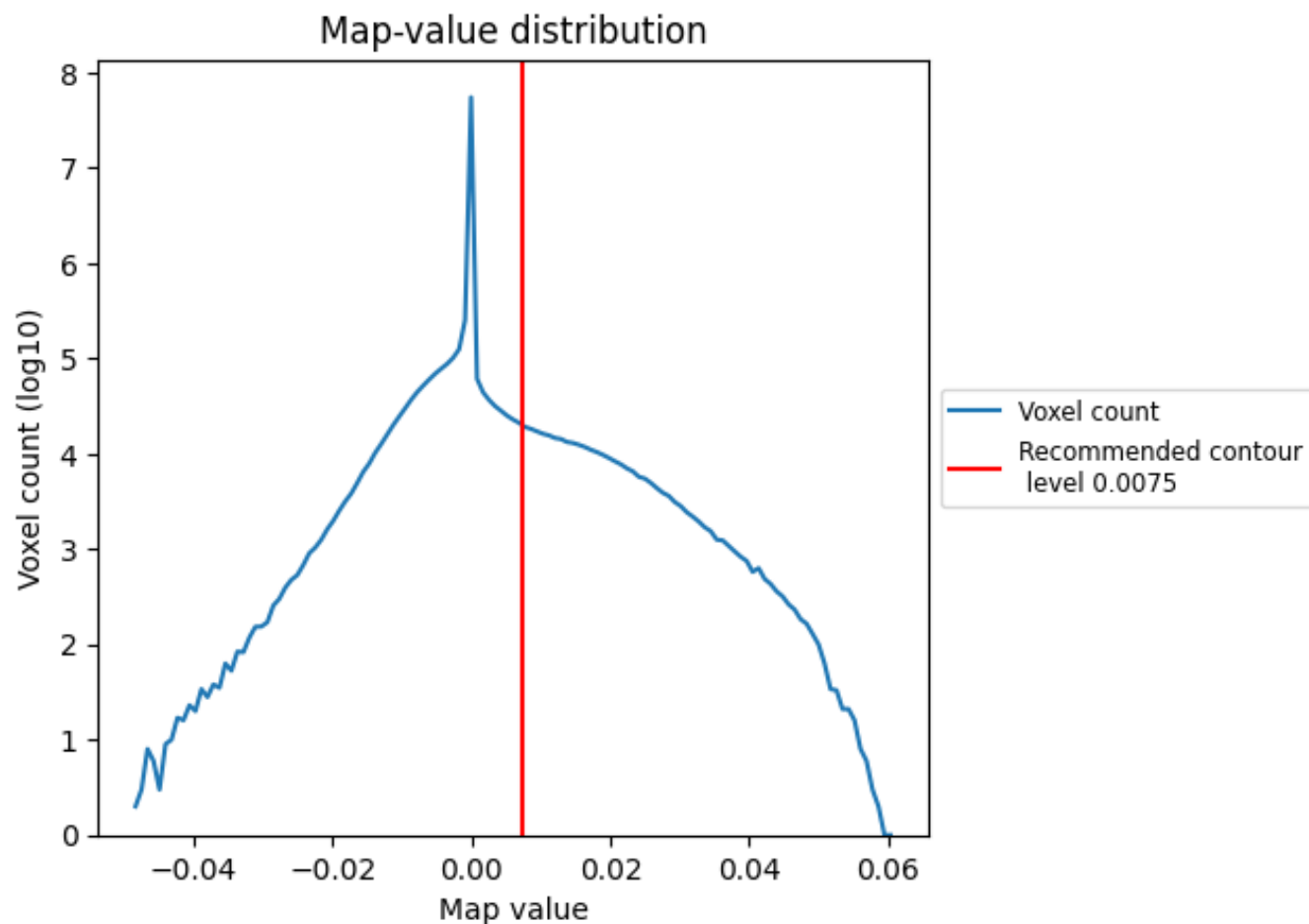
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

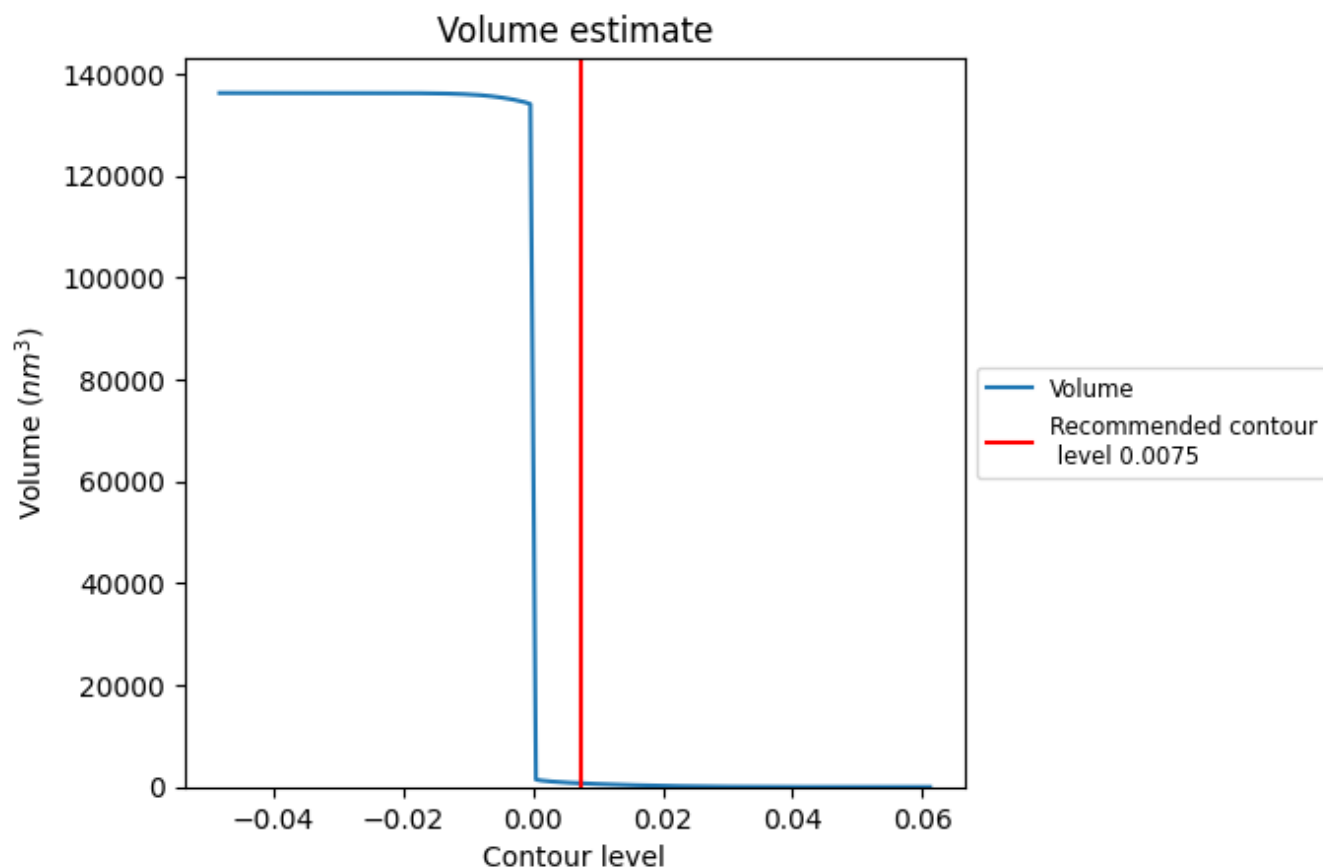
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

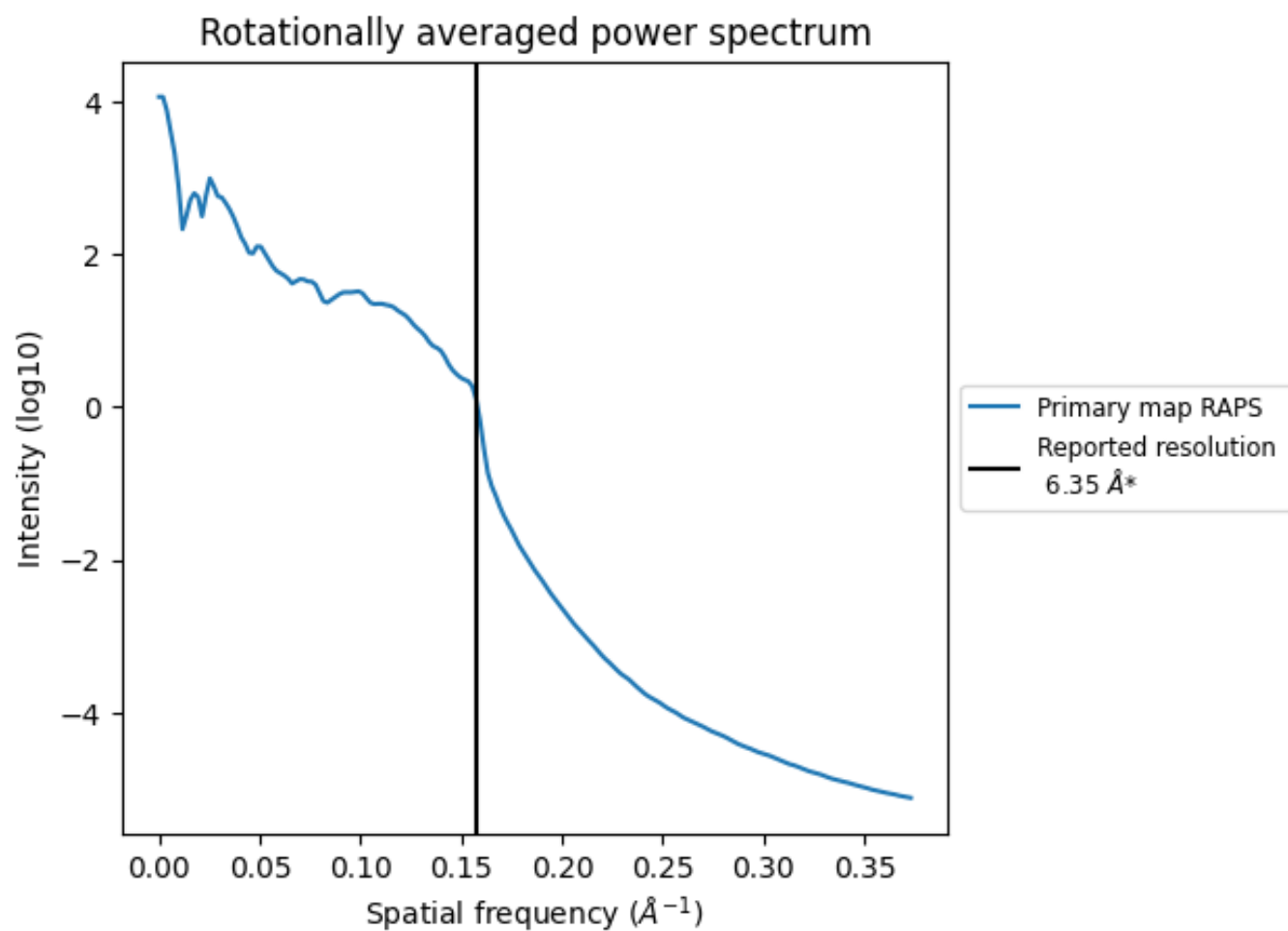
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 712 nm^3 ; this corresponds to an approximate mass of 643 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.157 Å⁻¹

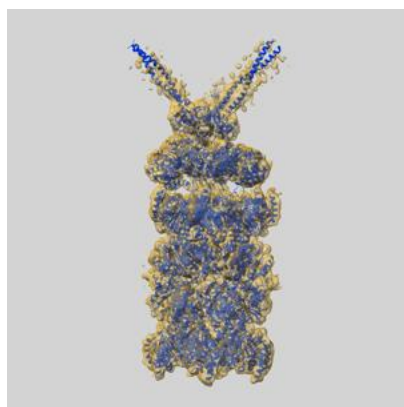
8 Fourier-Shell correlation

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

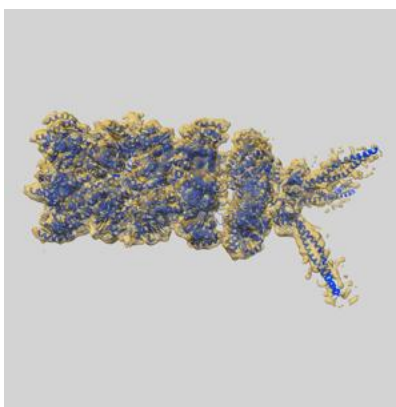
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0213 and PDB model 6HE9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

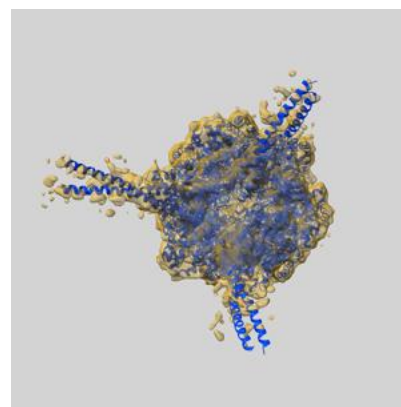
9.1 Map-model overlay [i](#)



X



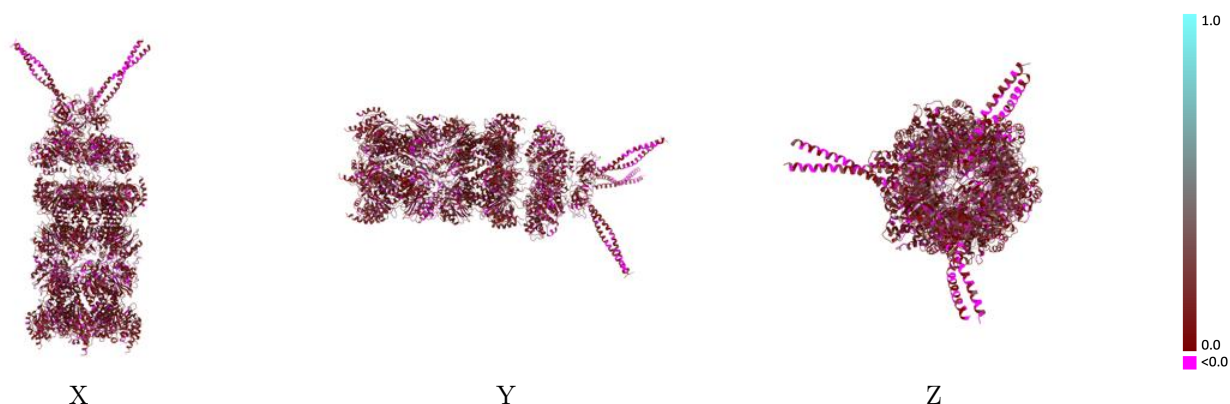
Y



Z

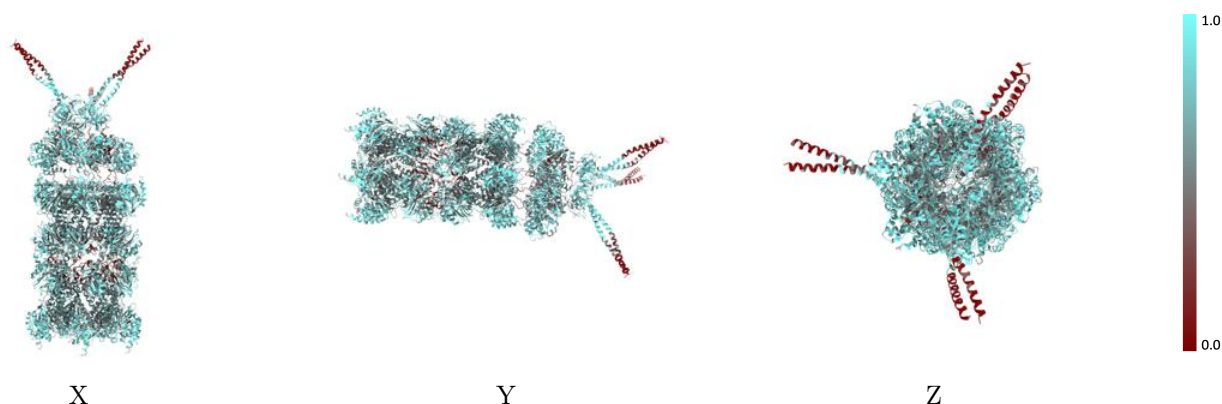
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



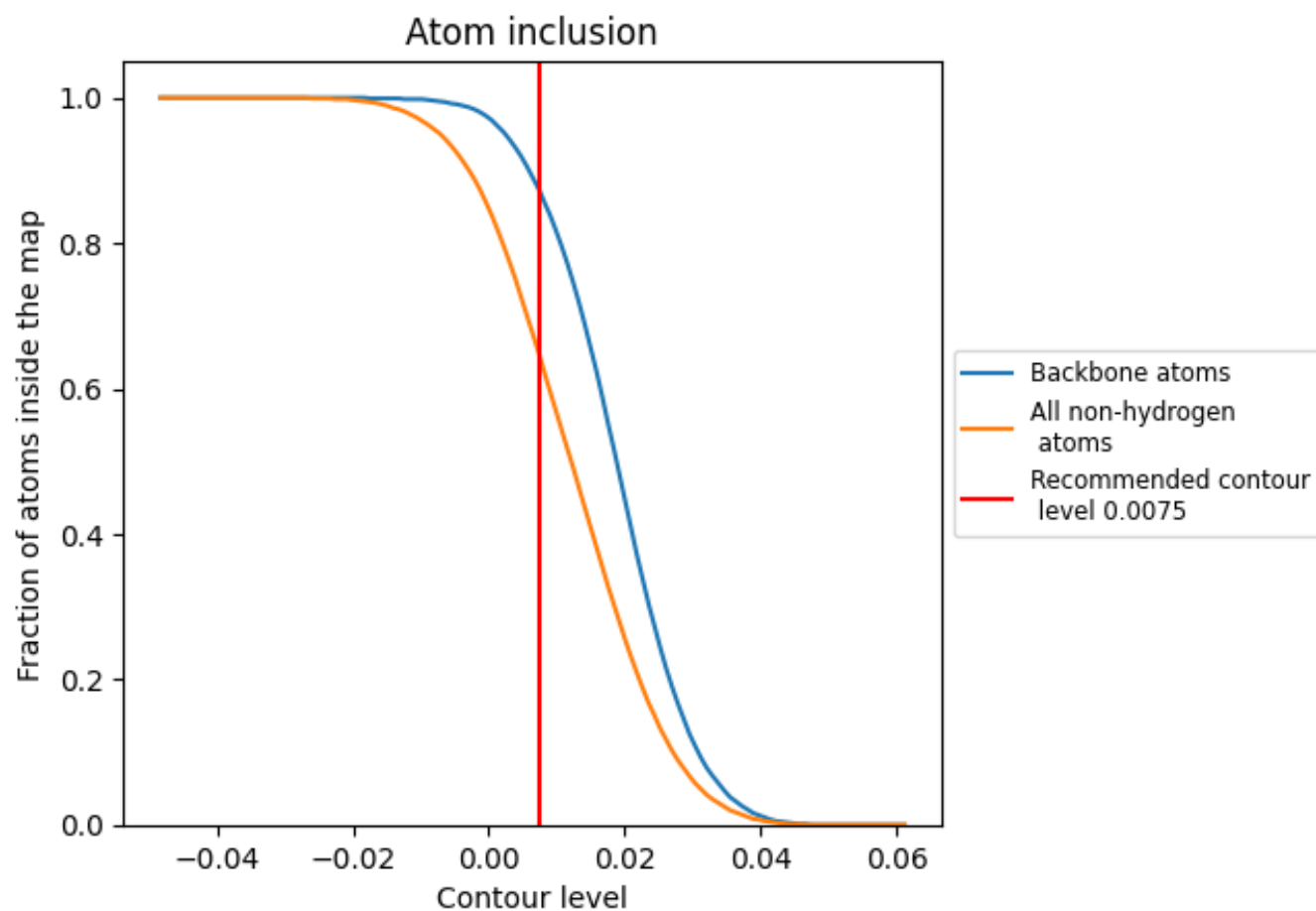
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 64% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.1230
1	 0.5980	 0.1270
2	 0.6120	 0.1290
3	 0.6270	 0.1220
4	 0.6040	 0.1280
5	 0.6220	 0.1270
6	 0.6220	 0.1300
7	 0.6120	 0.1190
A	 0.6910	 0.1380
B	 0.6840	 0.1410
C	 0.6690	 0.1330
D	 0.6750	 0.1360
E	 0.6740	 0.1380
F	 0.6860	 0.1390
G	 0.6720	 0.1350
H	 0.6500	 0.1130
I	 0.6380	 0.1080
J	 0.6510	 0.1130
K	 0.6410	 0.1130
L	 0.6220	 0.1100
M	 0.6420	 0.1160
a	 0.6800	 0.1260
b	 0.6630	 0.1280
c	 0.6730	 0.1300
d	 0.6770	 0.1320
e	 0.6750	 0.1360
f	 0.6680	 0.1230
g	 0.6790	 0.1320
h	 0.6100	 0.1110
i	 0.6030	 0.1170
j	 0.6090	 0.1140
k	 0.6100	 0.1070
l	 0.6060	 0.1200
m	 0.6050	 0.1100
n	 0.6020	 0.1110

