



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:06 PM UTC

PDB ID : 6HE8 / pdb_00006he8
EMDB ID : EMD-0212
Title : PAN-proteasome in state 1
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 6.86 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:

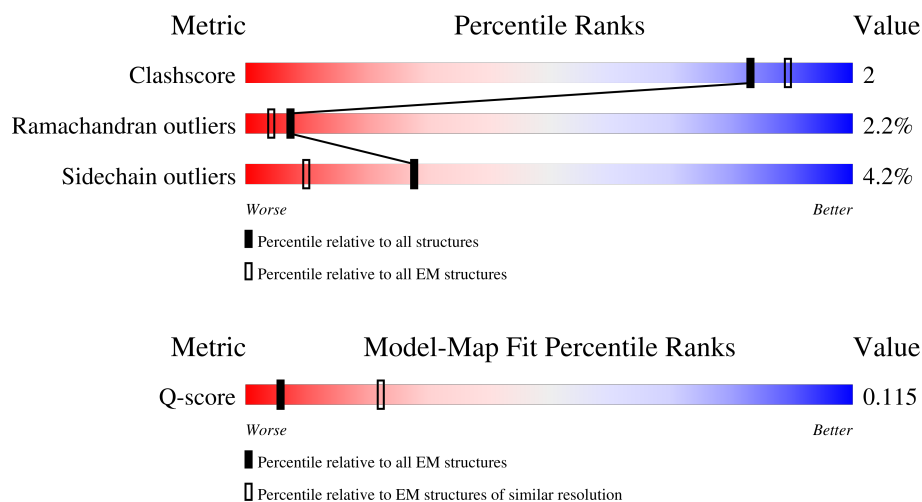
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.86 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	457 (6.36 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	A	242	8% 47% 46% 6%
1	B	242	6% 43% 51% 5%
1	C	242	7% 45% 48% 6%
1	D	242	7% 44% 49% 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	24% 39% 49% 10%
3	J	390	24% 39% 51% 10%
3	K	390	23% 39% 51% 9%
3	L	390	30% 36% 54% 10%
3	M	390	30% 44% 47% 7%

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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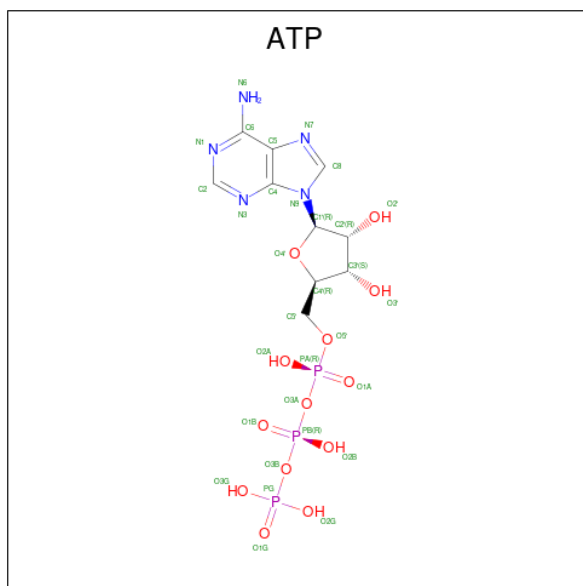
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	i	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	j	202	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: $C_{10}H_{16}N_5O_{13}P_3$).

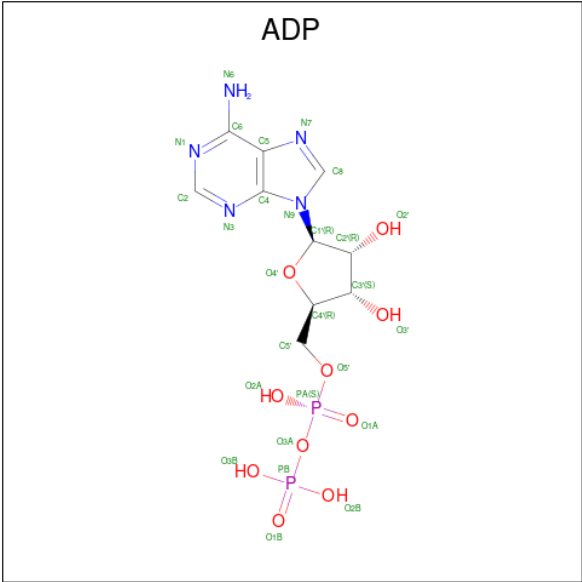


Mol	Chain	Residues	Atoms					AltConf
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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

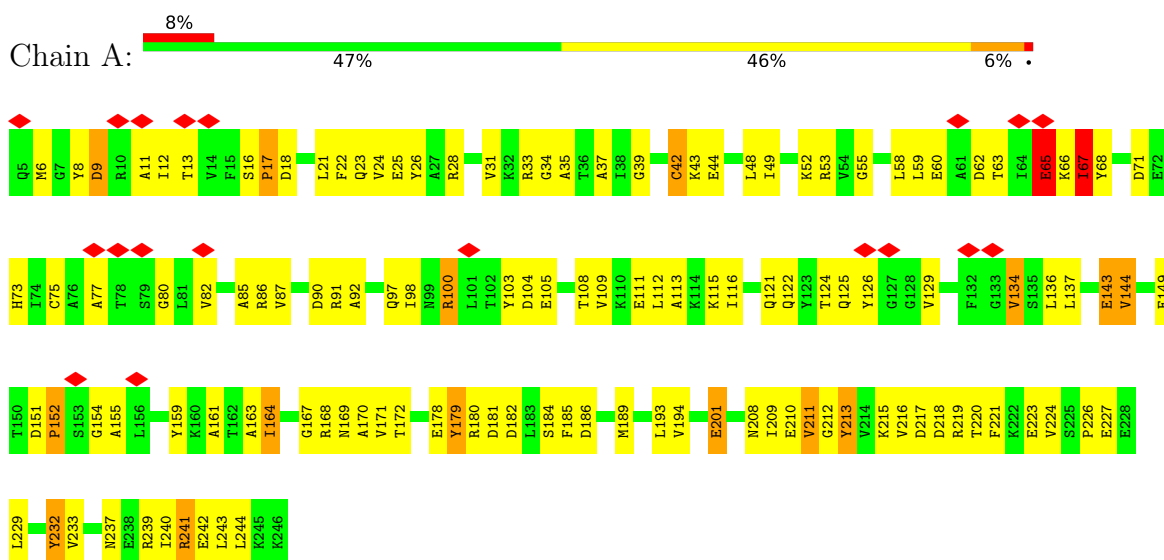


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	M	1	27	10	5	10	2	0

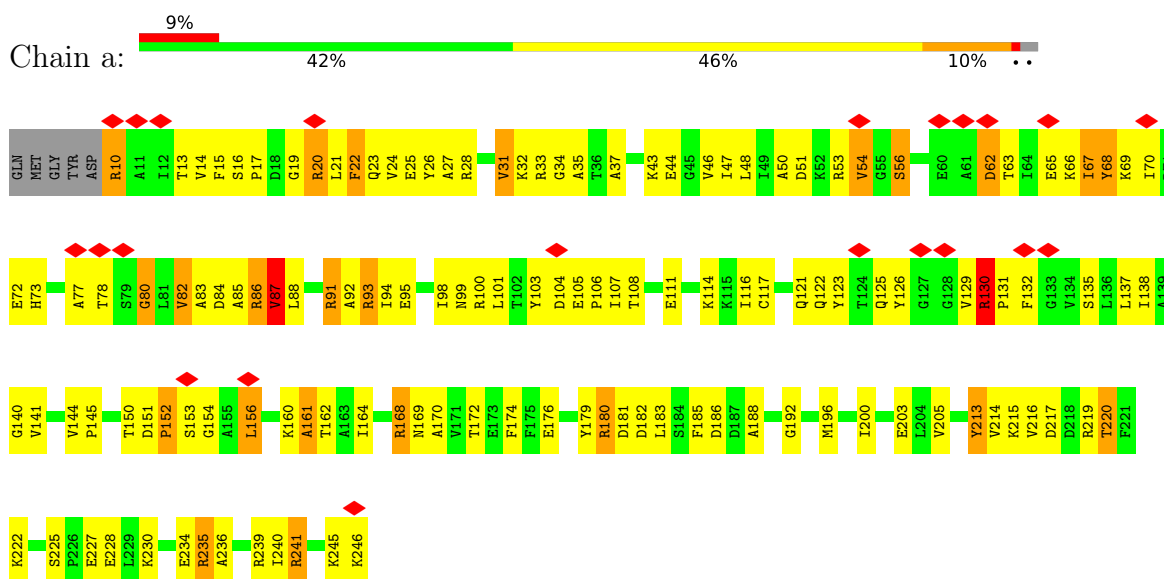
3 Residue-property plots

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

- Molecule 1: Proteasome subunit alpha

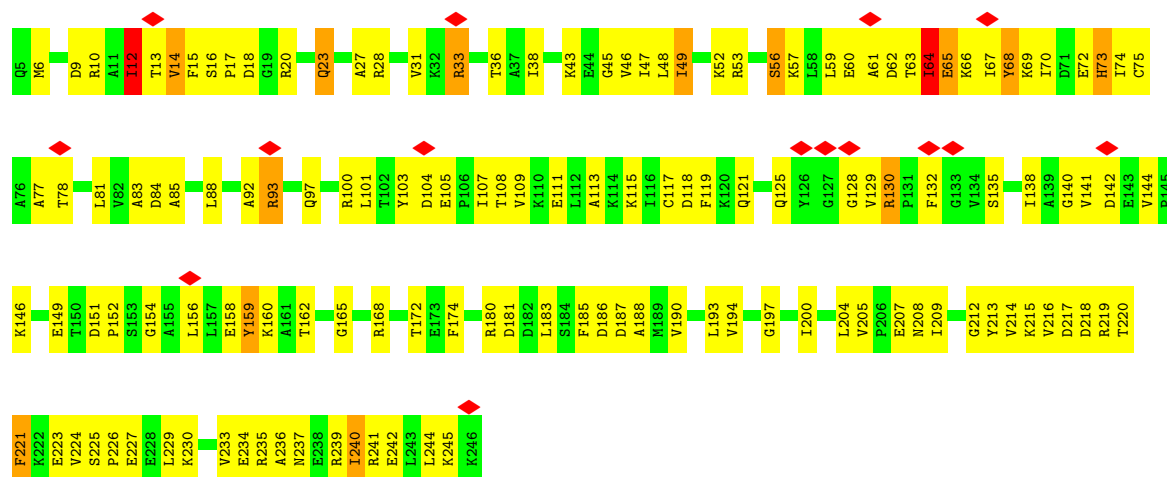


- Molecule 1: Proteasome subunit alpha



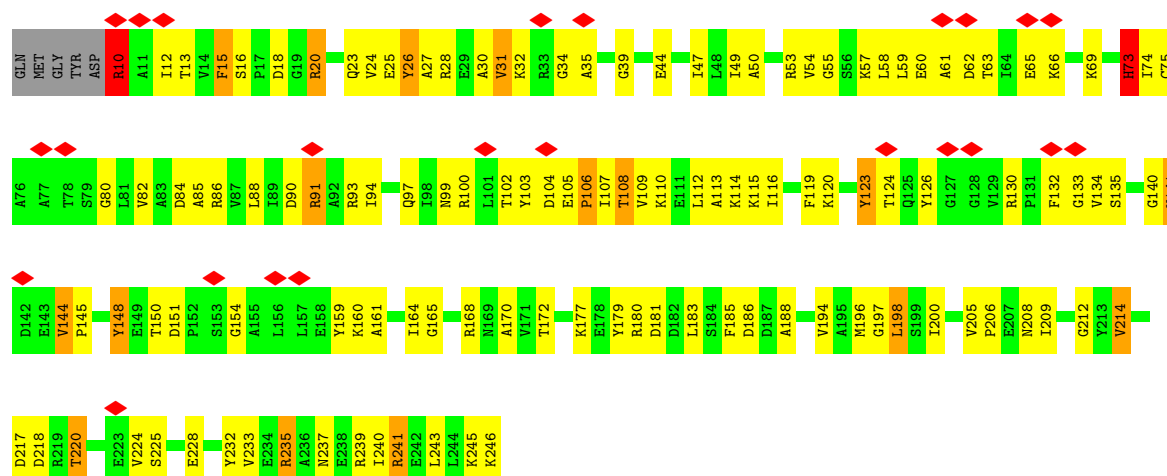
- Molecule 1: Proteasome subunit alpha

Chain B: 



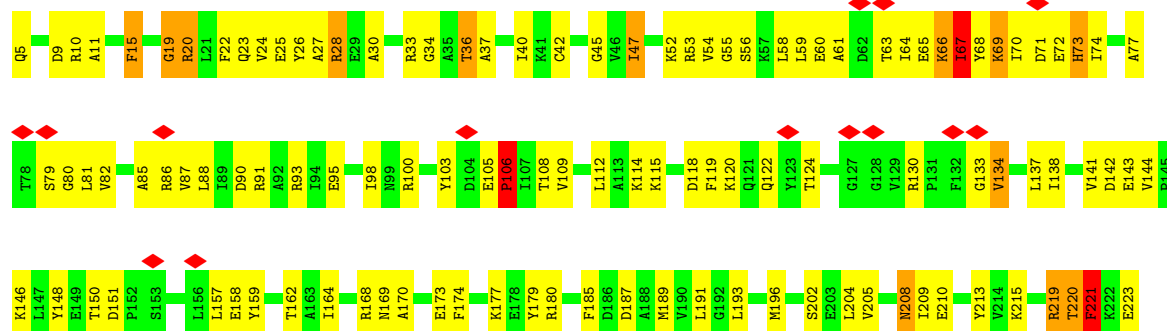
• Molecule 1: Proteasome subunit alpha

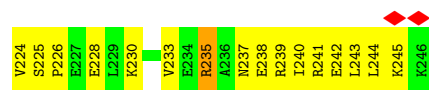
Chain b: 



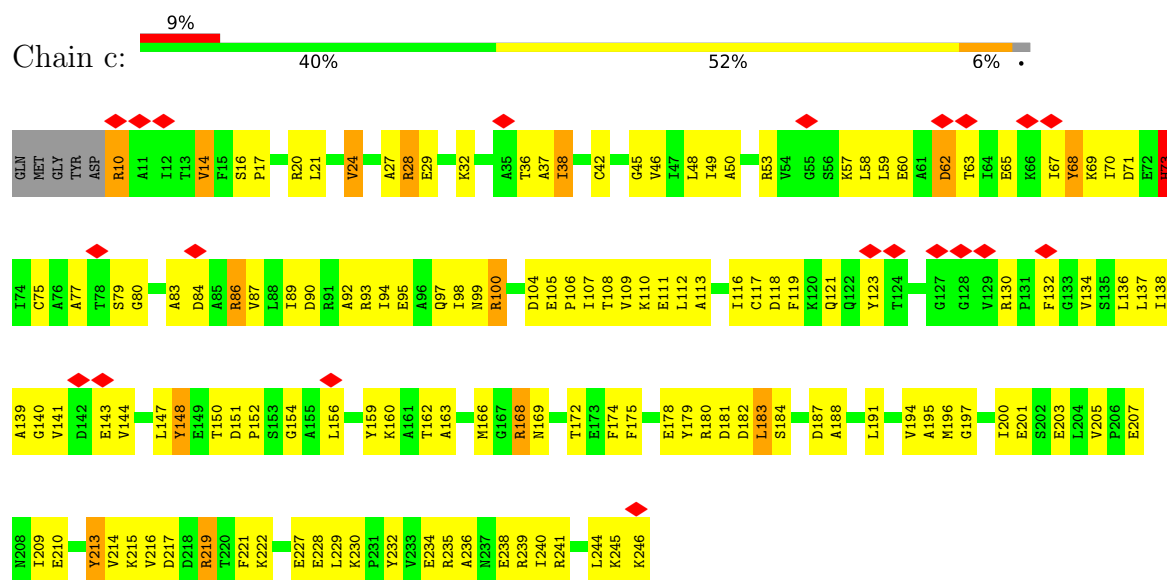
• Molecule 1: Proteasome subunit alpha

Chain C: 

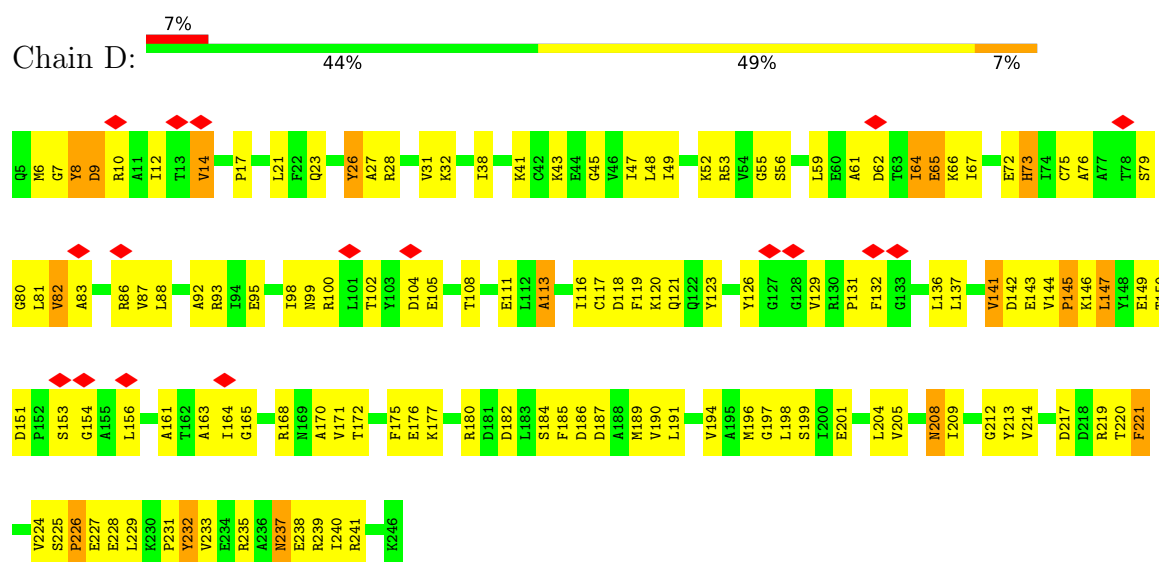




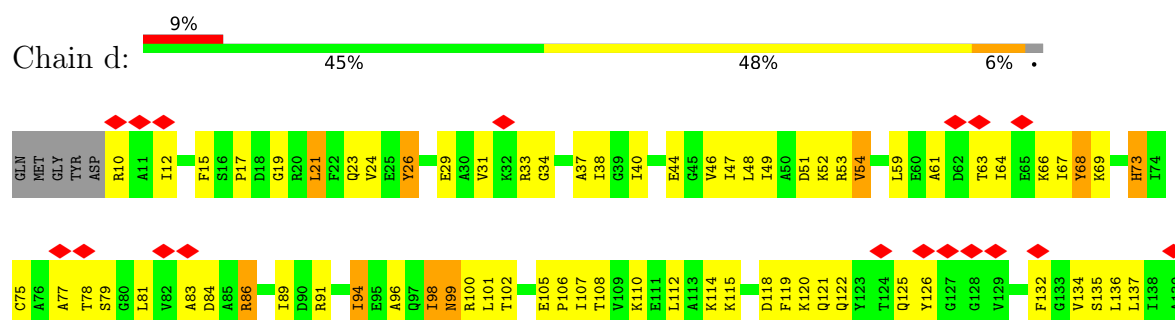
• Molecule 1: Proteasome subunit alpha

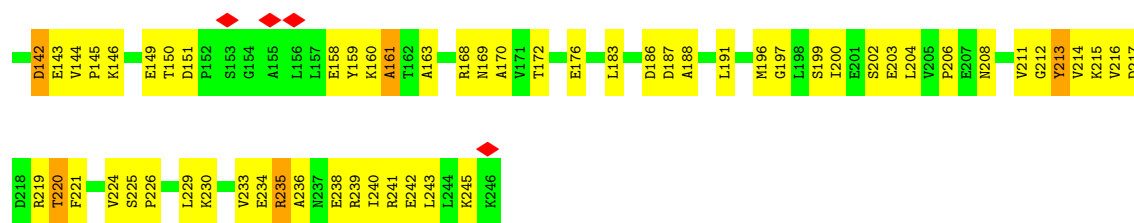


• Molecule 1: Proteasome subunit alpha

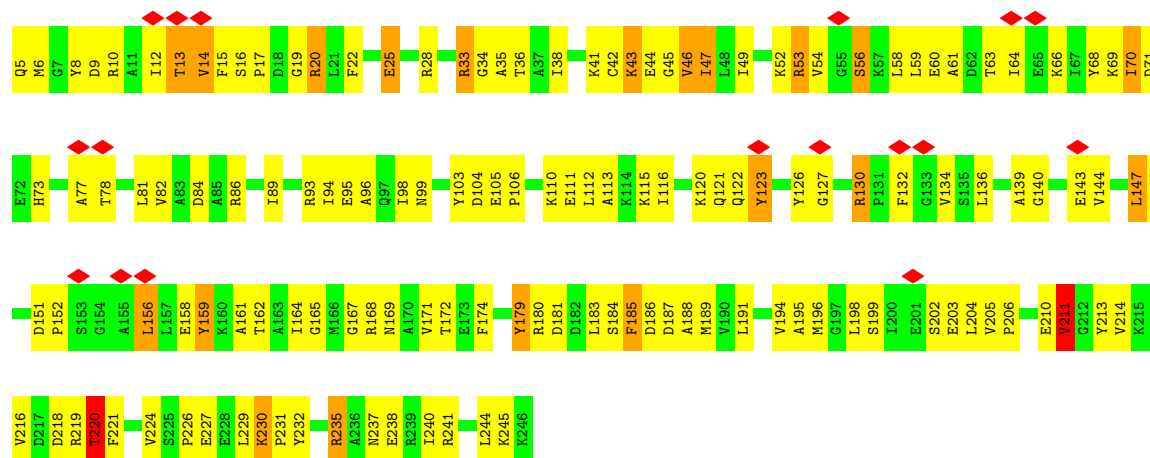


• Molecule 1: Proteasome subunit alpha

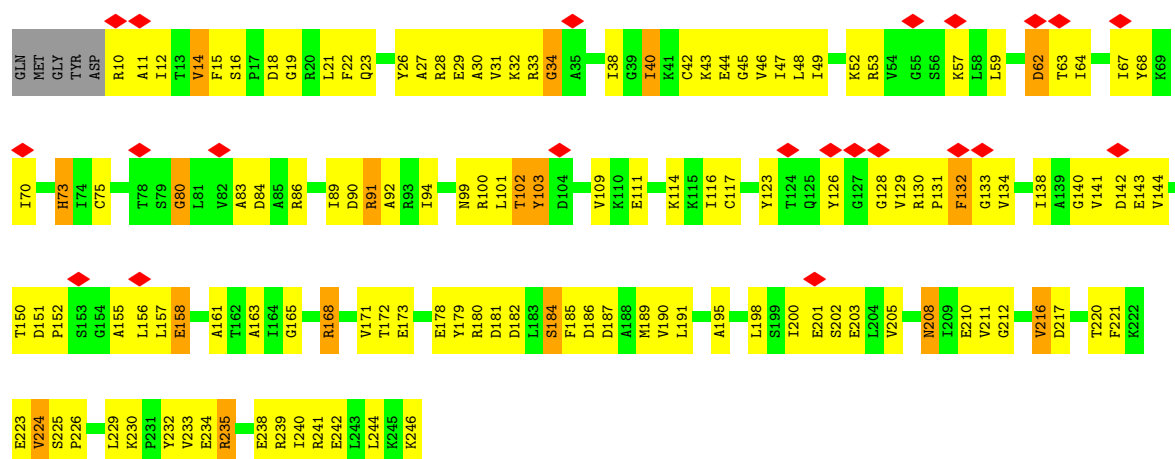
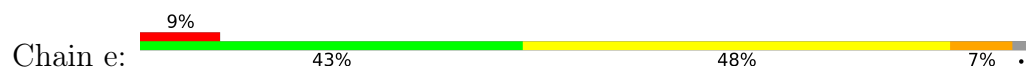




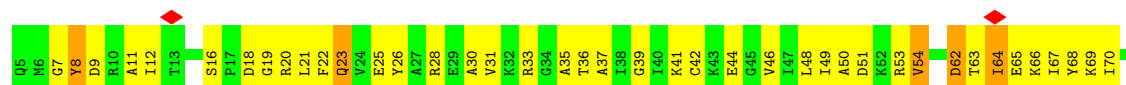
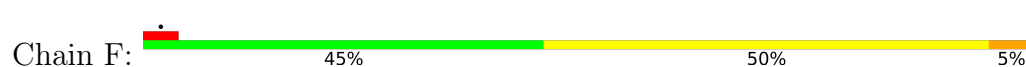
• Molecule 1: Proteasome subunit alpha

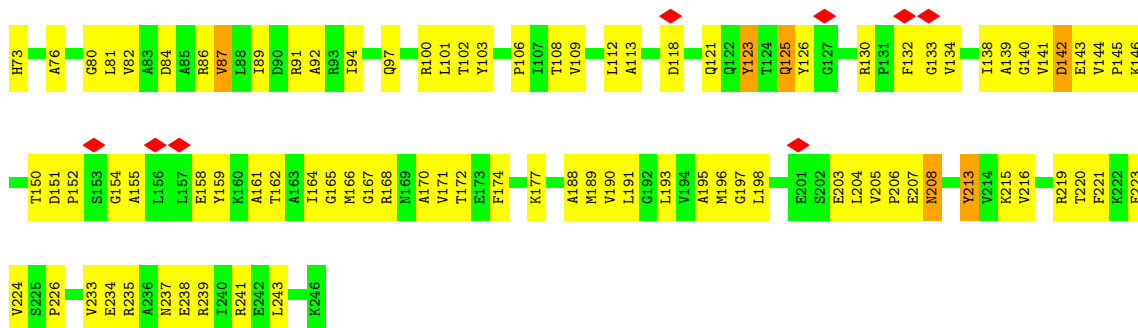


• Molecule 1: Proteasome subunit alpha

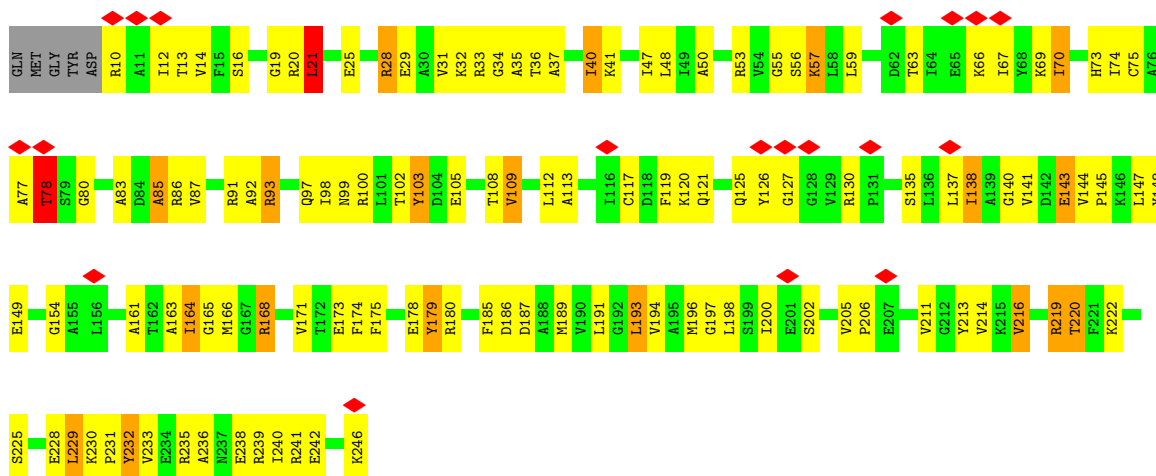


• Molecule 1: Proteasome subunit alpha

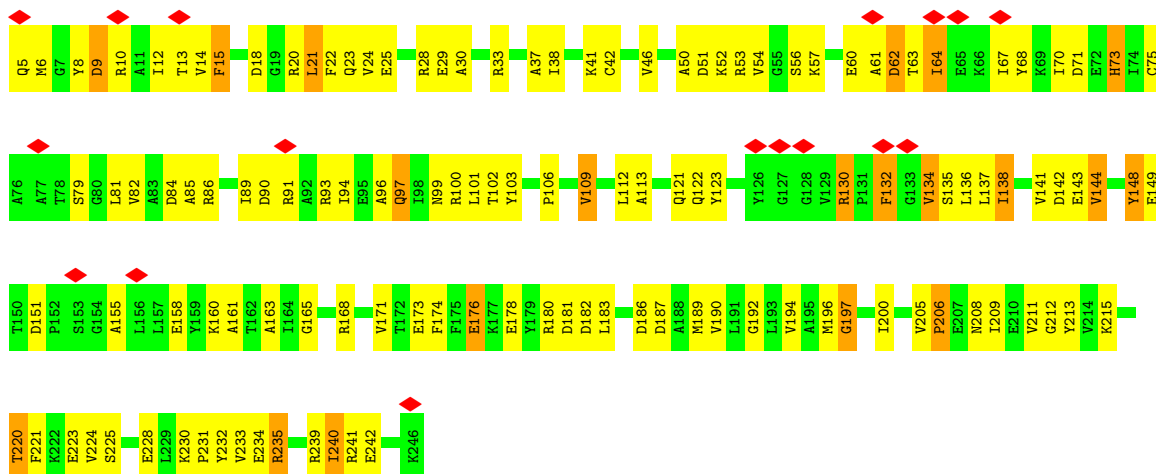




• Molecule 1: Proteasome subunit alpha

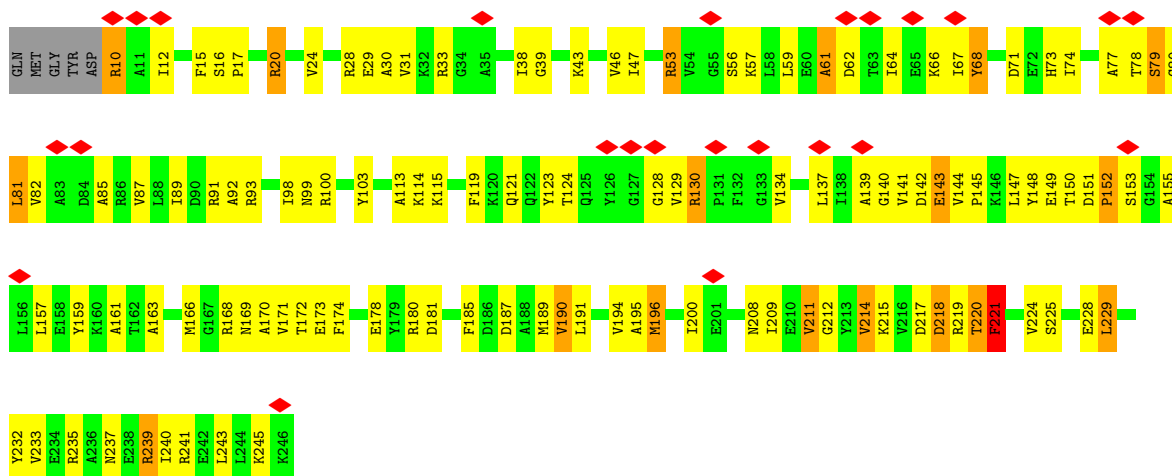


• Molecule 1: Proteasome subunit alpha

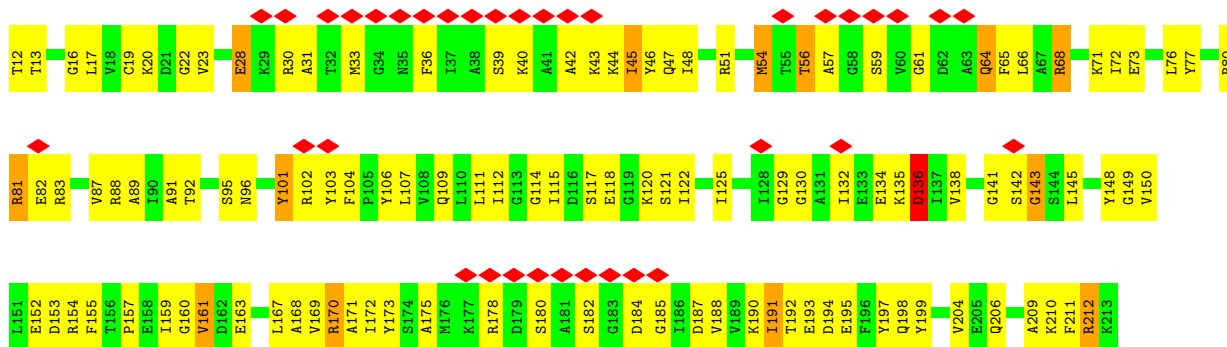
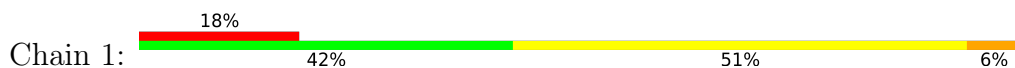


• Molecule 1: Proteasome subunit alpha

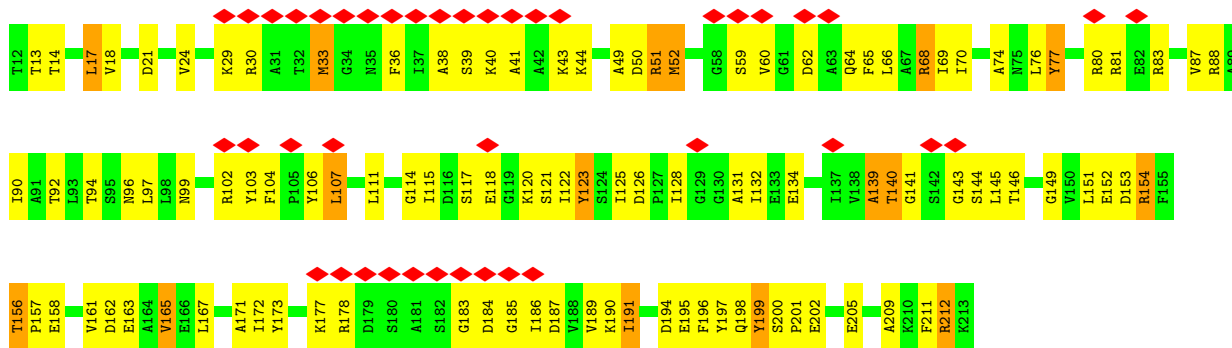




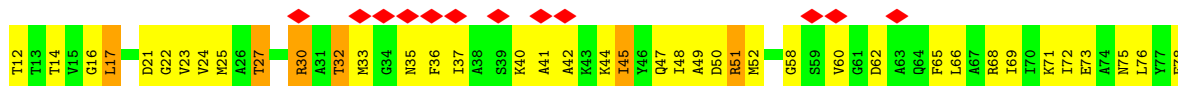
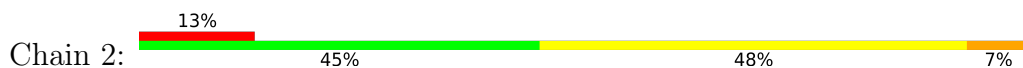
• Molecule 2: Proteasome subunit beta

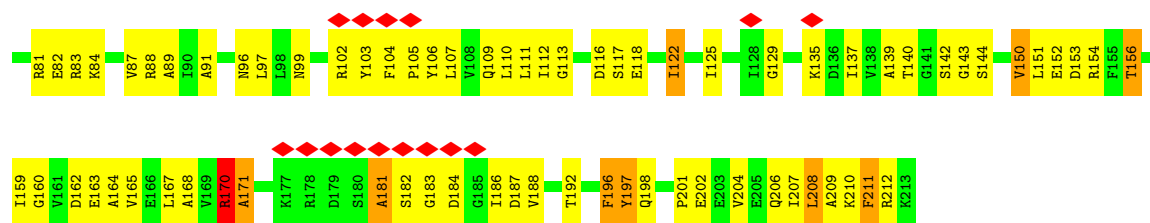


• Molecule 2: Proteasome subunit beta

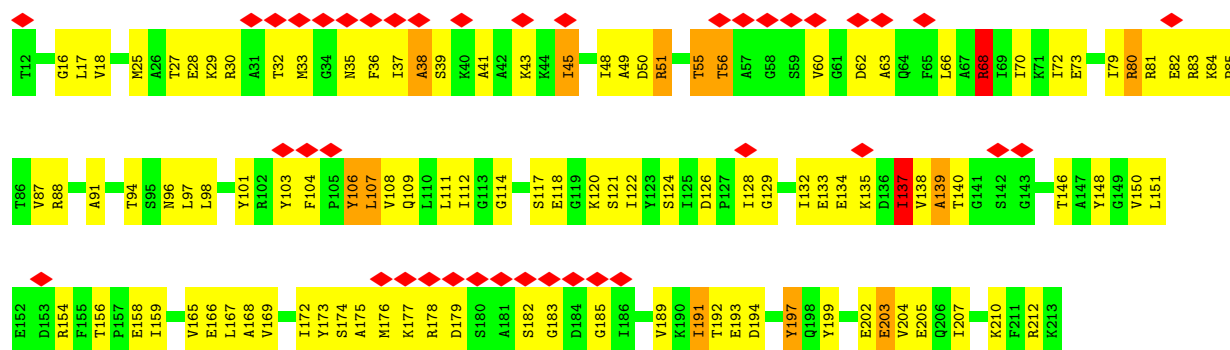
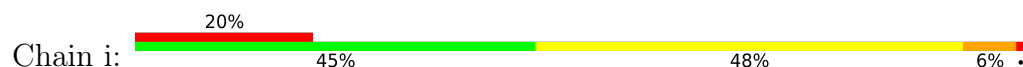


• Molecule 2: Proteasome subunit beta

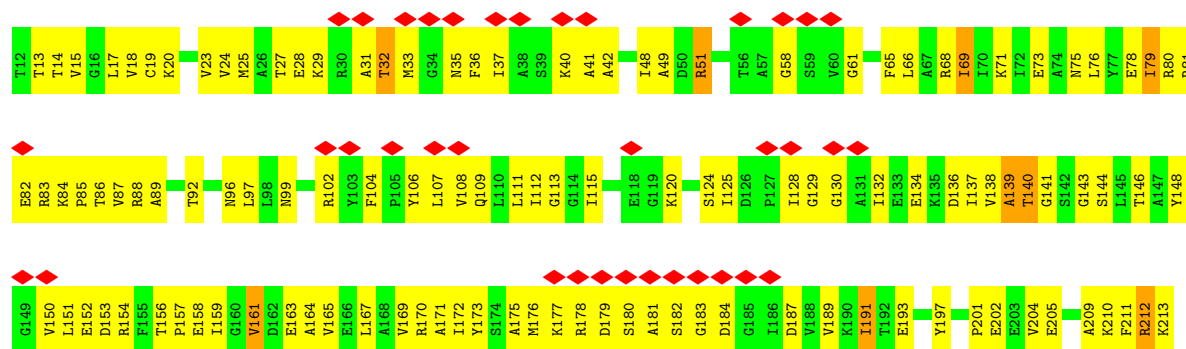




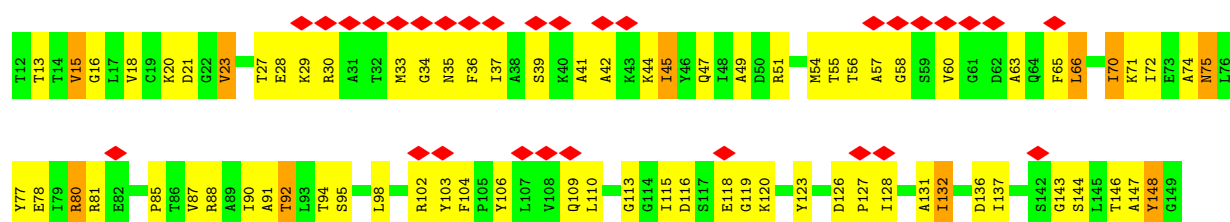
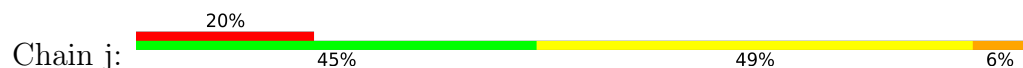
• Molecule 2: Proteasome subunit beta

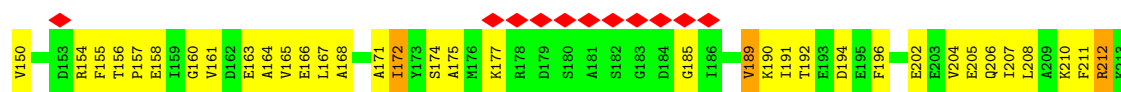


• Molecule 2: Proteasome subunit beta

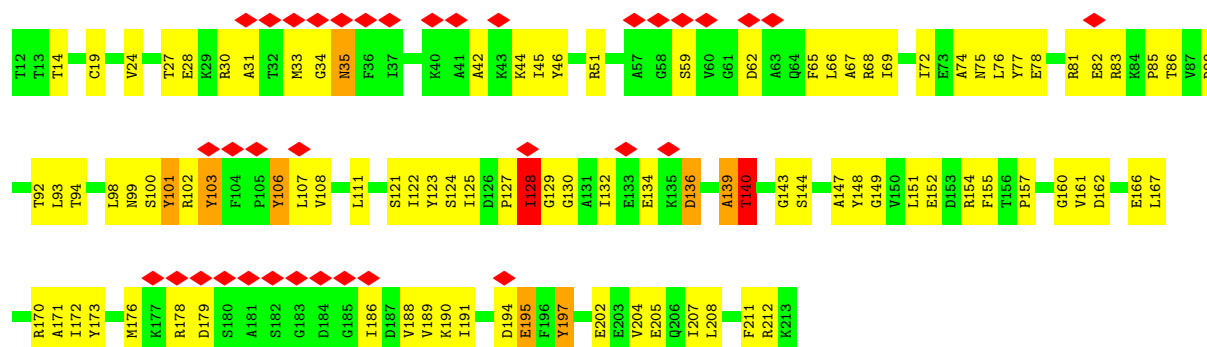


• Molecule 2: Proteasome subunit beta

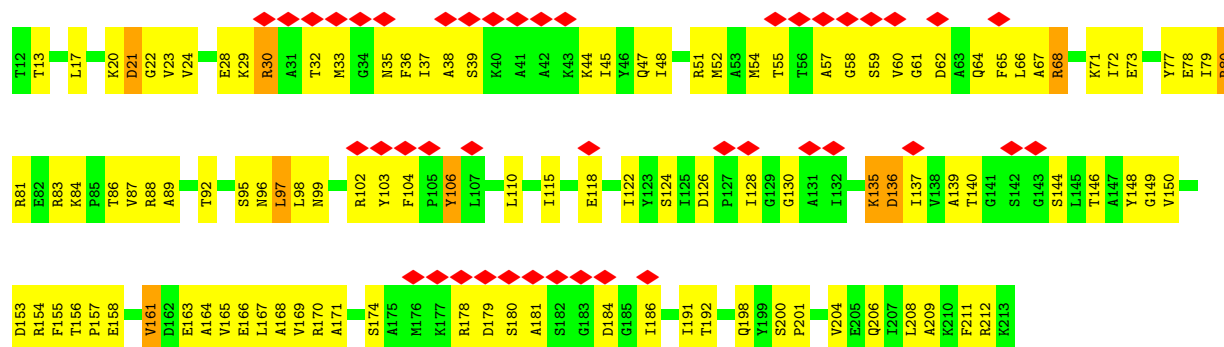
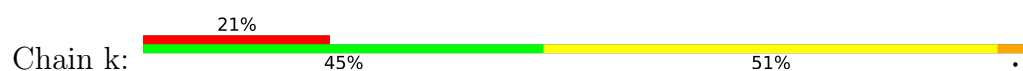




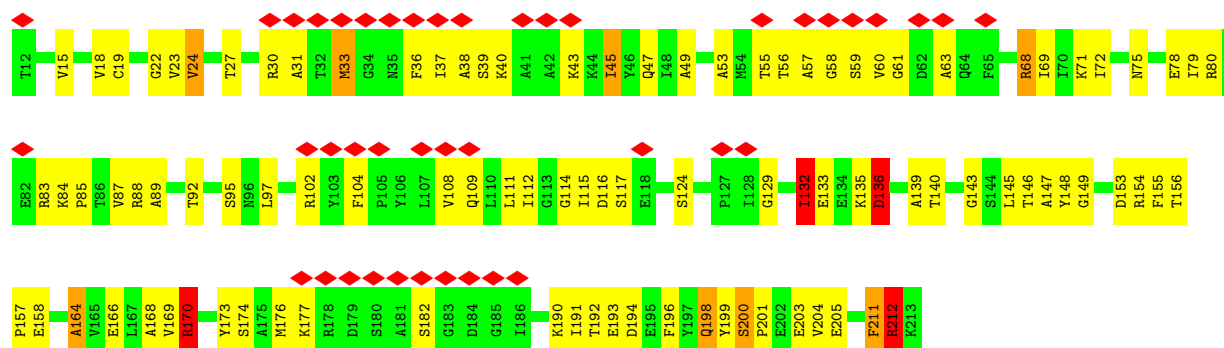
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

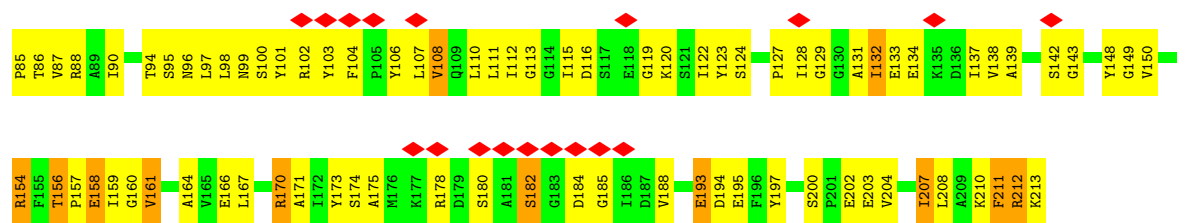


- Molecule 2: Proteasome subunit beta

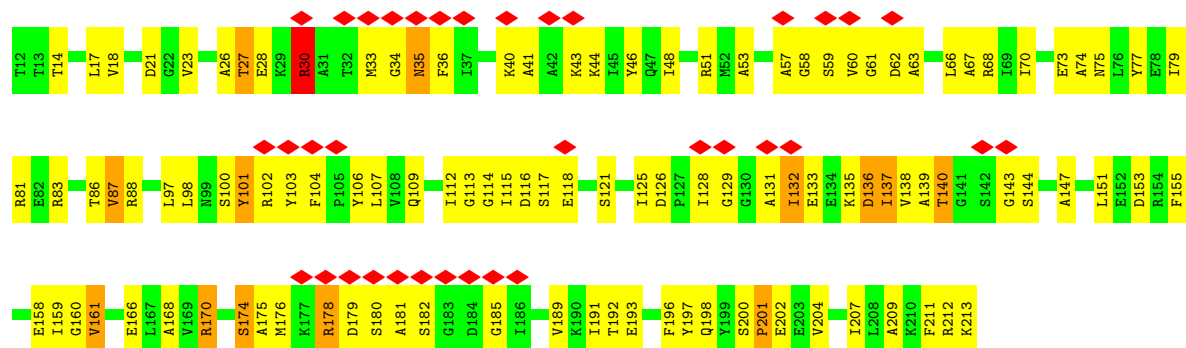


- Molecule 2: Proteasome subunit beta

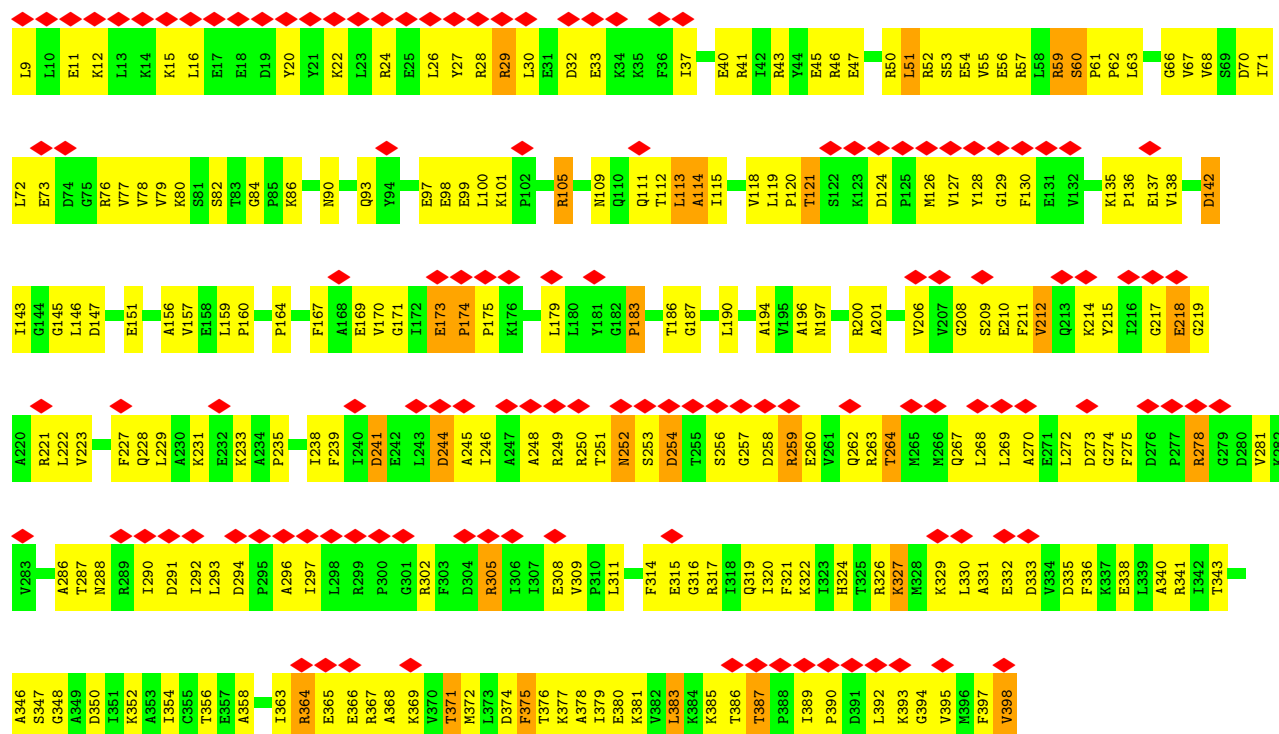
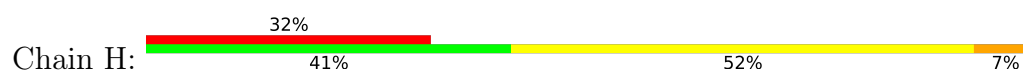




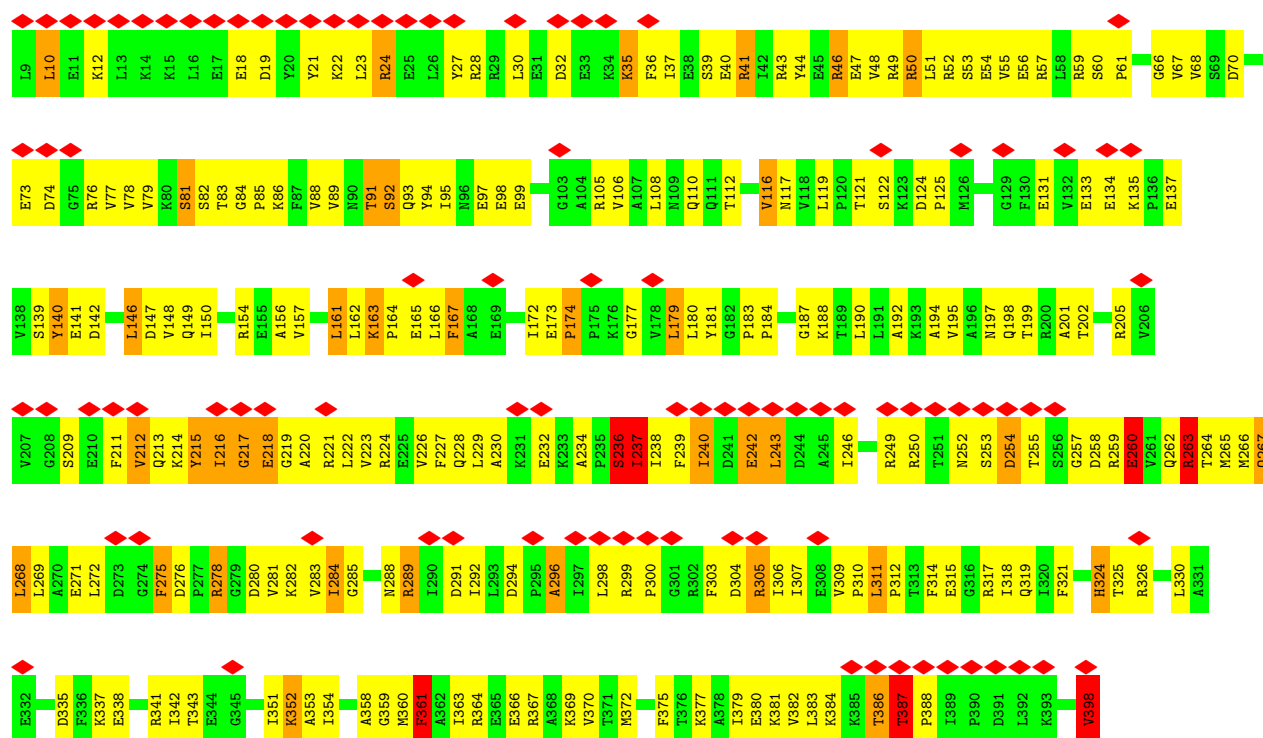
• Molecule 2: Proteasome subunit beta



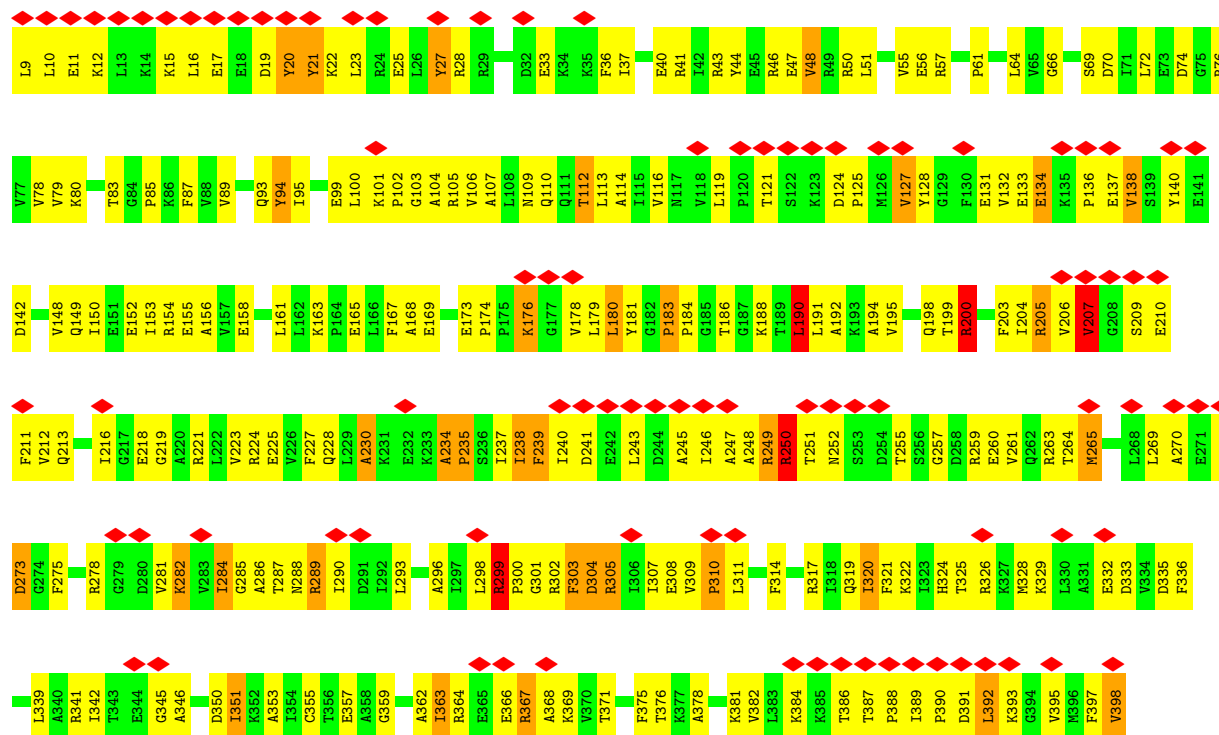
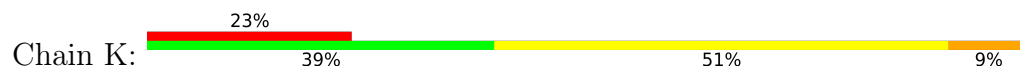
• Molecule 3: Proteasome-activating nucleotidase



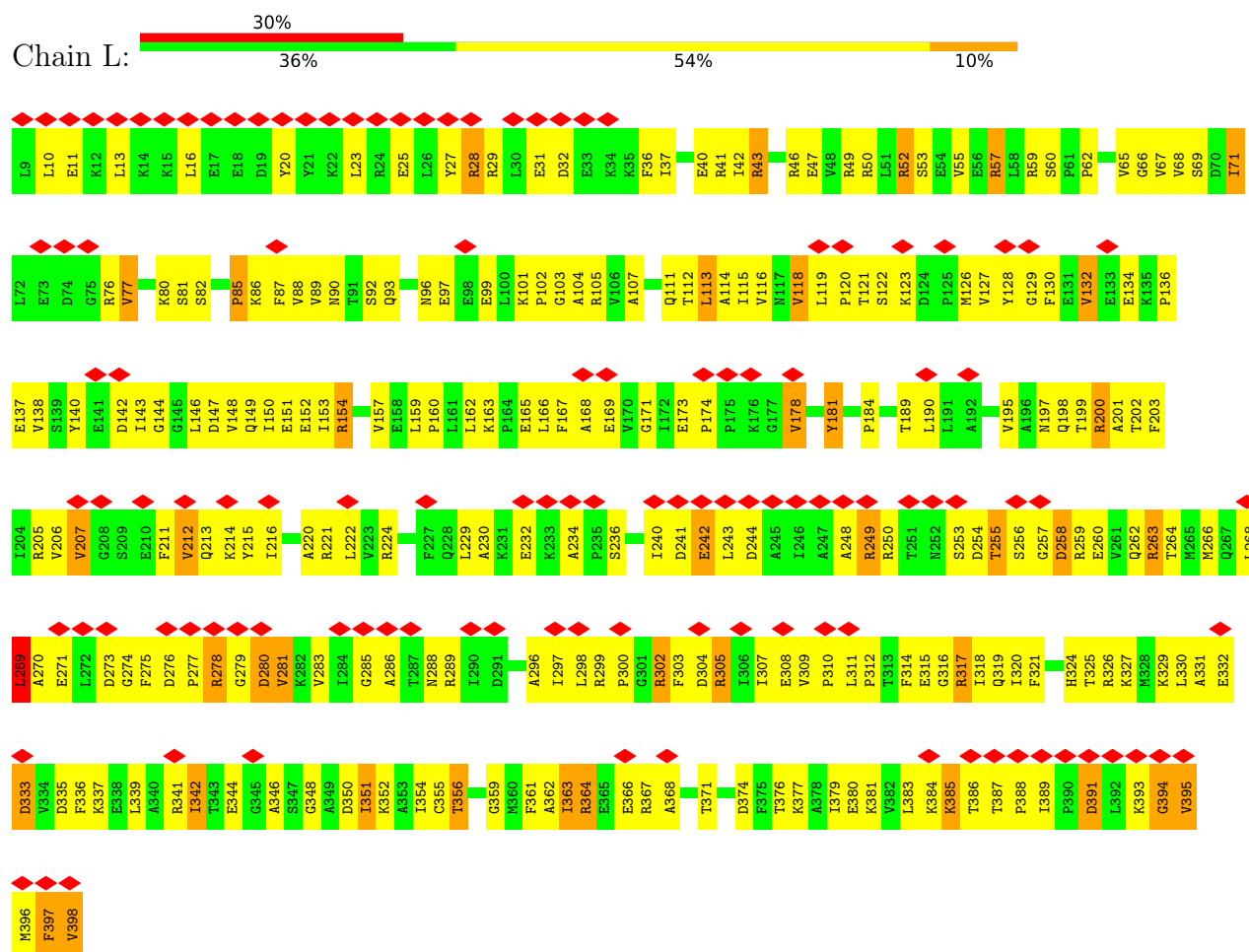
• Molecule 3: Proteasome-activating nucleotidase



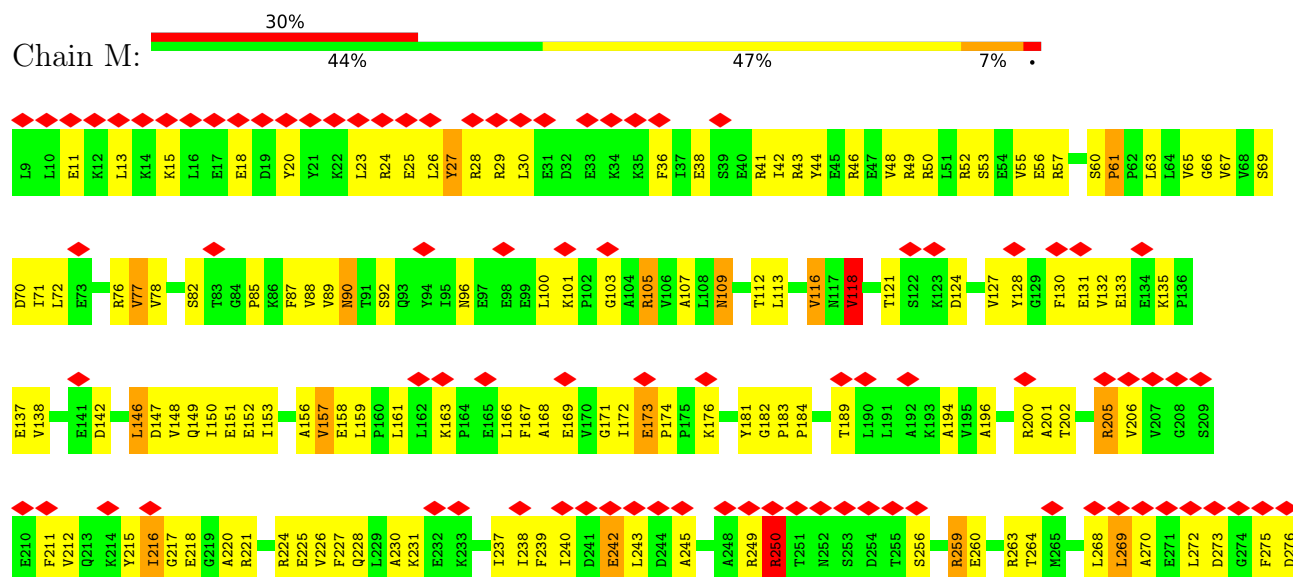
• Molecule 3: Proteasome-activating nucleotidase

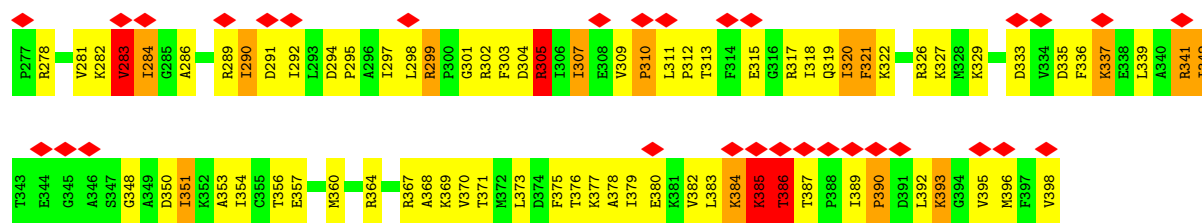


- Molecule 3: Proteasome-activating nucleotidase

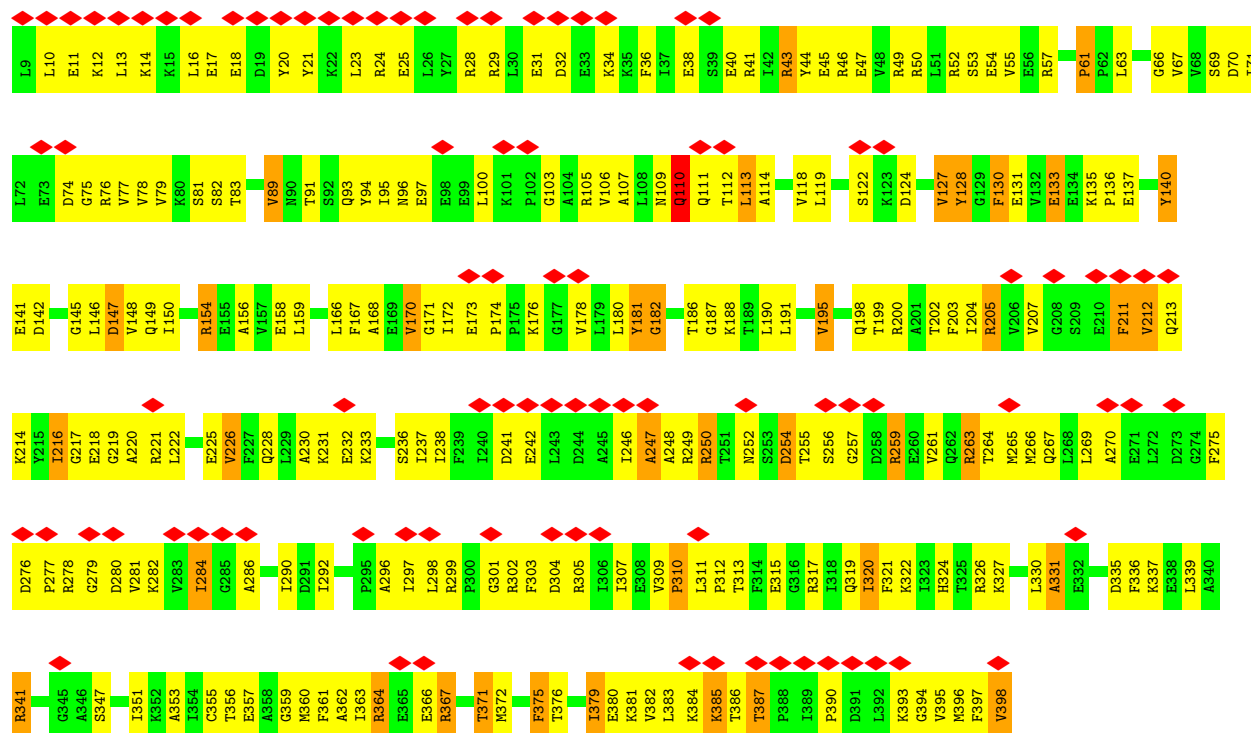


- Molecule 3: Proteasome-activating nucleotidase





• 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	38230	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	0.043	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.23	71/1934 (3.7%)	2.44	107/2605 (4.1%)
1	B	2.27	74/1934 (3.8%)	2.41	145/2605 (5.6%)
1	C	2.32	87/1934 (4.5%)	2.40	105/2605 (4.0%)
1	D	2.22	61/1934 (3.2%)	2.46	123/2605 (4.7%)
1	E	2.28	67/1934 (3.5%)	2.43	120/2605 (4.6%)
1	F	2.28	77/1934 (4.0%)	2.38	104/2605 (4.0%)
1	G	2.25	70/1934 (3.6%)	2.42	112/2605 (4.3%)
1	a	2.27	70/1892 (3.7%)	2.46	131/2549 (5.1%)
1	b	2.29	75/1892 (4.0%)	2.37	112/2549 (4.4%)
1	c	2.22	72/1892 (3.8%)	2.47	130/2549 (5.1%)
1	d	2.30	75/1892 (4.0%)	2.41	110/2549 (4.3%)
1	e	2.23	74/1892 (3.9%)	2.41	122/2549 (4.8%)
1	f	2.25	63/1892 (3.3%)	2.43	116/2549 (4.6%)
1	g	2.28	73/1892 (3.9%)	2.43	107/2549 (4.2%)
2	1	2.38	71/1573 (4.5%)	2.45	110/2121 (5.2%)
2	2	2.27	65/1573 (4.1%)	2.36	87/2121 (4.1%)
2	3	2.35	75/1573 (4.8%)	2.47	111/2121 (5.2%)
2	4	2.28	56/1573 (3.6%)	2.37	69/2121 (3.3%)
2	5	3.12	55/1573 (3.5%)	2.50	105/2121 (5.0%)
2	6	2.22	58/1573 (3.7%)	2.47	93/2121 (4.4%)
2	7	2.37	78/1573 (5.0%)	2.44	105/2121 (5.0%)
2	h	2.31	59/1573 (3.8%)	2.42	99/2121 (4.7%)
2	i	2.33	66/1573 (4.2%)	2.38	93/2121 (4.4%)
2	j	2.29	70/1573 (4.5%)	2.43	101/2121 (4.8%)
2	k	2.30	67/1573 (4.3%)	2.45	110/2121 (5.2%)
2	l	3.14	64/1573 (4.1%)	2.56	129/2121 (6.1%)
2	m	2.38	69/1573 (4.4%)	2.42	95/2121 (4.5%)
2	n	2.21	55/1573 (3.5%)	2.41	94/2121 (4.4%)
3	H	2.27	129/3146 (4.1%)	2.43	209/4240 (4.9%)
3	I	2.28	115/3146 (3.7%)	2.51	244/4240 (5.8%)
3	J	2.25	110/3146 (3.5%)	2.50	244/4240 (5.8%)
3	K	2.27	114/3146 (3.6%)	2.53	240/4240 (5.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
3	L	2.23	121/3146 (3.8%)	2.46	235/4240 (5.5%)
3	M	2.25	115/3146 (3.7%)	2.43	197/4240 (4.6%)
All	All	2.32	2621/67680 (3.9%)	2.44	4414/91212 (4.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	6
1	C	0	12
1	D	0	5
1	E	0	12
1	F	0	6
1	G	0	9
1	a	0	15
1	b	0	10
1	c	0	10
1	d	0	8
1	e	0	7
1	f	0	11
1	g	0	8
2	1	0	7
2	2	0	8
2	3	0	1
2	4	0	6
2	5	0	4
2	6	0	7
2	7	0	7
2	h	0	9
2	i	0	8
2	j	0	5
2	k	0	3
2	l	0	3
2	m	0	7
2	n	0	9
3	H	0	15
3	I	0	24
3	J	0	15
3	K	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	24
3	M	0	17
All	All	0	323

All (2621) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	170	ARG	CZ-NH1	61.50	2.18	1.32
2	1	170	ARG	CZ-NH1	55.67	2.10	1.32
2	1	211	PHE	CG-CD2	35.80	2.14	1.38
2	1	211	PHE	CG-CD1	34.05	2.10	1.38
2	5	211	PHE	CG-CD2	32.22	2.06	1.38
2	5	211	PHE	CG-CD1	30.95	2.03	1.38
2	5	211	PHE	CE1-CZ	22.93	2.07	1.38
2	1	211	PHE	CE1-CZ	22.38	2.05	1.38
2	5	211	PHE	CE2-CZ	21.43	2.02	1.38
2	1	211	PHE	CD2-CE2	21.40	2.02	1.38
2	1	211	PHE	CD1-CE1	21.34	2.02	1.38
2	5	211	PHE	CD1-CE1	21.05	2.01	1.38
2	5	211	PHE	CD2-CE2	20.64	2.00	1.38
2	1	211	PHE	CE2-CZ	20.59	2.00	1.38
2	2	51	ARG	CA-CB	11.86	1.62	1.53
1	g	53	ARG	CD-NE	11.71	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
1	f	53	ARG	NE-CZ	11.07	1.45	1.33
1	e	238	GLU	CA-C	-10.96	1.39	1.52
1	b	212	GLY	CA-C	-10.94	1.41	1.52
3	I	221	ARG	NE-CZ	10.90	1.45	1.33
1	e	80	GLY	CA-C	-10.52	1.40	1.52
3	L	309	VAL	CA-CB	-10.35	1.46	1.54
2	m	88	ARG	CD-NE	10.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLY	CA-C	10.04	1.60	1.52
2	m	123	TYR	CA-C	-10.02	1.40	1.52
3	M	71	ILE	CA-C	-10.02	1.39	1.52
2	7	178	ARG	NE-CZ	9.97	1.44	1.33
1	G	56	SER	CA-C	-9.97	1.47	1.52
1	b	50	ALA	CA-C	-9.95	1.40	1.52
3	M	77	VAL	CA-C	-9.93	1.40	1.52
1	d	168	ARG	CD-NE	9.84	1.60	1.46
2	3	32	THR	CA-C	-9.76	1.41	1.52
3	L	143	ILE	CA-C	-9.76	1.42	1.52
3	K	289	ARG	NE-CZ	9.68	1.43	1.33
1	e	165	GLY	CA-C	-9.68	1.41	1.52
1	b	235	ARG	NE-CZ	9.66	1.43	1.33
1	G	148	TYR	CA-C	-9.66	1.40	1.52
2	6	39	SER	CA-C	-9.59	1.40	1.52
1	A	194	VAL	CA-C	-9.54	1.40	1.52
2	i	88	ARG	NE-CZ	9.54	1.43	1.33
2	m	163	GLU	CA-C	-9.51	1.39	1.52
2	4	69	ILE	N-CA	-9.47	1.35	1.46
2	1	187	ASP	CA-C	-9.47	1.40	1.52
2	m	117	SER	CA-CB	9.42	1.68	1.53
1	g	212	GLY	CA-C	-9.42	1.41	1.51
2	i	51	ARG	NE-CZ	9.38	1.43	1.33
3	J	222	LEU	CA-C	-9.37	1.40	1.52
3	I	370	VAL	CA-CB	-9.32	1.42	1.54
2	m	22	GLY	C-O	-9.32	1.17	1.23
2	7	113	GLY	N-CA	-9.31	1.35	1.45
2	7	80	ARG	N-CA	-9.30	1.35	1.46
2	1	46	TYR	CA-C	-9.28	1.41	1.52
3	K	50	ARG	NE-CZ	9.26	1.43	1.33
2	6	123	TYR	CA-C	-9.24	1.41	1.52
2	1	154	ARG	NE-CZ	9.22	1.43	1.33
1	g	219	ARG	CD-NE	9.19	1.59	1.46
2	7	154	ARG	NE-CZ	9.17	1.43	1.33
3	K	41	ARG	NE-CZ	9.15	1.43	1.33
1	g	149	GLU	CA-C	-9.13	1.41	1.52
1	B	207	GLU	CA-C	-9.12	1.40	1.52
2	4	24	VAL	CA-CB	-9.12	1.42	1.54
3	K	66	GLY	CA-C	-9.12	1.43	1.52
2	1	195	GLU	N-CA	-9.10	1.33	1.45
2	k	22	GLY	CA-C	-9.10	1.41	1.52
1	f	222	LYS	CA-C	-9.05	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	VAL	N-CA	-9.02	1.37	1.46
3	M	29	ARG	N-CA	-9.01	1.35	1.46
1	f	120	LYS	CA-C	-9.00	1.41	1.52
3	H	218	GLU	CA-CB	9.00	1.68	1.53
3	K	249	ARG	NE-CZ	8.96	1.43	1.33
1	E	230	LYS	CA-C	8.95	1.61	1.52
2	i	41	ALA	CA-C	8.94	1.64	1.52
3	M	315	GLU	CA-C	-8.92	1.41	1.52
2	2	186	ILE	CA-C	-8.91	1.42	1.52
2	l	194	ASP	CA-C	-8.87	1.43	1.52
1	f	135	SER	CA-C	-8.82	1.41	1.52
3	H	331	ALA	N-CA	-8.79	1.36	1.46
1	G	20	ARG	CD-NE	8.77	1.58	1.46
1	B	144	VAL	C-N	8.76	1.45	1.33
1	F	224	VAL	CA-CB	-8.76	1.43	1.53
1	a	20	ARG	NE-CZ	8.75	1.42	1.33
1	G	225	SER	CA-C	-8.72	1.42	1.53
2	h	106	TYR	CA-C	-8.70	1.44	1.53
1	d	225	SER	CA-C	-8.69	1.44	1.53
3	J	200	ARG	CD-NE	8.68	1.58	1.46
3	I	85	PRO	CA-C	-8.68	1.42	1.52
1	B	239	ARG	CD-NE	8.64	1.58	1.46
3	H	274	GLY	C-N	8.63	1.44	1.33
3	M	105	ARG	CD-NE	8.62	1.58	1.46
1	G	134	VAL	N-CA	-8.62	1.36	1.46
2	7	56	THR	CA-C	-8.60	1.42	1.52
1	b	224	VAL	CA-CB	-8.60	1.44	1.54
2	k	115	ILE	N-CA	-8.60	1.36	1.46
2	2	102	ARG	CD-NE	8.60	1.58	1.46
2	j	54	MET	C-N	8.59	1.46	1.33
3	J	367	ARG	CA-C	-8.58	1.42	1.52
2	l	68	ARG	NE-CZ	8.58	1.42	1.33
1	D	147	LEU	N-CA	-8.56	1.35	1.46
1	A	240	ILE	CA-C	-8.55	1.41	1.52
3	K	205	ARG	CD-NE	8.54	1.58	1.46
3	K	136	PRO	C-N	8.49	1.45	1.33
3	L	355	CYS	N-CA	-8.48	1.35	1.46
1	B	93	ARG	NE-CZ	8.45	1.42	1.33
1	E	33	ARG	NE-CZ	8.45	1.42	1.33
1	e	48	LEU	CA-C	-8.45	1.42	1.52
1	e	44	GLU	CA-C	-8.45	1.42	1.52
1	b	12	ILE	CA-CB	-8.44	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	30	ARG	CD-NE	8.43	1.58	1.46
2	n	58	GLY	C-O	-8.42	1.18	1.24
1	b	63	THR	N-CA	-8.42	1.38	1.46
1	F	39	GLY	CA-C	-8.41	1.44	1.51
2	l	80	ARG	CA-C	-8.36	1.42	1.52
1	C	28	ARG	NE-CZ	8.36	1.42	1.33
3	K	28	ARG	NE-CZ	8.35	1.42	1.33
3	J	250	ARG	CA-C	-8.34	1.42	1.53
2	j	58	GLY	CA-C	-8.34	1.41	1.52
1	d	208	ASN	N-CA	-8.33	1.37	1.46
2	7	122	ILE	CA-C	-8.33	1.42	1.52
3	K	243	LEU	C-N	8.32	1.45	1.33
2	2	117	SER	CA-C	-8.32	1.42	1.52
2	2	212	ARG	NE-CZ	8.32	1.42	1.33
1	A	53	ARG	CD-NE	8.32	1.57	1.46
2	3	107	LEU	CA-C	-8.31	1.42	1.52
3	M	183	PRO	CA-C	8.31	1.59	1.52
1	d	10	ARG	NE-CZ	8.30	1.42	1.33
1	D	219	ARG	CD-NE	8.29	1.57	1.46
2	l	188	VAL	CA-C	-8.27	1.42	1.52
1	G	20	ARG	NE-CZ	8.26	1.42	1.33
1	D	86	ARG	C-N	8.25	1.44	1.33
2	m	82	GLU	CA-C	-8.25	1.45	1.53
1	E	169	ASN	CA-CB	8.24	1.66	1.53
3	H	113	LEU	CA-C	-8.23	1.41	1.52
3	M	174	PRO	CA-C	-8.22	1.46	1.52
1	f	50	ALA	CA-C	-8.22	1.42	1.52
1	G	73	HIS	CA-C	-8.22	1.42	1.52
3	K	64	LEU	CA-C	-8.22	1.42	1.52
2	1	81	ARG	CD-NE	8.21	1.57	1.46
2	5	80	ARG	NE-CZ	8.19	1.42	1.33
3	M	96	ASN	CA-C	-8.18	1.41	1.53
3	H	126	MET	CA-CB	8.17	1.64	1.53
1	g	100	ARG	CD-NE	8.16	1.57	1.46
2	4	195	GLU	N-CA	-8.12	1.35	1.45
2	m	155	PHE	CA-C	-8.11	1.42	1.52
2	h	134	GLU	CA-C	-8.09	1.42	1.52
2	i	80	ARG	CZ-NH1	8.09	1.44	1.32
1	E	187	ASP	N-CA	-8.09	1.35	1.46
1	f	87	VAL	CA-CB	-8.09	1.44	1.54
2	j	212	ARG	CD-NE	8.09	1.57	1.46
3	H	221	ARG	CD-NE	8.09	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	68	ARG	CD-NE	8.08	1.57	1.46
3	K	342	ILE	CA-C	-8.06	1.41	1.52
3	J	220	ALA	CA-CB	8.06	1.66	1.53
1	B	229	LEU	CA-C	-8.06	1.42	1.52
1	a	145	PRO	CA-C	-8.05	1.41	1.52
1	D	131	PRO	CA-C	-8.05	1.43	1.52
1	E	126	TYR	CA-CB	8.04	1.66	1.53
3	M	380	GLU	N-CA	-8.04	1.36	1.46
2	k	83	ARG	NE-CZ	8.03	1.41	1.33
1	B	225	SER	CA-C	-8.02	1.43	1.53
1	B	240	ILE	CA-CB	-8.02	1.45	1.54
2	7	131	ALA	CA-C	-8.02	1.42	1.52
1	G	13	THR	C-N	8.01	1.41	1.33
2	1	80	ARG	NE-CZ	8.01	1.41	1.33
3	M	339	LEU	CA-CB	8.00	1.66	1.53
3	H	24	ARG	CD-NE	8.00	1.57	1.46
1	F	165	GLY	CA-C	-8.00	1.43	1.52
2	2	196	PHE	C-N	8.00	1.44	1.33
2	3	18	VAL	CA-C	-7.99	1.42	1.52
3	H	367	ARG	N-CA	-7.98	1.36	1.46
1	c	152	PRO	C-N	7.98	1.44	1.33
2	5	212	ARG	NE-CZ	7.98	1.41	1.33
2	k	102	ARG	CD-NE	7.97	1.57	1.46
2	j	80	ARG	CD-NE	7.97	1.57	1.46
2	n	80	ARG	NE-CZ	7.96	1.41	1.33
2	h	81	ARG	NE-CZ	7.95	1.41	1.33
1	E	73	HIS	N-CA	-7.95	1.38	1.46
2	7	202	GLU	CA-C	-7.95	1.43	1.52
3	M	29	ARG	NE-CZ	7.94	1.41	1.33
2	3	33	MET	CA-C	-7.93	1.41	1.52
3	I	223	VAL	CA-C	-7.93	1.42	1.52
1	A	91	ARG	CA-C	-7.92	1.42	1.52
2	k	45	ILE	N-CA	-7.92	1.37	1.46
2	5	109	GLN	CA-C	-7.91	1.43	1.52
2	l	162	ASP	CA-CB	7.90	1.65	1.53
2	5	88	ARG	NE-CZ	7.90	1.41	1.33
3	K	250	ARG	NE-CZ	7.90	1.41	1.33
1	E	45	GLY	CA-C	-7.90	1.44	1.52
1	e	241	ARG	CA-C	-7.89	1.42	1.52
1	g	137	LEU	CA-C	-7.88	1.43	1.52
2	k	146	THR	N-CA	-7.88	1.36	1.46
1	A	241	ARG	CZ-NH1	7.87	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	49	ARG	CD-NE	7.85	1.57	1.46
1	b	49	ILE	CA-C	-7.84	1.43	1.52
2	6	99	ASN	CA-C	-7.83	1.42	1.52
2	4	68	ARG	NE-CZ	7.83	1.41	1.33
2	4	162	ASP	CA-CB	7.83	1.65	1.53
3	K	335	ASP	CA-C	-7.82	1.43	1.52
1	e	94	ILE	N-CA	-7.80	1.36	1.46
1	a	34	GLY	CA-C	-7.80	1.45	1.52
1	g	219	ARG	NE-CZ	7.80	1.41	1.33
2	4	88	ARG	NE-CZ	7.79	1.41	1.33
1	D	235	ARG	CZ-NH2	7.79	1.43	1.33
2	3	146	THR	C-N	7.79	1.44	1.33
3	H	90	ASN	CA-CB	7.79	1.64	1.53
2	i	168	ALA	N-CA	-7.78	1.37	1.46
3	J	61	PRO	CA-C	-7.78	1.47	1.52
1	c	160	LYS	C-N	7.77	1.43	1.33
1	a	68	TYR	CA-C	-7.76	1.43	1.52
1	a	66	LYS	CA-C	-7.76	1.43	1.53
1	d	212	GLY	CA-C	-7.76	1.44	1.52
1	e	239	ARG	NE-CZ	7.76	1.41	1.33
2	n	137	ILE	C-N	7.75	1.41	1.33
3	K	305	ARG	CZ-NH2	7.75	1.43	1.33
3	H	201	ALA	CA-C	-7.75	1.42	1.53
3	K	263	ARG	CD-NE	7.75	1.57	1.46
1	E	43	LYS	CA-C	-7.74	1.42	1.52
3	H	302	ARG	CZ-NH2	7.73	1.43	1.33
1	D	6	MET	CA-C	-7.73	1.42	1.52
1	c	178	GLU	N-CA	-7.72	1.37	1.46
2	l	126	ASP	CA-C	-7.72	1.43	1.53
3	M	380	GLU	CA-C	-7.71	1.43	1.52
1	g	93	ARG	CD-NE	7.70	1.57	1.46
2	3	80	ARG	CD-NE	7.70	1.57	1.46
2	5	24	VAL	CA-C	-7.70	1.43	1.52
1	g	241	ARG	NE-CZ	7.70	1.41	1.33
1	d	142	ASP	N-CA	-7.69	1.36	1.46
1	F	86	ARG	NE-CZ	7.69	1.41	1.33
3	L	169	GLU	CA-C	-7.69	1.42	1.52
3	J	182	GLY	C-N	-7.65	1.24	1.33
2	2	181	ALA	CA-C	-7.65	1.42	1.52
3	L	50	ARG	CA-CB	7.65	1.65	1.53
3	J	326	ARG	CD-NE	7.65	1.56	1.46
1	c	28	ARG	CD-NE	7.65	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	51	ARG	N-CA	-7.64	1.38	1.46
2	m	138	VAL	CA-C	-7.64	1.43	1.52
3	H	251	THR	CA-C	-7.63	1.43	1.52
2	3	86	THR	C-N	7.63	1.43	1.33
2	6	162	ASP	N-CA	-7.63	1.37	1.46
3	K	149	GLN	N-CA	-7.62	1.37	1.46
1	a	10	ARG	NE-CZ	7.62	1.41	1.33
2	1	122	ILE	CA-C	-7.62	1.43	1.52
3	K	369	LYS	CA-C	-7.60	1.43	1.52
1	F	73	HIS	ND1-CE1	7.60	1.40	1.32
3	J	137	GLU	N-CA	-7.59	1.37	1.46
3	I	52	ARG	NE-CZ	7.59	1.41	1.33
1	d	202	SER	CA-C	-7.59	1.43	1.52
1	C	64	ILE	CA-C	-7.58	1.44	1.52
3	H	330	LEU	CA-CB	7.58	1.64	1.53
1	E	60	GLU	N-CA	7.57	1.55	1.46
2	3	178	ARG	NE-CZ	7.57	1.41	1.33
2	3	172	ILE	CA-CB	-7.57	1.44	1.54
3	L	394	GLY	C-N	7.57	1.44	1.33
3	K	317	ARG	NE-CZ	7.55	1.41	1.33
2	i	56	THR	CA-C	-7.54	1.43	1.52
2	j	147	ALA	CA-CB	7.54	1.65	1.53
2	i	158	GLU	C-N	7.53	1.42	1.33
1	B	118	ASP	N-CA	-7.53	1.36	1.46
1	A	87	VAL	N-CA	-7.52	1.37	1.46
3	M	53	SER	N-CA	-7.52	1.37	1.46
1	A	136	LEU	CA-C	-7.52	1.43	1.52
2	7	184	ASP	CA-C	-7.52	1.43	1.52
1	D	111	GLU	N-CA	-7.50	1.37	1.46
1	B	38	ILE	CA-C	-7.50	1.43	1.52
2	2	22	GLY	C-O	7.48	1.28	1.23
1	F	203	GLU	CA-C	-7.48	1.43	1.52
2	m	32	THR	N-CA	-7.47	1.36	1.45
2	m	42	ALA	CA-C	-7.47	1.43	1.52
1	D	196	MET	C-N	7.47	1.43	1.33
2	1	115	ILE	CA-CB	-7.47	1.45	1.54
1	g	74	ILE	C-N	7.46	1.43	1.33
2	l	21	ASP	CA-CB	7.46	1.64	1.53
2	3	171	ALA	CA-C	-7.45	1.43	1.52
1	b	168	ARG	CZ-NH2	7.45	1.43	1.33
3	H	364	ARG	NE-CZ	7.44	1.41	1.33
3	L	299	ARG	CA-C	-7.44	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	50	ARG	N-CA	-7.43	1.37	1.46
2	i	18	VAL	CA-C	-7.43	1.43	1.52
3	L	29	ARG	N-CA	-7.43	1.37	1.46
1	e	22	PHE	CA-C	-7.43	1.43	1.52
1	e	172	THR	C-N	7.43	1.44	1.33
2	l	83	ARG	NE-CZ	7.42	1.41	1.33
2	h	107	LEU	C-N	7.41	1.43	1.33
1	A	179	TYR	C-N	7.41	1.42	1.33
1	b	165	GLY	CA-C	-7.39	1.43	1.52
3	K	230	ALA	CA-C	-7.39	1.43	1.52
1	D	171	VAL	CA-CB	-7.39	1.44	1.54
3	L	224	ARG	C-N	7.39	1.43	1.33
1	c	117	CYS	C-N	7.39	1.43	1.33
1	e	114	LYS	N-CA	-7.39	1.37	1.46
2	4	128	ILE	CA-CB	7.38	1.64	1.54
1	g	239	ARG	NE-CZ	7.37	1.41	1.33
3	J	200	ARG	NE-CZ	7.36	1.41	1.33
3	L	27	TYR	CA-CB	7.36	1.65	1.53
3	J	159	LEU	N-CA	-7.34	1.39	1.46
1	c	219	ARG	C-N	7.34	1.43	1.33
2	k	170	ARG	NE-CZ	7.34	1.41	1.33
3	M	44	TYR	CA-C	-7.34	1.43	1.52
2	7	64	GLN	N-CA	-7.34	1.37	1.46
1	G	86	ARG	CA-CB	7.33	1.65	1.53
3	K	359	GLY	CA-C	-7.33	1.43	1.52
1	d	163	ALA	N-CA	-7.33	1.36	1.45
2	i	139	ALA	C-N	7.32	1.42	1.33
3	L	29	ARG	CZ-NH2	7.30	1.43	1.33
1	c	235	ARG	NE-CZ	7.30	1.41	1.33
2	5	170	ARG	CD-NE	7.29	1.56	1.46
3	M	387	THR	N-CA	-7.28	1.39	1.46
3	M	60	SER	C-N	-7.27	1.24	1.33
3	I	326	ARG	CA-C	-7.26	1.43	1.52
3	L	222	LEU	N-CA	-7.26	1.37	1.46
2	6	170	ARG	NE-CZ	7.26	1.41	1.33
3	H	124	ASP	CA-CB	7.26	1.65	1.52
1	F	21	LEU	CA-C	-7.26	1.44	1.52
3	K	270	ALA	CA-C	-7.25	1.43	1.52
1	A	12	ILE	CA-CB	-7.25	1.46	1.54
1	d	68	TYR	N-CA	-7.24	1.37	1.45
1	b	240	ILE	C-N	7.24	1.43	1.33
2	i	168	ALA	C-N	7.24	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	83	ARG	CZ-NH1	7.23	1.42	1.32
2	6	67	ALA	C-N	7.22	1.43	1.33
2	h	18	VAL	CA-C	-7.22	1.44	1.52
2	3	159	ILE	CA-CB	7.22	1.62	1.54
3	K	302	ARG	CA-CB	7.21	1.64	1.54
3	M	250	ARG	NE-CZ	7.21	1.41	1.33
1	B	186	ASP	CA-C	-7.21	1.43	1.52
3	I	24	ARG	CA-C	-7.21	1.43	1.52
3	K	221	ARG	NE-CZ	7.20	1.41	1.33
1	E	59	LEU	CA-CB	7.20	1.64	1.53
1	f	189	MET	CA-C	-7.20	1.43	1.52
3	H	238	ILE	C-N	7.19	1.43	1.33
1	C	177	LYS	CA-C	-7.17	1.44	1.52
1	F	234	GLU	CA-CB	7.17	1.64	1.53
3	H	390	PRO	CA-C	-7.17	1.44	1.52
1	g	169	ASN	CA-C	-7.17	1.43	1.52
1	f	193	LEU	N-CA	-7.17	1.37	1.46
2	h	144	SER	CA-C	-7.17	1.43	1.52
1	C	11	ALA	CA-C	-7.17	1.43	1.52
1	F	7	GLY	C-N	7.17	1.43	1.33
1	f	205	VAL	N-CA	-7.17	1.37	1.46
3	M	385	LYS	C-N	7.16	1.43	1.33
3	L	76	ARG	NE-CZ	7.15	1.41	1.33
2	6	67	ALA	N-CA	-7.14	1.37	1.46
2	h	99	ASN	N-CA	-7.14	1.37	1.46
1	e	212	GLY	CA-C	-7.13	1.46	1.52
1	g	224	VAL	CA-C	-7.13	1.44	1.52
1	g	214	VAL	CA-C	-7.13	1.43	1.52
1	A	219	ARG	CD-NE	7.12	1.56	1.46
2	3	191	ILE	CA-C	-7.12	1.43	1.52
2	7	212	ARG	CD-NE	7.12	1.56	1.46
3	M	312	PRO	C-N	7.12	1.42	1.33
1	F	133	GLY	C-N	7.12	1.43	1.33
1	g	145	PRO	N-CA	-7.11	1.38	1.47
1	E	66	LYS	C-N	7.11	1.42	1.33
2	j	57	ALA	CA-C	-7.11	1.43	1.52
1	A	35	ALA	CA-C	-7.10	1.43	1.52
2	m	79	ILE	CA-CB	-7.10	1.45	1.54
3	I	50	ARG	CD-NE	7.10	1.56	1.46
1	b	115	LYS	N-CA	-7.10	1.38	1.46
3	I	46	ARG	NE-CZ	7.10	1.40	1.33
3	H	187	GLY	CA-C	-7.10	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	185	PHE	CA-C	-7.10	1.43	1.52
2	2	45	ILE	CA-CB	7.09	1.63	1.54
2	i	97	LEU	CA-C	-7.09	1.43	1.52
1	d	206	PRO	N-CA	-7.09	1.38	1.47
1	G	10	ARG	CZ-NH2	7.08	1.42	1.33
1	B	214	VAL	CA-C	-7.07	1.43	1.52
2	k	130	GLY	N-CA	-7.07	1.35	1.45
1	E	136	LEU	CA-C	-7.06	1.44	1.52
1	f	78	THR	CA-C	-7.06	1.44	1.52
3	K	105	ARG	NE-CZ	7.06	1.40	1.33
2	i	16	GLY	CA-C	-7.06	1.42	1.51
2	4	107	LEU	C-N	7.06	1.40	1.33
2	m	139	ALA	CA-C	-7.05	1.44	1.52
1	B	103	TYR	N-CA	-7.04	1.38	1.46
1	b	208	ASN	CA-CB	7.04	1.64	1.53
2	7	157	PRO	CA-C	-7.04	1.45	1.52
2	1	107	LEU	CA-CB	7.03	1.63	1.53
1	E	53	ARG	CZ-NH1	7.03	1.42	1.32
2	6	112	ILE	N-CA	-7.03	1.38	1.46
2	i	68	ARG	CD-NE	7.03	1.56	1.46
3	H	352	LYS	CA-CB	7.03	1.64	1.53
1	D	163	ALA	N-CA	-7.02	1.37	1.45
2	k	179	ASP	CA-C	-7.02	1.43	1.53
2	n	136	ASP	CA-CB	7.02	1.65	1.53
1	c	139	ALA	N-CA	-7.01	1.37	1.46
3	H	100	LEU	N-CA	-7.01	1.37	1.46
2	1	112	ILE	CA-C	-7.01	1.44	1.52
2	j	49	ALA	CA-C	-7.01	1.44	1.52
2	5	61	GLY	CA-C	-7.01	1.43	1.51
3	H	366	GLU	CA-C	-7.00	1.44	1.53
2	2	162	ASP	C-N	7.00	1.44	1.33
2	h	184	ASP	N-CA	-7.00	1.37	1.46
1	B	187	ASP	CA-C	-7.00	1.43	1.52
2	1	68	ARG	CD-NE	7.00	1.56	1.46
1	d	216	VAL	CA-C	-6.99	1.43	1.52
3	H	286	ALA	C-N	6.99	1.42	1.33
2	k	88	ARG	CA-C	-6.99	1.43	1.52
2	1	66	LEU	N-CA	-6.99	1.37	1.46
2	2	21	ASP	N-CA	-6.99	1.36	1.46
2	5	33	MET	C-N	6.99	1.42	1.33
2	3	176	MET	CA-C	-6.98	1.43	1.52
2	3	212	ARG	CZ-NH1	6.98	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	42	ILE	N-CA	-6.98	1.38	1.46
3	I	352	LYS	N-CA	-6.97	1.38	1.46
3	L	253	SER	C-N	6.97	1.42	1.33
2	l	63	ALA	CA-C	-6.97	1.44	1.52
1	E	180	ARG	NE-CZ	6.97	1.40	1.33
2	1	120	LYS	CA-C	-6.97	1.44	1.52
2	6	143	GLY	C-O	-6.96	1.19	1.24
1	a	91	ARG	CD-NE	6.96	1.55	1.46
3	K	156	ALA	CA-C	-6.96	1.43	1.52
3	I	257	GLY	C-N	6.95	1.42	1.33
1	e	75	CYS	N-CA	-6.95	1.36	1.45
3	I	105	ARG	NE-CZ	6.95	1.40	1.33
3	L	374	ASP	N-CA	-6.95	1.38	1.46
2	j	171	ALA	CA-C	-6.94	1.43	1.52
2	h	122	ILE	N-CA	-6.94	1.38	1.46
2	4	134	GLU	CA-C	-6.94	1.44	1.52
2	m	30	ARG	NE-CZ	6.94	1.40	1.33
1	c	29	GLU	CA-C	-6.94	1.43	1.52
3	L	105	ARG	N-CA	-6.93	1.37	1.46
3	L	59	ARG	NE-CZ	6.93	1.40	1.33
1	G	212	GLY	CA-C	-6.93	1.46	1.52
1	E	168	ARG	CA-C	-6.93	1.43	1.52
1	d	149	GLU	CA-C	-6.92	1.44	1.52
2	n	168	ALA	CA-CB	6.92	1.64	1.53
1	c	180	ARG	CD-NE	6.92	1.55	1.46
1	A	67	ILE	CA-C	-6.92	1.44	1.52
2	n	41	ALA	C-N	6.92	1.42	1.33
1	c	10	ARG	CD-NE	6.91	1.55	1.46
1	G	158	GLU	CA-CB	6.91	1.64	1.53
3	I	364	ARG	CD-NE	6.91	1.55	1.46
3	J	154	ARG	NE-CZ	6.91	1.40	1.33
3	K	57	ARG	NE-CZ	6.91	1.40	1.33
1	b	140	GLY	C-N	6.90	1.42	1.33
1	C	239	ARG	NE-CZ	6.90	1.40	1.33
1	e	130	ARG	CZ-NH1	6.90	1.42	1.32
1	G	239	ARG	CD-NE	6.90	1.55	1.46
2	j	77	TYR	CA-CB	6.90	1.64	1.53
2	4	144	SER	N-CA	-6.90	1.38	1.46
1	E	47	ILE	C-N	6.89	1.42	1.33
3	J	47	GLU	CA-C	-6.89	1.44	1.52
2	h	156	THR	CA-C	-6.89	1.45	1.52
2	m	29	LYS	CA-CB	6.89	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	167	PHE	N-CA	-6.88	1.37	1.46
1	c	175	PHE	CA-C	-6.88	1.43	1.52
1	g	113	ALA	CA-C	-6.88	1.43	1.52
1	C	33	ARG	CA-C	-6.88	1.43	1.52
2	i	151	LEU	N-CA	-6.88	1.38	1.46
1	c	75	CYS	C-N	6.87	1.42	1.33
3	H	41	ARG	CD-NE	6.87	1.55	1.46
1	D	98	ILE	CA-CB	-6.87	1.45	1.54
2	3	137	ILE	CA-CB	-6.87	1.46	1.54
3	M	319	GLN	CA-C	-6.87	1.44	1.52
1	f	41	LYS	CA-C	-6.86	1.44	1.52
1	a	227	GLU	C-N	6.86	1.43	1.33
1	a	47	ILE	C-N	6.86	1.42	1.33
1	f	219	ARG	CD-NE	6.86	1.55	1.46
3	K	300	PRO	N-CA	-6.86	1.39	1.47
1	C	86	ARG	CD-NE	6.85	1.55	1.46
2	1	31	ALA	N-CA	-6.85	1.37	1.46
1	G	233	VAL	CA-C	-6.84	1.44	1.52
3	L	316	GLY	CA-C	-6.84	1.43	1.52
3	J	69	SER	CA-CB	6.84	1.64	1.53
2	l	116	ASP	CA-C	-6.84	1.44	1.52
3	J	191	LEU	C-N	6.84	1.42	1.33
3	M	292	ILE	C-N	6.84	1.43	1.33
1	b	133	GLY	C-N	6.83	1.42	1.33
2	i	45	ILE	CA-CB	6.82	1.62	1.54
3	I	112	THR	CA-C	-6.82	1.43	1.52
2	i	51	ARG	CD-NE	6.82	1.55	1.46
1	G	240	ILE	CA-C	-6.82	1.44	1.52
2	n	83	ARG	CZ-NH1	6.81	1.42	1.32
2	h	120	LYS	CA-C	-6.81	1.44	1.52
1	a	51	ASP	CA-CB	6.80	1.62	1.53
2	7	120	LYS	CA-C	-6.80	1.44	1.52
3	I	282	LYS	C-N	6.80	1.42	1.33
3	I	164	PRO	N-CD	6.80	1.57	1.47
3	K	27	TYR	C-N	6.80	1.42	1.33
2	7	24	VAL	CA-C	-6.79	1.44	1.52
1	F	235	ARG	NE-CZ	6.79	1.40	1.33
1	C	130	ARG	CZ-NH1	6.79	1.42	1.32
1	f	239	ARG	CZ-NH2	6.79	1.42	1.33
1	F	130	ARG	CA-C	-6.79	1.43	1.52
1	a	19	GLY	CA-C	-6.79	1.42	1.51
1	E	132	PHE	C-N	6.78	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	177	LYS	CA-C	-6.78	1.44	1.52
1	A	233	VAL	C-N	6.78	1.43	1.33
3	L	299	ARG	CD-NE	6.78	1.55	1.46
2	3	134	GLU	CA-CB	6.78	1.61	1.53
1	C	40	ILE	CA-C	-6.77	1.44	1.52
1	A	218	ASP	N-CA	-6.77	1.38	1.46
1	a	140	GLY	CA-C	-6.77	1.43	1.51
2	l	14	THR	CA-C	-6.77	1.44	1.52
1	B	212	GLY	CA-C	-6.76	1.42	1.51
2	h	123	TYR	N-CA	-6.76	1.37	1.46
2	4	124	SER	CA-C	6.76	1.61	1.52
1	A	121	GLN	CA-C	-6.76	1.44	1.52
2	h	153	ASP	CA-C	-6.76	1.44	1.52
2	5	22	GLY	C-N	6.76	1.41	1.33
2	6	74	ALA	C-N	6.76	1.42	1.33
1	G	235	ARG	CZ-NH2	6.75	1.42	1.33
2	j	33	MET	CA-C	-6.75	1.45	1.53
1	E	198	LEU	CA-CB	6.75	1.64	1.53
2	l	36	PHE	C-N	6.75	1.42	1.33
3	J	366	GLU	CA-C	-6.75	1.45	1.53
1	F	69	LYS	CA-C	-6.74	1.44	1.52
3	J	28	ARG	NE-CZ	6.74	1.40	1.33
1	b	20	ARG	CA-CB	6.74	1.63	1.53
2	4	149	GLY	N-CA	-6.74	1.37	1.45
1	B	46	VAL	N-CA	6.74	1.54	1.46
3	H	76	ARG	NE-CZ	6.74	1.40	1.33
3	I	181	TYR	C-O	-6.74	1.16	1.23
1	F	123	TYR	N-CA	6.73	1.54	1.46
1	c	90	ASP	CA-C	-6.73	1.44	1.52
1	e	144	VAL	C-N	6.73	1.42	1.33
1	g	119	PHE	CA-C	-6.73	1.44	1.52
2	h	51	ARG	NE-CZ	6.72	1.40	1.33
2	4	69	ILE	CA-C	6.72	1.61	1.52
2	k	122	ILE	N-CA	6.72	1.54	1.46
3	M	364	ARG	NE-CZ	6.72	1.40	1.33
3	L	47	GLU	C-N	6.72	1.42	1.33
3	M	28	ARG	NE-CZ	6.72	1.40	1.33
2	k	154	ARG	NE-CZ	6.72	1.40	1.33
3	I	317	ARG	NE-CZ	6.72	1.40	1.33
3	L	254	ASP	CA-C	-6.71	1.47	1.53
2	l	178	ARG	CZ-NH1	6.71	1.42	1.32
1	c	95	GLU	C-N	6.71	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	241	ARG	CD-NE	6.71	1.55	1.46
1	g	178	GLU	C-N	6.71	1.42	1.33
3	K	173	GLU	C-N	6.71	1.41	1.33
3	I	309	VAL	CA-C	6.71	1.58	1.53
1	C	70	ILE	CA-C	-6.70	1.44	1.52
1	E	54	VAL	CA-C	6.70	1.60	1.52
1	g	214	VAL	CA-CB	-6.70	1.45	1.54
2	1	180	SER	CA-C	-6.70	1.43	1.52
3	M	29	ARG	C-N	6.70	1.43	1.33
2	5	111	LEU	C-N	6.70	1.41	1.33
2	m	75	ASN	CA-CB	6.70	1.63	1.53
1	C	100	ARG	CA-C	6.70	1.62	1.52
1	G	141	VAL	CA-C	-6.70	1.44	1.52
3	I	173	GLU	CA-CB	6.69	1.63	1.53
2	j	16	GLY	CA-C	-6.69	1.42	1.51
3	M	218	GLU	CA-C	-6.68	1.44	1.52
3	I	324	HIS	CE1-NE2	6.68	1.39	1.32
2	h	199	TYR	CA-C	6.68	1.61	1.52
2	j	205	GLU	N-CA	-6.68	1.38	1.46
1	d	169	ASN	N-CA	-6.67	1.38	1.46
3	I	117	ASN	C-N	6.67	1.41	1.33
2	j	206	GLN	N-CA	-6.67	1.38	1.46
3	L	76	ARG	N-CA	-6.67	1.36	1.46
3	M	270	ALA	C-N	6.67	1.43	1.34
3	H	302	ARG	NE-CZ	6.67	1.40	1.33
1	g	161	ALA	N-CA	-6.67	1.38	1.46
2	5	155	PHE	N-CA	6.66	1.54	1.46
3	M	116	VAL	CA-C	-6.66	1.44	1.52
2	1	56	THR	CA-C	-6.66	1.44	1.52
2	4	86	THR	CA-C	-6.66	1.44	1.53
2	1	185	GLY	N-CA	6.65	1.56	1.45
2	4	170	ARG	NE-CZ	6.65	1.40	1.33
2	k	154	ARG	CD-NE	6.65	1.55	1.46
3	K	41	ARG	CZ-NH1	6.65	1.42	1.32
1	g	195	ALA	N-CA	-6.65	1.38	1.46
1	A	210	GLU	C-N	6.65	1.43	1.33
2	5	56	THR	C-N	6.65	1.43	1.33
2	6	88	ARG	NE-CZ	6.65	1.40	1.33
1	A	85	ALA	C-N	6.65	1.42	1.33
1	C	33	ARG	CD-NE	6.64	1.55	1.46
1	d	121	GLN	C-N	6.64	1.43	1.33
2	3	37	ILE	CA-CB	-6.64	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	200	SER	CA-CB	6.64	1.64	1.53
2	6	160	GLY	N-CA	-6.64	1.39	1.44
1	C	64	ILE	CA-CB	-6.63	1.46	1.54
1	g	62	ASP	N-CA	-6.63	1.41	1.47
3	K	50	ARG	CD-NE	6.63	1.55	1.46
2	4	148	TYR	CA-CB	6.63	1.63	1.53
1	B	218	ASP	CA-C	-6.62	1.44	1.52
1	C	157	LEU	CA-C	-6.62	1.44	1.52
1	G	38	ILE	CA-C	6.62	1.60	1.52
2	4	143	GLY	CA-C	-6.62	1.43	1.51
3	M	315	GLU	CA-CB	6.62	1.63	1.53
1	C	242	GLU	C-N	6.61	1.43	1.33
2	6	76	LEU	N-CA	-6.61	1.38	1.46
1	E	41	LYS	CA-C	-6.61	1.44	1.52
1	E	93	ARG	NE-CZ	6.61	1.40	1.33
2	k	144	SER	CA-CB	6.61	1.63	1.53
3	M	130	PHE	CA-CB	6.61	1.62	1.53
1	F	41	LYS	CA-C	-6.60	1.44	1.52
3	J	176	LYS	C-N	6.60	1.40	1.32
1	F	67	ILE	CA-C	-6.59	1.44	1.52
2	n	180	SER	N-CA	-6.59	1.38	1.46
2	l	33	MET	N-CA	-6.59	1.38	1.46
1	e	53	ARG	NE-CZ	6.59	1.40	1.33
1	e	171	VAL	CA-CB	-6.59	1.45	1.54
1	F	28	ARG	CD-NE	6.59	1.55	1.46
1	C	238	GLU	N-CA	-6.58	1.38	1.46
3	K	210	GLU	C-N	6.58	1.43	1.33
1	C	73	HIS	N-CA	-6.58	1.40	1.46
1	F	139	ALA	C-N	-6.58	1.25	1.33
2	i	107	LEU	CA-C	-6.58	1.44	1.52
2	m	107	LEU	CA-CB	6.58	1.62	1.53
1	b	217	ASP	CA-CB	6.58	1.64	1.53
3	H	352	LYS	C-N	6.58	1.42	1.34
3	J	320	ILE	CA-C	-6.58	1.44	1.52
1	d	84	ASP	CA-C	-6.57	1.43	1.52
3	L	352	LYS	CA-CB	6.57	1.63	1.53
3	J	13	LEU	CA-C	6.57	1.61	1.52
1	f	69	LYS	CA-C	-6.57	1.44	1.52
1	g	20	ARG	CZ-NH2	6.56	1.42	1.33
2	n	44	LYS	CA-C	6.56	1.61	1.52
3	L	132	VAL	C-N	6.56	1.42	1.33
1	D	239	ARG	NE-CZ	6.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	137	ILE	CA-C	-6.56	1.44	1.52
2	1	36	PHE	C-N	6.55	1.41	1.33
1	f	53	ARG	CZ-NH1	6.55	1.42	1.32
3	J	105	ARG	NE-CZ	6.55	1.40	1.33
1	A	75	CYS	CA-C	-6.55	1.44	1.52
1	E	161	ALA	CA-C	-6.55	1.44	1.52
2	1	115	ILE	CA-C	-6.55	1.45	1.52
3	J	187	GLY	N-CA	-6.55	1.35	1.45
1	g	143	GLU	C-N	6.55	1.38	1.33
1	C	20	ARG	CZ-NH2	6.54	1.42	1.33
3	L	150	ILE	CA-CB	-6.54	1.46	1.54
3	M	105	ARG	NE-CZ	6.54	1.40	1.33
2	m	17	LEU	CA-C	-6.54	1.44	1.52
2	6	95	SER	C-N	6.53	1.42	1.33
3	K	79	VAL	CA-C	-6.53	1.44	1.52
2	m	57	ALA	CA-C	-6.53	1.44	1.52
1	A	112	LEU	C-N	6.53	1.43	1.34
2	h	171	ALA	CA-C	-6.53	1.44	1.52
3	H	197	ASN	N-CA	-6.53	1.38	1.46
2	7	170	ARG	CD-NE	6.52	1.55	1.46
3	K	61	PRO	CA-C	-6.52	1.46	1.52
3	H	333	ASP	C-N	6.52	1.41	1.33
1	f	35	ALA	C-N	6.52	1.42	1.33
2	h	162	ASP	C-N	6.52	1.43	1.33
2	2	183	GLY	C-N	6.52	1.42	1.33
3	I	341	ARG	CZ-NH2	6.52	1.42	1.33
1	f	130	ARG	NE-CZ	6.51	1.40	1.33
1	a	182	ASP	C-N	6.51	1.42	1.33
1	C	106	PRO	C-N	6.51	1.42	1.33
2	3	58	GLY	N-CA	-6.51	1.35	1.45
2	6	154	ARG	NE-CZ	6.51	1.40	1.33
2	2	40	LYS	C-N	6.50	1.42	1.33
2	h	196	PHE	CA-C	-6.50	1.45	1.53
1	a	87	VAL	C-N	6.50	1.42	1.33
1	d	136	LEU	CA-C	-6.50	1.44	1.52
2	i	134	GLU	C-N	6.50	1.42	1.33
3	M	305	ARG	CD-NE	6.50	1.55	1.46
2	3	148	TYR	N-CA	-6.50	1.38	1.46
3	M	278	ARG	N-CA	-6.50	1.38	1.46
1	A	134	VAL	N-CA	-6.50	1.38	1.46
1	C	67	ILE	C-N	6.49	1.41	1.33
2	3	31	ALA	CA-C	-6.49	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	171	ALA	C-N	6.49	1.42	1.33
1	D	217	ASP	C-N	6.49	1.43	1.33
3	L	341	ARG	CD-NE	6.49	1.55	1.46
1	F	66	LYS	CA-C	-6.49	1.44	1.52
3	J	264	THR	C-N	6.49	1.42	1.34
1	A	13	THR	C-N	6.49	1.41	1.33
2	7	156	THR	CA-C	-6.48	1.45	1.52
3	I	66	GLY	CA-C	-6.48	1.46	1.52
3	I	375	PHE	C-N	6.48	1.42	1.33
3	K	247	ALA	CA-C	-6.48	1.44	1.52
2	j	119	GLY	C-O	-6.47	1.20	1.24
2	6	45	ILE	CA-CB	-6.47	1.46	1.54
2	7	67	ALA	CA-C	-6.47	1.44	1.52
2	1	211	PHE	CA-CB	6.47	1.64	1.53
1	C	224	VAL	N-CA	-6.47	1.39	1.46
1	A	82	VAL	CA-CB	-6.46	1.46	1.54
1	d	119	PHE	CA-CB	6.46	1.63	1.53
2	2	51	ARG	CA-C	-6.46	1.46	1.53
2	k	167	LEU	CA-C	-6.46	1.44	1.52
1	f	91	ARG	C-N	6.46	1.42	1.34
1	f	149	GLU	C-O	-6.46	1.16	1.23
1	g	157	LEU	N-CA	-6.46	1.38	1.46
2	6	143	GLY	CA-C	-6.46	1.44	1.51
2	2	116	ASP	N-CA	-6.46	1.38	1.46
2	k	21	ASP	N-CA	-6.46	1.39	1.46
1	E	71	ASP	C-N	6.45	1.43	1.33
2	i	138	VAL	CA-C	-6.45	1.45	1.52
2	7	17	LEU	C-N	6.45	1.41	1.33
1	b	224	VAL	C-N	6.45	1.42	1.33
2	l	154	ARG	NE-CZ	6.45	1.40	1.33
1	G	12	ILE	CA-CB	-6.45	1.45	1.54
1	C	100	ARG	CZ-NH1	6.45	1.41	1.32
3	H	296	ALA	C-N	6.45	1.40	1.33
3	L	151	GLU	C-O	-6.45	1.16	1.24
1	a	100	ARG	CD-NE	6.44	1.55	1.46
1	g	31	VAL	N-CA	6.44	1.54	1.46
3	H	52	ARG	CD-NE	6.44	1.55	1.46
2	3	141	GLY	N-CA	6.44	1.52	1.45
3	L	241	ASP	C-N	6.44	1.42	1.33
2	m	166	GLU	CA-CB	6.44	1.63	1.53
2	1	178	ARG	CA-CB	6.43	1.63	1.53
2	j	158	GLU	N-CA	-6.43	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	63	ALA	C-N	6.43	1.42	1.33
3	H	70	ASP	C-N	6.43	1.41	1.33
1	C	37	ALA	CA-C	-6.43	1.44	1.52
1	g	87	VAL	CA-C	-6.43	1.42	1.52
3	H	28	ARG	NE-CZ	6.43	1.40	1.33
2	i	156	THR	CA-C	-6.42	1.46	1.52
2	m	23	VAL	C-N	6.42	1.42	1.33
1	A	168	ARG	NE-CZ	6.42	1.40	1.33
1	a	214	VAL	CA-C	-6.42	1.44	1.52
1	B	146	LYS	CA-C	-6.42	1.44	1.52
3	H	264	THR	CA-C	6.42	1.61	1.52
3	L	289	ARG	NE-CZ	6.42	1.40	1.33
3	H	29	ARG	NE-CZ	6.42	1.40	1.33
3	L	335	ASP	CA-C	-6.42	1.45	1.52
2	7	102	ARG	CD-NE	6.41	1.55	1.46
1	F	125	GLN	CA-C	-6.41	1.44	1.52
2	6	186	ILE	CA-CB	6.41	1.62	1.55
2	6	205	GLU	C-N	6.41	1.43	1.33
2	7	81	ARG	NE-CZ	6.41	1.40	1.33
3	H	335	ASP	CA-CB	6.41	1.61	1.53
1	b	75	CYS	CA-C	-6.41	1.44	1.52
1	g	240	ILE	CA-C	-6.41	1.45	1.52
1	A	53	ARG	CZ-NH1	6.41	1.41	1.32
1	b	107	ILE	CA-C	-6.40	1.46	1.53
2	i	55	THR	C-N	6.40	1.42	1.33
2	n	170	ARG	CZ-NH2	6.40	1.41	1.33
3	H	262	GLN	C-N	6.40	1.43	1.33
2	2	75	ASN	CA-C	-6.40	1.44	1.52
2	l	140	THR	C-N	6.40	1.42	1.32
3	H	239	PHE	N-CA	-6.40	1.38	1.46
3	I	284	ILE	C-N	6.40	1.39	1.33
2	m	51	ARG	CD-NE	6.40	1.55	1.46
1	c	104	ASP	CA-CB	6.39	1.62	1.53
1	d	17	PRO	N-CD	-6.39	1.38	1.47
2	n	161	VAL	CA-C	6.39	1.63	1.52
1	d	61	ALA	N-CA	-6.39	1.40	1.46
1	C	219	ARG	CZ-NH2	6.39	1.41	1.33
2	4	211	PHE	CA-C	-6.39	1.48	1.52
3	J	198	GLN	C-O	-6.39	1.16	1.23
2	5	198	GLN	N-CA	-6.38	1.39	1.46
3	I	137	GLU	C-N	6.38	1.41	1.33
3	J	20	TYR	C-N	6.38	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	197	GLY	CA-C	-6.38	1.45	1.52
3	K	395	VAL	CA-CB	-6.38	1.47	1.54
1	b	186	ASP	CA-CB	6.37	1.63	1.53
3	L	300	PRO	CA-C	-6.37	1.43	1.52
3	I	220	ALA	N-CA	-6.37	1.38	1.46
3	M	66	GLY	CA-C	-6.37	1.42	1.51
1	b	39	GLY	C-N	6.37	1.41	1.33
1	c	245	LYS	N-CA	-6.37	1.38	1.46
1	g	166	MET	CA-C	-6.37	1.44	1.52
2	j	44	LYS	C-N	6.37	1.41	1.33
3	K	251	THR	CA-C	-6.36	1.45	1.52
3	K	17	GLU	N-CA	-6.36	1.38	1.46
2	7	212	ARG	CA-C	6.36	1.59	1.53
1	C	180	ARG	NE-CZ	6.36	1.40	1.33
2	j	90	ILE	CA-CB	6.36	1.62	1.54
1	a	93	ARG	NE-CZ	6.36	1.40	1.33
1	B	13	THR	C-N	6.36	1.41	1.33
1	F	130	ARG	C-N	6.36	1.41	1.33
3	H	341	ARG	CZ-NH1	6.36	1.41	1.32
1	f	10	ARG	NE-CZ	6.36	1.40	1.33
1	B	81	LEU	CA-CB	6.35	1.62	1.53
1	g	10	ARG	CD-NE	6.35	1.55	1.46
2	2	105	PRO	CA-C	6.35	1.60	1.52
1	e	53	ARG	CZ-NH1	6.34	1.41	1.32
3	M	88	VAL	N-CA	-6.34	1.37	1.46
1	d	101	LEU	CA-CB	6.34	1.63	1.53
1	E	28	ARG	NE-CZ	6.34	1.40	1.33
2	k	212	ARG	NE-CZ	6.34	1.40	1.33
1	a	150	THR	CA-C	-6.34	1.45	1.52
1	B	108	THR	CA-C	-6.34	1.44	1.52
1	g	214	VAL	C-O	-6.33	1.17	1.24
1	e	201	GLU	CA-CB	6.33	1.62	1.53
3	L	221	ARG	CZ-NH1	6.33	1.41	1.32
2	i	88	ARG	N-CA	-6.33	1.38	1.46
1	f	219	ARG	CA-C	-6.33	1.45	1.53
3	L	305	ARG	CD-NE	6.32	1.55	1.46
1	b	74	ILE	CA-C	-6.32	1.44	1.52
3	I	67	VAL	C-N	6.32	1.41	1.33
2	i	194	ASP	C-N	6.32	1.41	1.33
2	4	74	ALA	CA-C	-6.32	1.44	1.52
3	M	130	PHE	CA-C	-6.32	1.44	1.52
3	M	392	LEU	N-CA	-6.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	155	ALA	CA-C	-6.32	1.45	1.52
1	e	241	ARG	CZ-NH1	6.32	1.41	1.32
3	M	299	ARG	NE-CZ	6.32	1.40	1.33
1	d	213	TYR	CA-C	-6.31	1.44	1.52
2	n	57	ALA	N-CA	-6.31	1.38	1.46
2	7	103	TYR	CA-CB	6.31	1.63	1.53
3	K	245	ALA	C-N	6.31	1.41	1.33
1	C	164	ILE	CB-CG1	6.31	1.66	1.53
3	L	25	GLU	N-CA	-6.31	1.38	1.46
3	I	43	ARG	NE-CZ	6.31	1.40	1.33
1	G	176	GLU	C-O	-6.30	1.16	1.24
3	I	216	ILE	C-N	6.30	1.41	1.33
3	H	159	LEU	C-O	-6.30	1.18	1.24
3	K	12	LYS	CA-C	-6.30	1.44	1.52
3	J	77	VAL	C-N	6.30	1.40	1.33
3	K	36	PHE	C-O	-6.30	1.16	1.24
1	E	73	HIS	ND1-CE1	6.30	1.38	1.32
2	i	55	THR	CA-C	-6.30	1.45	1.52
1	F	53	ARG	CZ-NH2	6.29	1.41	1.33
2	n	83	ARG	CA-C	-6.29	1.45	1.52
1	d	84	ASP	N-CA	-6.29	1.38	1.46
1	E	183	LEU	CA-C	6.29	1.60	1.52
1	E	206	PRO	N-CA	-6.29	1.40	1.47
2	2	160	GLY	C-N	6.29	1.41	1.33
2	3	61	GLY	C-N	6.29	1.42	1.33
1	A	169	ASN	CA-C	-6.29	1.44	1.52
1	d	169	ASN	CA-C	-6.29	1.45	1.52
2	7	69	ILE	N-CA	-6.29	1.39	1.46
1	A	215	LYS	C-N	6.29	1.42	1.33
3	J	109	ASN	C-N	6.29	1.43	1.33
1	C	79	SER	CA-C	-6.29	1.44	1.52
2	h	102	ARG	NE-CZ	6.29	1.40	1.33
1	d	219	ARG	CD-NE	6.28	1.55	1.46
3	L	53	SER	C-N	6.28	1.41	1.33
1	A	237	ASN	N-CA	-6.28	1.38	1.46
3	I	383	LEU	N-CA	-6.28	1.38	1.46
3	J	259	ARG	NE-CZ	6.28	1.40	1.33
1	b	53	ARG	CA-C	-6.28	1.44	1.52
3	K	41	ARG	CA-C	-6.28	1.44	1.52
2	3	167	LEU	CA-C	-6.28	1.44	1.52
3	K	155	GLU	CA-CB	6.27	1.63	1.53
2	i	156	THR	N-CA	-6.27	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	136	ASP	C-N	6.27	1.43	1.33
1	e	131	PRO	CA-C	-6.27	1.44	1.52
3	J	24	ARG	NE-CZ	6.27	1.40	1.33
2	n	102	ARG	CZ-NH1	6.27	1.41	1.32
3	J	205	ARG	N-CA	6.27	1.53	1.46
1	c	195	ALA	CA-C	-6.27	1.44	1.52
2	3	84	LYS	C-N	6.27	1.41	1.33
2	l	155	PHE	CA-C	-6.26	1.44	1.52
2	k	200	SER	C-N	6.26	1.43	1.33
1	d	75	CYS	CA-C	-6.26	1.45	1.52
2	n	109	GLN	CA-CB	6.26	1.63	1.53
3	M	28	ARG	N-CA	-6.26	1.38	1.46
2	1	44	LYS	CA-C	6.26	1.59	1.52
1	b	10	ARG	CD-NE	6.26	1.55	1.46
2	j	80	ARG	NE-CZ	6.26	1.40	1.33
2	k	36	PHE	C-N	6.26	1.42	1.33
1	B	113	ALA	CA-C	-6.25	1.44	1.52
2	1	87	VAL	N-CA	-6.25	1.38	1.46
2	m	180	SER	CA-C	-6.25	1.44	1.52
1	A	155	ALA	N-CA	6.25	1.54	1.45
3	H	46	ARG	CA-C	-6.25	1.44	1.52
3	H	302	ARG	CA-C	-6.25	1.44	1.52
2	1	114	GLY	CA-C	-6.24	1.44	1.52
3	I	216	ILE	N-CA	-6.24	1.39	1.46
1	f	242	GLU	CA-C	-6.24	1.44	1.52
3	H	333	ASP	CA-C	-6.24	1.44	1.52
3	L	80	LYS	CA-CB	6.24	1.61	1.53
1	a	25	GLU	C-N	6.24	1.42	1.33
1	f	74	ILE	N-CA	-6.24	1.38	1.46
1	b	86	ARG	CA-C	-6.24	1.44	1.52
1	D	64	ILE	N-CA	-6.24	1.38	1.46
2	5	63	ALA	C-N	6.24	1.42	1.33
3	I	367	ARG	CD-NE	6.24	1.54	1.46
2	i	169	VAL	CA-CB	-6.23	1.47	1.54
2	l	138	VAL	N-CA	-6.23	1.38	1.46
3	M	318	ILE	CA-C	-6.23	1.44	1.52
1	f	235	ARG	NE-CZ	6.23	1.40	1.33
2	l	115	ILE	CA-C	-6.23	1.45	1.52
3	H	82	SER	CA-CB	6.23	1.64	1.53
3	L	57	ARG	CD-NE	6.23	1.54	1.46
2	k	191	ILE	N-CA	-6.23	1.38	1.46
1	a	37	ALA	CA-C	-6.22	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	ARG	CZ-NH1	6.22	1.41	1.32
2	m	62	ASP	N-CA	-6.22	1.38	1.46
1	F	193	LEU	C-N	6.22	1.41	1.33
1	F	106	PRO	CA-C	-6.22	1.44	1.52
3	J	284	ILE	CA-C	-6.22	1.44	1.52
2	i	62	ASP	C-N	6.22	1.42	1.33
1	C	80	GLY	CA-C	-6.22	1.43	1.51
3	H	365	GLU	N-CA	-6.21	1.37	1.46
1	e	234	GLU	C-N	6.21	1.43	1.33
2	1	89	ALA	CA-C	-6.21	1.45	1.52
2	i	129	GLY	CA-C	-6.21	1.45	1.51
2	4	59	SER	CA-C	-6.21	1.44	1.52
3	M	370	VAL	N-CA	-6.21	1.38	1.46
1	g	243	LEU	N-CA	-6.21	1.38	1.46
2	n	155	PHE	CA-C	-6.21	1.45	1.52
2	3	81	ARG	NE-CZ	6.20	1.39	1.33
1	g	163	ALA	N-CA	-6.20	1.38	1.46
1	d	197	GLY	CA-C	-6.20	1.45	1.52
3	L	249	ARG	NE-CZ	6.20	1.39	1.33
3	M	90	ASN	CA-C	-6.19	1.44	1.52
2	j	60	VAL	C-O	-6.19	1.16	1.24
1	B	180	ARG	CZ-NH2	6.19	1.41	1.33
1	c	110	LYS	CA-C	-6.19	1.44	1.52
2	4	121	SER	N-CA	-6.19	1.38	1.46
3	K	363	ILE	C-N	6.19	1.43	1.33
2	3	111	LEU	CA-C	-6.19	1.45	1.52
1	d	53	ARG	C-N	6.18	1.42	1.33
3	H	290	ILE	C-N	6.18	1.43	1.33
3	J	78	VAL	C-N	6.18	1.41	1.33
2	5	104	PHE	N-CA	-6.18	1.40	1.46
3	M	307	ILE	CA-C	-6.18	1.45	1.52
1	G	99	ASN	CA-C	-6.18	1.44	1.52
1	B	235	ARG	CD-NE	6.17	1.54	1.46
2	n	204	VAL	CA-C	-6.17	1.44	1.52
2	5	124	SER	CA-C	-6.17	1.45	1.52
2	3	66	LEU	CA-CB	6.17	1.62	1.53
2	m	83	ARG	CA-C	-6.17	1.44	1.52
2	i	117	SER	N-CA	-6.17	1.38	1.46
1	C	58	LEU	CA-C	-6.16	1.45	1.52
1	f	21	LEU	C-N	6.16	1.42	1.33
2	4	19	CYS	CA-C	-6.16	1.45	1.52
3	I	10	LEU	CA-CB	6.16	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	217	GLY	C-N	6.16	1.42	1.33
1	d	176	GLU	CA-C	6.16	1.61	1.52
2	5	116	ASP	CA-CB	6.16	1.62	1.53
1	d	241	ARG	CD-NE	6.16	1.54	1.46
2	2	96	ASN	CA-C	-6.16	1.44	1.52
2	6	204	VAL	C-N	6.16	1.42	1.34
3	I	105	ARG	N-CA	6.16	1.53	1.46
1	D	38	ILE	CB-CG1	6.15	1.65	1.53
3	M	225	GLU	C-N	6.15	1.41	1.33
2	i	81	ARG	NE-CZ	6.15	1.39	1.33
2	j	81	ARG	CA-C	-6.15	1.44	1.52
1	D	209	ILE	N-CA	6.15	1.52	1.46
2	n	113	GLY	C-N	6.15	1.40	1.33
1	C	20	ARG	CD-NE	6.15	1.54	1.46
2	m	135	LYS	N-CA	-6.15	1.38	1.46
3	H	326	ARG	CZ-NH2	6.15	1.41	1.33
1	a	130	ARG	CA-C	-6.14	1.45	1.52
1	b	88	LEU	N-CA	-6.14	1.38	1.46
2	l	83	ARG	NE-CZ	6.14	1.39	1.33
1	D	123	TYR	CA-CB	6.14	1.63	1.53
2	i	36	PHE	C-N	6.14	1.41	1.33
3	H	358	ALA	CA-C	6.14	1.60	1.52
1	b	34	GLY	CA-C	-6.14	1.43	1.52
1	b	100	ARG	C-N	6.14	1.42	1.33
1	C	244	LEU	CA-C	-6.14	1.43	1.52
2	j	156	THR	CA-C	6.14	1.58	1.52
3	L	171	GLY	CA-C	-6.14	1.43	1.51
2	3	163	GLU	CA-C	-6.13	1.44	1.52
2	1	117	SER	CA-C	-6.13	1.44	1.52
2	7	203	GLU	CA-CB	6.13	1.62	1.53
3	L	184	PRO	CA-CB	6.13	1.62	1.53
1	F	141	VAL	C-O	-6.13	1.17	1.24
2	4	100	SER	N-CA	-6.13	1.39	1.46
2	m	169	VAL	CA-C	-6.13	1.44	1.52
2	k	17	LEU	C-N	6.13	1.41	1.33
2	7	106	TYR	C-N	6.12	1.41	1.33
3	M	85	PRO	CA-CB	6.12	1.61	1.53
1	f	220	THR	C-N	6.12	1.42	1.33
3	I	299	ARG	CD-NE	6.12	1.54	1.46
3	J	49	ARG	N-CA	6.12	1.53	1.46
3	M	100	LEU	CA-C	-6.12	1.45	1.52
1	C	85	ALA	C-N	6.12	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	17	PRO	N-CD	-6.12	1.39	1.47
2	1	197	TYR	C-O	-6.12	1.16	1.23
2	i	38	ALA	C-N	6.12	1.41	1.33
1	B	27	ALA	C-N	6.11	1.42	1.33
2	6	79	ILE	CA-C	-6.11	1.45	1.52
2	7	86	THR	CA-C	-6.11	1.44	1.53
3	I	199	THR	CA-C	-6.11	1.45	1.52
1	E	220	THR	CA-C	-6.11	1.44	1.52
1	e	201	GLU	CA-C	-6.11	1.45	1.53
3	M	250	ARG	CD-NE	6.11	1.54	1.46
3	H	368	ALA	C-N	6.11	1.42	1.33
2	l	68	ARG	CD-NE	6.10	1.54	1.46
2	4	166	GLU	CA-C	6.10	1.60	1.52
2	k	45	ILE	CA-CB	6.10	1.61	1.54
2	k	99	ASN	C-N	6.10	1.42	1.33
3	I	68	VAL	CA-CB	-6.10	1.47	1.54
2	j	39	SER	CA-C	-6.10	1.44	1.52
1	A	213	TYR	N-CA	-6.10	1.38	1.46
1	b	73	HIS	CD2-NE2	6.10	1.44	1.37
1	c	100	ARG	NE-CZ	6.10	1.39	1.33
3	J	278	ARG	CZ-NH2	6.10	1.41	1.33
1	d	176	GLU	CA-CB	6.10	1.63	1.53
2	i	30	ARG	NE-CZ	6.10	1.39	1.33
3	K	350	ASP	C-N	6.10	1.41	1.33
3	J	110	GLN	CA-CB	6.09	1.63	1.53
1	g	114	LYS	N-CA	6.09	1.53	1.46
1	e	241	ARG	N-CA	6.09	1.53	1.46
2	l	138	VAL	CA-C	-6.09	1.44	1.52
3	L	257	GLY	N-CA	-6.09	1.36	1.45
3	J	131	GLU	C-N	6.09	1.41	1.33
1	g	130	ARG	CZ-NH2	6.09	1.41	1.33
3	K	28	ARG	N-CA	-6.09	1.39	1.46
1	b	25	GLU	C-N	6.09	1.42	1.34
2	h	111	LEU	N-CA	-6.09	1.39	1.46
1	A	126	TYR	CA-CB	6.08	1.63	1.53
1	d	51	ASP	CA-CB	6.08	1.61	1.53
1	F	70	ILE	CA-CB	-6.08	1.46	1.54
2	4	102	ARG	CD-NE	6.08	1.54	1.46
2	5	154	ARG	CA-C	-6.08	1.44	1.52
3	L	52	ARG	CA-CB	6.08	1.62	1.53
3	M	52	ARG	CZ-NH1	6.08	1.41	1.32
1	a	35	ALA	CA-CB	6.08	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	36	PHE	CA-C	-6.08	1.45	1.52
3	I	259	ARG	NE-CZ	6.08	1.39	1.33
3	M	15	LYS	N-CA	-6.08	1.39	1.46
1	A	91	ARG	NE-CZ	6.08	1.39	1.33
1	G	220	THR	CA-C	-6.08	1.45	1.52
3	K	326	ARG	CD-NE	6.08	1.54	1.46
3	L	344	GLU	CA-C	-6.08	1.45	1.52
1	D	212	GLY	CA-C	-6.07	1.46	1.52
1	g	20	ARG	N-CA	-6.07	1.38	1.46
2	7	60	VAL	CA-C	-6.07	1.44	1.52
3	J	382	VAL	C-O	-6.07	1.16	1.24
1	B	47	ILE	CA-CB	6.07	1.62	1.54
1	b	233	VAL	C-N	6.07	1.41	1.33
3	J	75	GLY	CA-C	-6.07	1.41	1.51
2	7	116	ASP	CA-CB	6.07	1.63	1.53
3	H	50	ARG	NE-CZ	6.07	1.39	1.33
3	L	53	SER	CA-CB	6.07	1.62	1.53
1	F	101	LEU	N-CA	-6.07	1.39	1.46
2	2	25	MET	C-N	6.07	1.41	1.33
2	4	93	LEU	CA-C	-6.07	1.44	1.52
2	7	110	LEU	CA-C	-6.07	1.45	1.52
3	H	128	TYR	CA-C	6.06	1.60	1.52
1	f	47	ILE	CA-C	-6.06	1.45	1.52
2	j	191	ILE	CA-C	-6.06	1.44	1.52
1	G	53	ARG	CZ-NH2	6.06	1.41	1.33
1	B	209	ILE	CA-C	-6.06	1.45	1.52
2	k	67	ALA	CA-C	-6.06	1.45	1.52
1	A	73	HIS	CD2-NE2	6.06	1.44	1.37
1	e	241	ARG	CD-NE	6.05	1.54	1.46
1	f	163	ALA	C-N	6.05	1.41	1.33
3	I	97	GLU	N-CA	6.05	1.54	1.46
1	d	143	GLU	C-N	6.05	1.40	1.33
1	e	53	ARG	N-CA	6.04	1.53	1.46
3	M	172	ILE	N-CA	-6.04	1.38	1.46
1	f	97	GLN	N-CA	-6.04	1.38	1.46
2	j	126	ASP	N-CA	-6.04	1.38	1.45
3	K	364	ARG	NE-CZ	6.04	1.39	1.33
3	L	71	ILE	CA-CB	6.04	1.61	1.54
3	L	220	ALA	N-CA	-6.04	1.39	1.46
3	L	366	GLU	CA-C	-6.04	1.47	1.53
2	j	109	GLN	C-N	6.04	1.42	1.33
3	L	181	TYR	CA-C	-6.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	23	GLN	N-CA	-6.04	1.39	1.46
1	a	186	ASP	N-CA	-6.04	1.39	1.46
3	H	105	ARG	NE-CZ	6.04	1.39	1.33
1	D	208	ASN	CA-C	-6.04	1.45	1.53
3	J	23	LEU	C-N	6.04	1.41	1.33
3	J	396	MET	CA-C	-6.04	1.45	1.52
3	I	271	GLU	CA-CB	6.03	1.62	1.53
1	c	222	LYS	N-CA	6.03	1.53	1.45
3	I	211	PHE	CA-C	-6.03	1.45	1.52
3	M	315	GLU	N-CA	-6.03	1.39	1.46
1	G	165	GLY	CA-C	-6.03	1.43	1.51
2	j	204	VAL	N-CA	-6.03	1.39	1.46
2	j	58	GLY	C-N	6.03	1.41	1.33
3	J	242	GLU	CA-C	-6.03	1.45	1.52
2	h	186	ILE	C-O	-6.03	1.17	1.24
3	M	276	ASP	CA-CB	6.02	1.63	1.53
2	m	152	GLU	N-CA	-6.02	1.38	1.46
2	n	118	GLU	CA-C	-6.02	1.45	1.52
1	E	241	ARG	NE-CZ	6.02	1.39	1.33
2	j	88	ARG	NE-CZ	6.02	1.39	1.33
2	7	88	ARG	NE-CZ	6.02	1.39	1.33
3	H	40	GLU	N-CA	-6.02	1.39	1.46
3	L	249	ARG	CD-NE	6.02	1.54	1.46
1	A	208	ASN	C-N	6.01	1.40	1.33
1	a	176	GLU	C-N	6.01	1.42	1.33
3	K	41	ARG	CD-NE	6.01	1.54	1.46
1	A	33	ARG	NE-CZ	6.01	1.39	1.33
1	g	16	SER	CA-C	-6.01	1.46	1.52
2	5	47	GLN	N-CA	-6.01	1.39	1.46
1	C	133	GLY	CA-C	-6.01	1.43	1.51
3	K	228	GLN	CA-CB	6.01	1.62	1.53
1	B	28	ARG	NE-CZ	6.00	1.39	1.33
2	l	51	ARG	NE-CZ	6.00	1.39	1.33
1	F	189	MET	N-CA	-6.00	1.39	1.46
3	H	324	HIS	CD2-NE2	-6.00	1.31	1.37
3	J	326	ARG	NE-CZ	6.00	1.39	1.33
2	2	198	GLN	CA-CB	6.00	1.62	1.53
3	I	108	LEU	CA-C	-6.00	1.45	1.52
2	4	188	VAL	CA-C	-6.00	1.45	1.52
2	h	149	GLY	N-CA	-6.00	1.38	1.45
2	i	91	ALA	N-CA	-6.00	1.39	1.46
3	I	27	TYR	CA-CB	6.00	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	168	ARG	CD-NE	6.00	1.54	1.46
2	l	119	GLY	N-CA	6.00	1.51	1.45
2	1	16	GLY	C-N	6.00	1.41	1.33
2	7	106	TYR	CA-C	-6.00	1.45	1.52
2	7	127	PRO	N-CA	6.00	1.54	1.47
1	E	185	PHE	CA-CB	5.99	1.62	1.53
2	2	168	ALA	CA-C	-5.99	1.45	1.52
2	i	63	ALA	N-CA	-5.99	1.39	1.46
2	l	174	SER	C-N	5.99	1.41	1.33
1	a	116	ILE	CA-CB	-5.99	1.46	1.54
1	b	106	PRO	N-CA	-5.99	1.40	1.47
1	c	241	ARG	C-N	5.99	1.41	1.33
2	2	60	VAL	N-CA	-5.99	1.39	1.46
3	M	49	ARG	NE-CZ	5.99	1.39	1.33
2	5	80	ARG	CD-NE	5.99	1.54	1.46
3	I	291	ASP	CA-CB	5.99	1.62	1.53
2	2	52	MET	N-CA	-5.99	1.38	1.46
1	d	67	ILE	CA-CB	5.99	1.61	1.54
3	J	395	VAL	CA-C	-5.99	1.45	1.53
1	g	30	ALA	CA-CB	5.98	1.62	1.53
2	7	188	VAL	CA-C	-5.98	1.45	1.52
1	d	114	LYS	CA-C	-5.98	1.45	1.52
1	G	75	CYS	N-CA	-5.98	1.38	1.45
2	7	74	ALA	CA-CB	5.98	1.62	1.53
3	M	176	LYS	N-CA	5.98	1.53	1.46
3	L	327	LYS	CA-CB	5.98	1.63	1.53
3	M	69	SER	C-N	5.98	1.40	1.33
1	b	206	PRO	CA-C	-5.98	1.44	1.52
1	b	212	GLY	N-CA	-5.98	1.39	1.45
3	L	397	PHE	CA-C	-5.98	1.44	1.52
1	b	75	CYS	C-O	5.98	1.31	1.23
2	5	154	ARG	NE-CZ	5.97	1.39	1.33
2	5	139	ALA	CA-C	-5.97	1.45	1.52
2	3	138	VAL	C-N	5.97	1.42	1.33
2	4	154	ARG	CA-C	5.97	1.61	1.52
3	H	57	ARG	CZ-NH2	5.97	1.41	1.33
3	K	127	VAL	N-CA	-5.97	1.39	1.46
3	L	46	ARG	NE-CZ	5.97	1.39	1.33
2	k	32	THR	CA-C	5.97	1.59	1.52
1	A	43	LYS	CA-C	-5.96	1.44	1.52
1	c	20	ARG	CA-C	-5.96	1.45	1.52
1	E	68	TYR	N-CA	-5.96	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	191	LEU	C-N	5.96	1.41	1.34
3	H	316	GLY	CA-C	-5.96	1.45	1.52
3	I	372	MET	CA-C	-5.96	1.45	1.52
1	E	106	PRO	CA-CB	5.96	1.61	1.53
1	g	208	ASN	C-N	5.96	1.40	1.33
1	F	97	GLN	CA-C	-5.96	1.45	1.52
3	K	76	ARG	NE-CZ	5.96	1.39	1.33
1	c	69	LYS	CA-CB	5.96	1.61	1.53
1	D	10	ARG	CD-NE	5.96	1.54	1.46
3	M	196	ALA	CA-C	-5.95	1.45	1.52
1	D	197	GLY	N-CA	-5.95	1.38	1.45
3	L	103	GLY	C-N	5.95	1.41	1.33
1	G	234	GLU	CA-CB	5.95	1.62	1.53
2	5	199	TYR	CA-C	5.95	1.60	1.52
3	J	118	VAL	CA-C	-5.95	1.45	1.52
1	A	100	ARG	NE-CZ	5.95	1.39	1.33
2	n	101	TYR	CA-CB	5.95	1.61	1.53
3	M	357	GLU	CA-C	-5.95	1.45	1.52
1	F	189	MET	C-N	5.94	1.41	1.33
1	g	220	THR	C-N	5.94	1.42	1.33
2	k	110	LEU	N-CA	5.94	1.52	1.45
2	7	124	SER	C-N	5.94	1.41	1.33
2	6	81	ARG	CA-C	-5.94	1.44	1.52
1	b	164	ILE	C-N	5.94	1.41	1.32
2	h	145	LEU	CA-C	-5.94	1.45	1.52
1	d	66	LYS	C-N	5.94	1.40	1.33
2	j	65	PHE	CA-CB	5.94	1.62	1.53
2	6	170	ARG	CD-NE	5.94	1.54	1.46
3	M	24	ARG	NE-CZ	5.94	1.39	1.33
1	G	168	ARG	NE-CZ	5.93	1.39	1.33
3	K	20	TYR	CZ-OH	5.93	1.50	1.38
1	D	196	MET	CA-C	-5.93	1.44	1.52
1	G	37	ALA	CA-CB	5.93	1.63	1.53
2	1	154	ARG	CD-NE	5.93	1.54	1.46
2	1	155	PHE	C-O	-5.93	1.16	1.24
2	j	160	GLY	CA-C	-5.93	1.45	1.52
2	n	74	ALA	N-CA	-5.93	1.39	1.46
1	E	186	ASP	C-N	5.93	1.42	1.33
1	e	52	LYS	C-N	5.93	1.41	1.33
2	h	118	GLU	CA-C	-5.93	1.44	1.52
2	2	165	VAL	CA-CB	-5.93	1.46	1.54
3	I	319	GLN	C-N	5.93	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	71	LYS	CA-C	-5.93	1.45	1.52
2	7	81	ARG	CD-NE	5.93	1.54	1.46
1	b	30	ALA	CA-C	-5.93	1.45	1.52
1	C	28	ARG	CD-NE	5.93	1.54	1.46
1	E	93	ARG	CA-C	-5.93	1.45	1.52
2	j	60	VAL	CA-CB	5.93	1.62	1.54
2	m	51	ARG	C-N	5.93	1.42	1.33
1	B	235	ARG	NE-CZ	5.92	1.39	1.33
2	5	49	ALA	C-O	-5.92	1.18	1.24
2	l	104	PHE	CA-C	5.92	1.59	1.52
3	K	137	GLU	CA-CB	5.92	1.65	1.53
3	K	278	ARG	CD-NE	5.92	1.54	1.46
1	f	75	CYS	CA-C	-5.92	1.45	1.52
2	2	154	ARG	CZ-NH2	5.92	1.41	1.33
3	K	206	VAL	CA-C	-5.92	1.45	1.52
3	L	224	ARG	CD-NE	5.92	1.54	1.46
2	5	92	THR	C-N	5.92	1.42	1.33
3	J	180	LEU	C-N	5.92	1.40	1.33
1	b	23	GLN	CA-C	-5.92	1.45	1.52
2	4	103	TYR	C-N	5.92	1.43	1.33
1	F	141	VAL	CA-C	-5.92	1.45	1.52
2	7	212	ARG	CA-CB	5.92	1.59	1.54
3	J	280	ASP	CA-CB	5.92	1.61	1.53
3	J	304	ASP	CA-CB	5.92	1.62	1.53
2	4	92	THR	CA-C	-5.92	1.44	1.52
1	E	8	TYR	N-CA	-5.91	1.40	1.46
1	F	103	TYR	C-N	5.91	1.42	1.33
1	D	189	MET	C-N	5.91	1.41	1.33
3	H	338	GLU	CA-C	5.91	1.60	1.52
1	F	81	LEU	C-N	5.91	1.41	1.33
2	m	169	VAL	C-N	5.91	1.41	1.33
3	M	189	THR	N-CA	5.91	1.53	1.46
1	C	33	ARG	CZ-NH1	5.91	1.41	1.32
1	e	224	VAL	CA-C	-5.91	1.45	1.52
3	H	124	ASP	C-N	5.91	1.40	1.33
2	j	20	LYS	CA-C	-5.91	1.46	1.53
3	K	100	LEU	C-N	5.91	1.41	1.33
1	G	54	VAL	CA-CB	-5.90	1.46	1.54
3	I	89	VAL	N-CA	5.90	1.52	1.46
1	E	116	ILE	C-O	-5.90	1.17	1.24
1	c	213	TYR	CA-C	-5.90	1.45	1.52
1	d	219	ARG	C-N	5.90	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	177	GLY	CA-C	-5.90	1.45	1.51
3	L	41	ARG	NE-CZ	5.90	1.39	1.33
1	g	235	ARG	C-N	5.90	1.41	1.33
3	I	47	GLU	C-N	5.90	1.41	1.33
1	A	105	GLU	CA-C	-5.90	1.45	1.52
3	H	308	GLU	C-N	5.90	1.38	1.33
3	I	230	ALA	CA-C	-5.90	1.45	1.52
3	K	284	ILE	N-CA	-5.90	1.39	1.46
2	k	20	LYS	N-CA	-5.89	1.38	1.46
2	4	170	ARG	CD-NE	5.88	1.54	1.46
1	d	137	LEU	N-CA	-5.88	1.39	1.46
1	G	23	GLN	CD-NE2	5.88	1.45	1.33
2	1	142	SER	CA-C	-5.88	1.45	1.52
1	A	17	PRO	CA-C	5.88	1.62	1.52
1	D	32	LYS	C-N	5.88	1.41	1.33
3	M	348	GLY	CA-C	-5.88	1.45	1.52
2	k	166	GLU	CA-C	5.88	1.60	1.52
1	b	62	ASP	CA-C	-5.87	1.45	1.52
3	K	152	GLU	C-N	5.87	1.41	1.33
1	E	168	ARG	CZ-NH1	5.87	1.41	1.32
2	i	135	LYS	C-N	5.87	1.42	1.33
2	3	181	ALA	C-N	5.87	1.41	1.33
2	6	102	ARG	NE-CZ	5.87	1.39	1.33
1	C	19	GLY	CA-C	-5.87	1.43	1.51
3	J	113	LEU	CA-C	-5.87	1.48	1.53
2	k	79	ILE	C-N	5.87	1.41	1.33
1	d	47	ILE	CA-C	-5.86	1.45	1.52
2	5	30	ARG	CA-C	-5.86	1.45	1.52
2	n	137	ILE	CA-C	5.86	1.60	1.52
3	M	46	ARG	CA-C	-5.86	1.45	1.52
3	M	107	ALA	N-CA	-5.86	1.38	1.46
3	J	66	GLY	C-N	5.86	1.41	1.33
1	A	52	LYS	CA-C	-5.86	1.45	1.52
2	j	80	ARG	CA-C	-5.86	1.45	1.52
1	G	223	GLU	CA-CB	5.86	1.61	1.53
1	C	119	PHE	N-CA	-5.86	1.39	1.46
1	f	144	VAL	N-CA	-5.86	1.39	1.46
2	j	154	ARG	NE-CZ	5.86	1.39	1.33
2	j	206	GLN	C-N	5.86	1.41	1.33
2	m	76	LEU	CA-CB	5.86	1.62	1.53
3	K	314	PHE	CG-CD1	5.86	1.51	1.38
1	c	63	THR	C-N	5.85	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	38	ALA	C-N	5.85	1.40	1.33
3	J	339	LEU	CA-CB	5.85	1.62	1.53
1	g	229	LEU	CA-CB	5.85	1.62	1.53
3	L	213	GLN	C-N	5.85	1.42	1.33
1	f	119	PHE	C-N	5.85	1.41	1.33
2	3	164	ALA	N-CA	-5.85	1.38	1.46
3	H	66	GLY	C-N	5.85	1.41	1.33
1	A	77	ALA	N-CA	-5.84	1.39	1.45
1	C	209	ILE	C-O	-5.84	1.18	1.24
1	e	100	ARG	CD-NE	5.84	1.54	1.46
2	2	102	ARG	NE-CZ	5.84	1.39	1.33
2	j	18	VAL	CA-C	-5.84	1.45	1.52
2	j	80	ARG	CA-CB	5.84	1.62	1.53
2	k	78	GLU	N-CA	-5.84	1.39	1.46
1	a	17	PRO	CA-CB	-5.84	1.45	1.53
2	i	17	LEU	N-CA	-5.84	1.38	1.45
3	I	317	ARG	CD-NE	5.84	1.54	1.46
1	b	186	ASP	CA-C	-5.84	1.45	1.52
1	C	74	ILE	CA-C	-5.84	1.45	1.52
1	F	144	VAL	C-N	5.84	1.41	1.33
2	j	189	VAL	N-CA	-5.84	1.39	1.46
1	A	26	TYR	CA-C	-5.84	1.44	1.52
2	7	85	PRO	N-CA	-5.84	1.39	1.47
2	k	28	GLU	CA-C	-5.84	1.45	1.52
3	L	203	PHE	CA-CB	5.84	1.60	1.53
1	A	224	VAL	C-N	5.83	1.41	1.33
2	l	153	ASP	C-N	5.83	1.41	1.33
2	4	42	ALA	C-N	5.83	1.41	1.33
3	L	159	LEU	CA-C	-5.83	1.45	1.52
2	2	76	LEU	CA-C	-5.83	1.45	1.52
3	H	305	ARG	CD-NE	5.83	1.54	1.46
3	L	336	PHE	C-N	5.83	1.41	1.33
1	B	12	ILE	CA-CB	-5.83	1.48	1.54
2	1	152	GLU	N-CA	-5.83	1.38	1.46
1	B	107	ILE	N-CA	-5.83	1.39	1.46
2	5	196	PHE	CA-C	-5.83	1.46	1.53
3	J	256	SER	C-N	5.83	1.42	1.33
3	H	80	LYS	CA-CB	5.82	1.61	1.53
1	c	196	MET	CA-C	-5.82	1.45	1.52
2	l	122	ILE	C-O	-5.82	1.18	1.24
1	D	100	ARG	CZ-NH1	5.82	1.40	1.32
2	5	112	ILE	CA-CB	-5.82	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	211	PHE	C-N	5.82	1.41	1.33
3	H	381	LYS	C-N	5.82	1.41	1.33
3	I	289	ARG	CA-C	-5.82	1.45	1.52
3	H	196	ALA	CA-CB	5.82	1.62	1.53
3	K	296	ALA	C-N	5.82	1.38	1.33
1	c	239	ARG	C-N	5.81	1.41	1.33
3	L	11	GLU	N-CA	-5.81	1.38	1.46
2	1	153	ASP	CA-C	-5.81	1.45	1.52
2	l	129	GLY	CA-C	-5.81	1.46	1.52
2	l	197	TYR	CA-CB	5.81	1.63	1.53
1	f	231	PRO	N-CA	-5.81	1.40	1.47
2	3	23	VAL	CA-C	-5.81	1.45	1.52
3	I	154	ARG	CZ-NH1	5.81	1.40	1.32
3	K	15	LYS	N-CA	-5.81	1.39	1.46
3	L	121	THR	N-CA	-5.81	1.39	1.46
2	4	81	ARG	CA-CB	5.81	1.63	1.53
1	g	80	GLY	C-N	5.81	1.41	1.33
1	f	117	CYS	CA-C	-5.80	1.44	1.52
2	h	191	ILE	CA-C	-5.80	1.45	1.52
2	6	30	ARG	CZ-NH2	5.80	1.41	1.33
3	H	15	LYS	CA-C	-5.80	1.45	1.52
1	d	110	LYS	CA-CB	5.80	1.62	1.53
1	A	112	LEU	CB-CG	5.80	1.65	1.53
1	F	33	ARG	NE-CZ	5.80	1.39	1.33
3	K	326	ARG	NE-CZ	5.80	1.39	1.33
2	i	112	ILE	N-CA	-5.80	1.39	1.46
2	7	97	LEU	CA-C	-5.80	1.45	1.52
3	M	278	ARG	NE-CZ	5.80	1.39	1.33
3	J	230	ALA	C-N	5.80	1.41	1.33
2	m	181	ALA	C-N	5.79	1.41	1.33
1	d	235	ARG	NE-CZ	5.79	1.39	1.33
1	E	199	SER	CA-C	-5.79	1.45	1.52
1	G	160	LYS	CA-CB	5.79	1.62	1.53
3	M	228	GLN	CA-C	-5.79	1.45	1.52
2	i	159	ILE	N-CA	5.79	1.53	1.46
2	6	34	GLY	C-N	5.79	1.41	1.33
1	C	148	TYR	CA-C	-5.79	1.45	1.52
1	G	54	VAL	C-N	5.79	1.42	1.33
2	1	112	ILE	N-CA	-5.79	1.39	1.46
2	k	135	LYS	CA-C	-5.79	1.45	1.52
3	K	76	ARG	CD-NE	5.79	1.54	1.46
3	M	113	LEU	C-N	5.79	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	211	PHE	CA-C	-5.79	1.45	1.53
2	k	158	GLU	C-N	5.79	1.40	1.33
2	2	88	ARG	CZ-NH1	5.79	1.40	1.32
1	f	225	SER	C-N	5.78	1.40	1.33
2	m	179	ASP	N-CA	-5.78	1.38	1.46
1	B	23	GLN	N-CA	-5.78	1.39	1.46
1	f	70	ILE	CA-C	-5.78	1.46	1.52
2	5	30	ARG	CD-NE	5.78	1.54	1.46
2	6	131	ALA	CA-C	-5.78	1.45	1.52
2	7	134	GLU	CA-C	-5.78	1.45	1.52
3	L	43	ARG	CD-NE	5.78	1.54	1.46
1	G	100	ARG	CA-C	-5.78	1.44	1.52
3	L	230	ALA	C-N	5.78	1.41	1.33
1	B	149	GLU	CA-C	-5.77	1.45	1.52
3	H	43	ARG	CZ-NH2	5.77	1.41	1.33
3	M	395	VAL	N-CA	-5.77	1.39	1.46
1	a	32	LYS	N-CA	-5.77	1.39	1.46
2	l	66	LEU	CA-C	-5.77	1.45	1.52
2	h	80	ARG	NE-CZ	5.77	1.39	1.33
2	i	204	VAL	C-N	5.77	1.41	1.34
2	j	13	THR	CA-C	5.77	1.59	1.52
2	k	204	VAL	N-CA	5.77	1.53	1.46
1	C	137	LEU	CA-C	-5.77	1.45	1.52
1	E	20	ARG	NE-CZ	5.77	1.39	1.33
2	1	122	ILE	N-CA	5.77	1.53	1.46
2	2	52	MET	CA-C	-5.77	1.45	1.52
3	L	163	LYS	N-CA	-5.77	1.38	1.46
2	i	43	LYS	N-CA	-5.76	1.38	1.46
3	L	248	ALA	C-N	5.76	1.41	1.33
3	J	111	GLN	N-CA	-5.76	1.39	1.46
1	D	76	ALA	CA-C	-5.76	1.45	1.52
3	H	26	LEU	CA-C	-5.76	1.45	1.52
3	M	174	PRO	C-O	-5.76	1.19	1.24
1	a	182	ASP	CA-C	-5.76	1.45	1.52
1	A	186	ASP	C-N	5.76	1.41	1.33
2	2	210	LYS	CA-C	-5.76	1.44	1.52
1	A	86	ARG	NE-CZ	5.75	1.39	1.33
1	a	230	LYS	CA-CB	5.75	1.60	1.53
1	B	154	GLY	C-N	5.75	1.41	1.33
2	h	69	ILE	CA-CB	-5.75	1.47	1.54
2	j	127	PRO	C-N	5.75	1.40	1.33
2	6	80	ARG	NE-CZ	5.75	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	150	VAL	CA-C	-5.75	1.45	1.52
2	n	61	GLY	CA-C	-5.75	1.43	1.51
3	J	375	PHE	CA-CB	-5.75	1.44	1.53
2	l	54	MET	N-CA	-5.75	1.38	1.46
2	7	32	THR	CA-C	-5.75	1.45	1.52
1	B	78	THR	C-N	5.75	1.41	1.33
1	c	245	LYS	CA-C	5.75	1.60	1.52
1	d	19	GLY	N-CA	-5.75	1.37	1.45
2	2	188	VAL	N-CA	-5.75	1.39	1.46
1	B	219	ARG	CD-NE	5.75	1.54	1.46
1	c	156	LEU	CA-C	-5.74	1.45	1.52
2	m	134	GLU	CA-C	-5.74	1.45	1.52
1	B	45	GLY	C-N	5.74	1.40	1.33
2	6	40	LYS	CA-CB	5.74	1.63	1.53
1	A	211	VAL	N-CA	-5.74	1.39	1.46
3	K	99	GLU	N-CA	-5.74	1.38	1.46
3	L	162	LEU	CA-CB	5.74	1.62	1.54
3	K	155	GLU	N-CA	-5.74	1.39	1.46
1	a	69	LYS	CA-C	-5.73	1.45	1.52
1	f	28	ARG	CD-NE	5.73	1.54	1.46
1	E	168	ARG	CZ-NH2	5.73	1.41	1.33
1	G	189	MET	CA-C	-5.73	1.45	1.52
3	L	280	ASP	C-N	5.73	1.40	1.33
3	M	302	ARG	NE-CZ	5.73	1.39	1.33
3	J	31	GLU	N-CA	-5.73	1.39	1.46
1	G	18	ASP	CA-C	-5.73	1.44	1.52
2	l	76	LEU	CA-C	-5.73	1.45	1.52
1	a	104	ASP	CA-CB	5.73	1.61	1.53
2	3	51	ARG	NE-CZ	5.73	1.39	1.33
2	3	97	LEU	CA-C	5.73	1.60	1.52
3	M	317	ARG	N-CA	5.73	1.53	1.46
1	F	31	VAL	C-N	5.72	1.41	1.33
2	j	102	ARG	NE-CZ	5.72	1.39	1.33
3	L	248	ALA	CA-C	-5.72	1.46	1.52
1	d	54	VAL	CA-CB	-5.72	1.46	1.54
3	J	241	ASP	C-N	5.72	1.40	1.33
2	4	197	TYR	CA-C	-5.72	1.45	1.52
1	B	227	GLU	N-CA	-5.72	1.39	1.46
3	H	73	GLU	C-N	5.72	1.41	1.33
3	L	262	GLN	C-N	5.72	1.41	1.33
1	e	100	ARG	CZ-NH2	5.72	1.40	1.33
1	b	241	ARG	N-CA	-5.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	89	ALA	C-N	5.71	1.40	1.33
2	4	66	LEU	CA-C	-5.71	1.44	1.52
2	k	170	ARG	CA-C	-5.71	1.44	1.52
2	n	51	ARG	NE-CZ	5.71	1.39	1.33
3	K	325	THR	CA-CB	-5.71	1.44	1.53
3	M	167	PHE	CA-C	-5.71	1.45	1.52
1	a	130	ARG	CZ-NH2	5.71	1.40	1.33
1	a	161	ALA	N-CA	-5.71	1.38	1.46
2	l	153	ASP	CA-C	-5.71	1.45	1.52
1	B	57	LYS	CA-C	-5.71	1.44	1.52
2	4	75	ASN	CA-C	-5.71	1.45	1.52
3	K	310	PRO	CA-CB	-5.71	1.45	1.53
1	e	123	TYR	CA-CB	5.71	1.62	1.54
1	d	158	GLU	N-CA	5.71	1.53	1.46
1	F	23	GLN	C-N	5.71	1.40	1.33
1	G	231	PRO	CA-C	-5.71	1.43	1.52
2	2	170	ARG	CZ-NH1	5.71	1.40	1.32
1	c	183	LEU	C-N	5.71	1.41	1.33
1	c	219	ARG	CA-C	-5.71	1.45	1.53
3	L	354	ILE	CA-C	5.71	1.59	1.52
2	l	100	SER	N-CA	-5.70	1.38	1.46
2	m	199	TYR	CA-C	5.70	1.60	1.52
1	C	122	GLN	CA-CB	5.70	1.62	1.53
3	H	200	ARG	CD-NE	5.70	1.54	1.46
2	l	30	ARG	CZ-NH2	5.70	1.40	1.33
2	m	18	VAL	CA-C	-5.70	1.46	1.52
2	n	114	GLY	N-CA	5.70	1.52	1.45
1	b	24	VAL	CA-C	-5.70	1.45	1.52
1	e	42	CYS	C-N	5.70	1.42	1.33
2	7	112	ILE	CA-CB	-5.70	1.47	1.54
3	M	341	ARG	CD-NE	5.70	1.54	1.46
2	m	128	ILE	CA-C	-5.70	1.45	1.52
1	C	93	ARG	C-O	-5.70	1.17	1.24
2	j	51	ARG	C-N	5.70	1.41	1.33
3	J	330	LEU	CA-C	-5.70	1.45	1.52
1	d	31	VAL	CA-CB	-5.69	1.47	1.54
1	f	239	ARG	CD-NE	5.69	1.54	1.46
2	k	212	ARG	CA-C	-5.69	1.45	1.52
3	M	256	SER	CA-CB	5.69	1.62	1.53
3	J	171	GLY	N-CA	-5.69	1.36	1.45
1	a	86	ARG	CA-C	-5.69	1.45	1.52
1	D	21	LEU	C-N	5.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	150	ILE	N-CA	-5.69	1.39	1.46
2	j	110	LEU	N-CA	-5.69	1.39	1.45
2	7	107	LEU	C-N	5.69	1.40	1.33
3	I	218	GLU	CA-C	5.69	1.60	1.52
3	L	395	VAL	C-N	5.69	1.41	1.33
3	J	213	GLN	CA-CB	5.69	1.63	1.53
3	J	364	ARG	C-N	5.69	1.41	1.33
1	B	75	CYS	C-N	5.68	1.41	1.33
1	b	91	ARG	CD-NE	5.68	1.54	1.46
2	2	167	LEU	N-CA	-5.68	1.39	1.46
3	I	341	ARG	CD-NE	5.68	1.54	1.46
3	L	80	LYS	C-N	5.68	1.40	1.33
1	B	61	ALA	CA-C	-5.68	1.45	1.52
2	7	41	ALA	C-N	5.68	1.41	1.33
1	e	91	ARG	NE-CZ	5.68	1.39	1.33
3	I	326	ARG	NE-CZ	5.68	1.39	1.33
1	d	86	ARG	CA-C	-5.68	1.45	1.52
2	m	191	ILE	N-CA	-5.67	1.39	1.46
2	k	184	ASP	CA-CB	5.67	1.61	1.53
1	e	10	ARG	CZ-NH1	5.67	1.40	1.32
2	k	36	PHE	CA-CB	5.67	1.61	1.53
1	A	216	VAL	CA-CB	-5.67	1.46	1.54
2	1	143	GLY	C-N	5.67	1.41	1.33
2	2	112	ILE	CA-C	-5.67	1.45	1.52
2	n	30	ARG	CZ-NH2	5.67	1.40	1.33
1	F	215	LYS	CA-C	-5.67	1.45	1.52
3	J	158	GLU	N-CA	-5.67	1.39	1.46
1	B	10	ARG	NE-CZ	5.67	1.39	1.33
1	B	52	LYS	CA-CB	5.67	1.61	1.53
1	b	27	ALA	N-CA	-5.66	1.39	1.46
3	I	85	PRO	N-CA	-5.66	1.40	1.47
1	b	82	VAL	N-CA	-5.66	1.39	1.46
1	b	148	TYR	N-CA	-5.66	1.38	1.45
1	D	177	LYS	CA-C	-5.66	1.45	1.53
2	l	30	ARG	NE-CZ	5.66	1.39	1.33
3	L	249	ARG	CZ-NH2	5.66	1.40	1.33
1	b	116	ILE	CA-C	-5.66	1.44	1.52
2	3	128	ILE	C-N	5.66	1.44	1.33
2	4	62	ASP	CA-C	-5.66	1.45	1.52
2	n	138	VAL	C-N	5.66	1.41	1.33
3	M	52	ARG	C-N	5.66	1.41	1.33
3	M	69	SER	CA-CB	5.66	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	219	GLY	N-CA	-5.66	1.38	1.45
1	a	91	ARG	NE-CZ	5.66	1.39	1.33
1	a	105	GLU	CA-C	-5.66	1.46	1.52
2	4	72	ILE	CA-CB	5.66	1.61	1.54
2	i	197	TYR	CA-C	-5.65	1.46	1.52
3	K	89	VAL	C-N	5.65	1.41	1.33
1	A	193	LEU	C-N	5.65	1.41	1.33
3	L	107	ALA	N-CA	-5.65	1.38	1.45
3	I	79	VAL	CA-C	5.65	1.59	1.52
2	6	26	ALA	CA-C	-5.65	1.45	1.52
1	A	159	TYR	CA-C	-5.65	1.45	1.52
2	2	202	GLU	N-CA	5.65	1.53	1.46
2	l	128	ILE	CB-CG1	5.65	1.64	1.53
2	m	180	SER	C-N	5.65	1.42	1.33
3	H	206	VAL	CA-C	-5.65	1.45	1.52
1	b	130	ARG	CA-C	-5.65	1.45	1.52
2	6	180	SER	CA-C	-5.65	1.47	1.52
3	J	247	ALA	C-O	-5.65	1.16	1.24
2	1	159	ILE	C-O	-5.64	1.18	1.24
2	h	103	TYR	CZ-OH	5.64	1.50	1.38
3	I	53	SER	CA-C	-5.64	1.45	1.52
1	C	10	ARG	CZ-NH2	5.64	1.40	1.33
1	c	238	GLU	CA-C	-5.64	1.45	1.52
1	f	214	VAL	N-CA	-5.64	1.39	1.46
2	1	209	ALA	N-CA	-5.64	1.38	1.46
1	a	235	ARG	NE-CZ	5.63	1.39	1.33
1	C	243	LEU	CA-CB	5.63	1.62	1.53
1	c	138	ILE	CB-CG1	5.63	1.64	1.53
1	d	200	ILE	CA-CB	-5.63	1.47	1.54
1	e	133	GLY	C-N	5.63	1.38	1.33
3	K	314	PHE	N-CA	-5.63	1.39	1.46
1	C	164	ILE	CA-C	-5.63	1.45	1.52
1	B	158	GLU	CA-C	-5.63	1.46	1.52
1	D	137	LEU	CA-C	-5.63	1.46	1.52
2	3	202	GLU	C-N	5.63	1.41	1.33
3	H	146	LEU	CA-C	-5.63	1.44	1.52
1	D	233	VAL	CA-C	5.63	1.59	1.52
1	F	103	TYR	CA-C	-5.63	1.44	1.52
1	F	132	PHE	C-N	5.63	1.41	1.33
1	g	147	LEU	C-N	5.63	1.40	1.33
3	I	48	VAL	C-N	5.63	1.41	1.34
3	K	101	LYS	CA-C	-5.63	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	171	ALA	CA-CB	5.62	1.62	1.53
3	I	70	ASP	CA-C	-5.62	1.45	1.52
1	B	64	ILE	C-N	5.62	1.41	1.33
2	k	64	GLN	C-N	5.62	1.41	1.33
2	5	173	TYR	C-N	5.62	1.41	1.33
1	g	10	ARG	CZ-NH2	5.62	1.40	1.33
2	4	139	ALA	CA-C	-5.62	1.45	1.52
3	I	197	ASN	CG-ND2	5.62	1.45	1.33
1	c	45	GLY	C-N	5.62	1.39	1.33
2	j	51	ARG	CD-NE	5.62	1.54	1.46
2	m	142	SER	C-N	5.62	1.40	1.33
2	n	212	ARG	CZ-NH1	5.62	1.40	1.32
3	H	54	GLU	C-N	5.62	1.40	1.34
3	J	43	ARG	CD-NE	5.62	1.54	1.46
3	L	76	ARG	CD-NE	5.61	1.54	1.46
2	k	39	SER	CA-CB	5.61	1.61	1.53
1	b	120	LYS	CA-C	-5.61	1.45	1.52
1	d	52	LYS	CA-C	-5.61	1.45	1.52
1	g	171	VAL	CA-CB	-5.61	1.47	1.54
1	e	150	THR	C-N	5.61	1.41	1.33
1	G	67	ILE	CA-C	-5.61	1.46	1.52
2	4	204	VAL	CA-C	-5.61	1.44	1.52
3	I	310	PRO	CA-C	-5.61	1.47	1.53
1	f	206	PRO	CA-C	-5.60	1.45	1.52
1	b	112	LEU	N-CA	5.60	1.53	1.46
1	e	229	LEU	C-N	5.60	1.41	1.33
1	e	229	LEU	CA-CB	5.60	1.62	1.53
1	D	241	ARG	NE-CZ	5.60	1.39	1.33
2	7	138	VAL	N-CA	-5.60	1.39	1.46
1	c	187	ASP	CA-C	-5.60	1.45	1.52
1	d	145	PRO	CA-C	-5.60	1.46	1.52
1	f	240	ILE	CA-C	5.60	1.59	1.52
3	K	9	LEU	CA-C	-5.60	1.41	1.52
1	C	179	TYR	CA-C	-5.59	1.45	1.52
1	f	219	ARG	CZ-NH2	5.59	1.40	1.33
2	k	13	THR	C-N	5.59	1.41	1.33
3	K	364	ARG	CZ-NH2	5.59	1.40	1.33
2	i	121	SER	CA-C	5.59	1.59	1.52
1	b	113	ALA	N-CA	-5.59	1.39	1.46
2	3	179	ASP	N-CA	-5.59	1.38	1.45
3	I	285	GLY	CA-C	-5.59	1.45	1.51
1	F	138	ILE	CA-C	-5.59	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	68	ARG	C-N	5.59	1.41	1.33
2	k	110	LEU	C-N	5.59	1.40	1.33
3	J	304	ASP	N-CA	-5.59	1.39	1.46
1	d	91	ARG	CA-C	-5.59	1.45	1.52
3	H	317	ARG	CZ-NH2	5.59	1.40	1.33
3	L	190	LEU	C-N	5.59	1.41	1.33
3	L	132	VAL	N-CA	-5.58	1.39	1.46
1	F	142	ASP	CA-CB	5.58	1.62	1.53
2	3	73	GLU	C-N	5.58	1.41	1.33
3	L	260	GLU	CA-C	-5.58	1.45	1.52
1	d	125	GLN	C-N	5.58	1.41	1.33
1	d	235	ARG	CD-NE	5.58	1.54	1.46
2	j	177	LYS	N-CA	-5.58	1.39	1.46
3	H	137	GLU	N-CA	-5.58	1.39	1.46
1	a	154	GLY	C-N	5.58	1.40	1.33
3	I	183	PRO	CA-C	5.58	1.57	1.52
3	L	224	ARG	CA-C	-5.58	1.45	1.52
3	H	119	LEU	C-N	5.58	1.40	1.33
3	I	177	GLY	C-O	-5.58	1.18	1.23
2	1	175	ALA	CA-CB	5.57	1.62	1.53
2	3	136	ASP	CA-CB	5.57	1.62	1.53
2	2	208	LEU	CA-C	-5.57	1.44	1.52
1	g	92	ALA	N-CA	5.57	1.53	1.46
2	3	212	ARG	CD-NE	5.57	1.54	1.46
2	4	155	PHE	CA-C	-5.57	1.45	1.52
2	4	162	ASP	N-CA	-5.57	1.39	1.46
3	M	217	GLY	C-N	5.57	1.41	1.33
1	b	126	TYR	N-CA	-5.57	1.39	1.46
1	c	144	VAL	N-CA	-5.57	1.39	1.46
2	l	198	GLN	CA-C	-5.57	1.46	1.52
1	C	210	GLU	C-N	5.57	1.40	1.33
1	E	194	VAL	CA-CB	-5.57	1.47	1.54
3	H	229	LEU	CA-C	-5.57	1.45	1.52
3	K	174	PRO	N-CD	-5.57	1.40	1.47
3	L	384	LYS	C-O	-5.57	1.17	1.24
3	J	46	ARG	CZ-NH1	5.57	1.40	1.32
1	C	219	ARG	NE-CZ	5.56	1.39	1.33
2	6	190	LYS	N-CA	-5.56	1.39	1.46
3	K	249	ARG	CA-C	-5.56	1.45	1.53
3	K	278	ARG	NE-CZ	5.56	1.39	1.33
2	n	100	SER	CA-CB	5.56	1.62	1.53
2	m	50	ASP	C-N	5.56	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	125	ILE	CA-C	-5.56	1.45	1.52
2	l	145	LEU	N-CA	-5.56	1.39	1.46
1	d	91	ARG	N-CA	-5.55	1.39	1.46
2	m	178	ARG	NE-CZ	5.55	1.39	1.33
3	H	378	ALA	C-N	5.55	1.41	1.33
1	E	210	GLU	N-CA	-5.55	1.39	1.46
3	H	394	GLY	N-CA	-5.55	1.38	1.45
3	K	259	ARG	CZ-NH2	5.55	1.40	1.33
3	M	147	ASP	CA-C	5.55	1.60	1.52
1	C	219	ARG	CD-NE	5.55	1.54	1.46
2	2	81	ARG	CZ-NH2	5.55	1.40	1.33
2	3	17	LEU	CA-CB	-5.55	1.44	1.53
3	I	221	ARG	CZ-NH2	5.55	1.40	1.33
1	C	54	VAL	CA-C	5.55	1.58	1.52
1	f	161	ALA	CA-C	-5.55	1.45	1.52
1	c	105	GLU	C-O	-5.55	1.17	1.24
2	j	63	ALA	C-O	-5.55	1.17	1.24
1	c	203	GLU	N-CA	-5.54	1.38	1.45
2	i	137	ILE	N-CA	-5.54	1.40	1.46
3	M	322	LYS	CA-C	5.54	1.59	1.52
2	j	65	PHE	C-O	-5.54	1.17	1.24
2	n	175	ALA	C-N	5.54	1.41	1.33
1	b	194	VAL	CA-C	-5.54	1.46	1.52
1	E	144	VAL	C-N	5.54	1.40	1.33
1	E	147	LEU	N-CA	-5.54	1.39	1.46
1	e	156	LEU	C-N	5.54	1.41	1.33
1	G	208	ASN	CA-CB	5.54	1.61	1.53
2	h	197	TYR	C-N	5.54	1.41	1.33
1	a	54	VAL	CA-CB	-5.54	1.47	1.54
1	B	235	ARG	CZ-NH1	5.54	1.40	1.32
2	5	111	LEU	CA-C	-5.54	1.45	1.52
3	J	89	VAL	CA-C	-5.54	1.46	1.52
2	i	84	LYS	CA-C	-5.54	1.46	1.53
3	H	274	GLY	N-CA	-5.54	1.38	1.45
3	K	113	LEU	N-CA	-5.54	1.38	1.46
3	I	218	GLU	C-N	5.53	1.41	1.33
3	I	258	ASP	N-CA	5.53	1.52	1.46
1	C	73	HIS	CB-CG	5.53	1.57	1.50
1	a	245	LYS	CA-CB	5.53	1.62	1.54
1	D	170	ALA	C-O	-5.53	1.17	1.24
3	H	22	LYS	C-N	5.53	1.41	1.34
3	M	70	ASP	CA-CB	5.53	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	88	ARG	NE-CZ	5.53	1.39	1.33
2	i	199	TYR	CA-C	-5.53	1.45	1.52
1	F	11	ALA	CA-CB	5.53	1.62	1.53
2	5	140	THR	CA-C	-5.53	1.45	1.52
2	4	106	TYR	CA-C	-5.52	1.46	1.52
2	k	118	GLU	CA-CB	5.52	1.63	1.53
2	6	80	ARG	CA-C	-5.52	1.45	1.52
3	H	57	ARG	CD-NE	5.52	1.53	1.46
3	L	129	GLY	N-CA	-5.52	1.38	1.45
3	L	269	LEU	CA-C	-5.52	1.45	1.52
1	F	223	GLU	CA-C	-5.52	1.45	1.52
2	3	85	PRO	CA-C	-5.52	1.47	1.53
1	e	140	GLY	CA-C	-5.52	1.45	1.51
1	F	188	ALA	C-O	-5.52	1.17	1.24
3	M	384	LYS	C-O	5.52	1.30	1.24
1	c	154	GLY	C-N	5.52	1.41	1.33
2	2	153	ASP	CA-C	-5.52	1.45	1.52
2	j	15	VAL	N-CA	-5.52	1.40	1.46
2	6	170	ARG	CA-C	-5.52	1.45	1.52
2	h	114	GLY	CA-C	-5.51	1.44	1.52
2	j	98	LEU	C-N	5.51	1.41	1.33
3	K	333	ASP	CA-CB	5.51	1.62	1.53
3	J	168	ALA	C-N	5.51	1.41	1.33
1	C	191	LEU	C-N	5.51	1.40	1.33
1	d	48	LEU	CA-C	-5.51	1.46	1.52
2	h	186	ILE	CA-C	5.51	1.59	1.52
2	n	26	ALA	CA-C	-5.51	1.45	1.52
1	C	243	LEU	C-N	5.51	1.40	1.33
2	2	24	VAL	CA-C	-5.51	1.45	1.52
1	g	78	THR	C-N	5.51	1.40	1.33
3	I	321	PHE	C-N	5.51	1.40	1.33
3	K	265	MET	C-N	5.51	1.41	1.34
3	H	143	ILE	CA-CB	-5.50	1.47	1.54
1	b	232	TYR	CA-CB	5.50	1.62	1.53
2	2	170	ARG	NE-CZ	5.50	1.39	1.33
2	j	196	PHE	CA-C	-5.50	1.45	1.53
2	7	173	TYR	CA-C	-5.50	1.45	1.52
3	J	57	ARG	NE-CZ	5.50	1.39	1.33
1	a	200	ILE	CA-CB	-5.50	1.47	1.54
2	1	153	ASP	C-O	-5.50	1.17	1.24
2	1	199	TYR	CA-C	-5.50	1.45	1.52
3	I	367	ARG	CA-CB	5.50	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	362	ALA	N-CA	-5.50	1.39	1.46
1	c	50	ALA	N-CA	-5.50	1.39	1.46
1	D	47	ILE	N-CA	-5.50	1.39	1.46
1	a	182	ASP	CA-CB	5.50	1.62	1.53
2	l	95	SER	CA-C	-5.50	1.45	1.52
2	6	60	VAL	CA-C	-5.50	1.45	1.52
3	H	52	ARG	NE-CZ	5.50	1.39	1.33
3	M	368	ALA	CA-C	-5.50	1.46	1.53
1	d	203	GLU	CA-C	5.50	1.59	1.52
2	1	170	ARG	NE-CZ	5.50	1.39	1.33
3	H	210	GLU	C-N	5.50	1.40	1.33
3	L	111	GLN	CA-C	-5.50	1.45	1.52
3	M	28	ARG	CA-C	5.50	1.59	1.52
1	A	143	GLU	C-N	5.49	1.39	1.33
1	B	100	ARG	C-N	5.49	1.40	1.33
1	E	42	CYS	CA-C	-5.49	1.45	1.52
1	f	25	GLU	C-N	5.49	1.41	1.33
1	g	152	PRO	CA-CB	-5.49	1.46	1.53
2	3	170	ARG	NE-CZ	5.49	1.39	1.33
2	m	206	GLN	C-N	5.49	1.41	1.33
3	K	142	ASP	CA-C	-5.49	1.45	1.53
1	C	100	ARG	NE-CZ	5.49	1.39	1.33
2	2	206	GLN	C-N	5.49	1.40	1.33
2	7	54	MET	N-CA	-5.49	1.39	1.46
3	H	341	ARG	C-N	5.49	1.40	1.33
3	L	319	GLN	CA-CB	-5.49	1.44	1.53
3	L	351	ILE	CA-C	-5.49	1.45	1.52
3	J	248	ALA	CA-CB	5.49	1.62	1.53
1	a	183	LEU	CA-C	-5.48	1.46	1.52
1	E	168	ARG	NE-CZ	5.48	1.39	1.33
1	e	138	ILE	CA-CB	-5.48	1.47	1.54
2	k	51	ARG	CZ-NH1	5.48	1.40	1.32
1	B	221	PHE	N-CA	-5.48	1.39	1.46
1	G	205	VAL	C-N	-5.48	1.28	1.34
1	g	67	ILE	N-CA	-5.48	1.39	1.46
2	2	125	ILE	CA-C	-5.48	1.45	1.52
2	5	203	GLU	CA-C	-5.48	1.45	1.52
1	D	86	ARG	NE-CZ	5.48	1.39	1.33
2	1	121	SER	C-N	5.48	1.40	1.33
3	H	46	ARG	CZ-NH2	5.48	1.40	1.33
3	H	380	GLU	CA-C	-5.48	1.45	1.52
3	L	28	ARG	CZ-NH2	5.48	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	214	LYS	CA-CB	5.47	1.62	1.53
1	G	233	VAL	C-O	-5.47	1.18	1.24
2	6	54	MET	CA-C	-5.47	1.45	1.52
2	6	82	GLU	C-N	5.47	1.40	1.33
1	a	33	ARG	NE-CZ	5.47	1.39	1.33
1	b	93	ARG	CZ-NH1	5.47	1.40	1.32
1	b	239	ARG	CD-NE	5.47	1.53	1.46
1	C	119	PHE	CB-CG	5.47	1.63	1.50
2	5	204	VAL	CA-C	-5.47	1.45	1.52
3	H	379	ILE	N-CA	-5.47	1.40	1.46
3	J	113	LEU	N-CA	-5.47	1.39	1.46
1	F	22	PHE	N-CA	-5.47	1.39	1.46
3	K	239	PHE	C-O	-5.47	1.17	1.24
1	a	44	GLU	C-N	5.47	1.43	1.33
1	E	14	VAL	CA-C	-5.47	1.46	1.52
1	g	28	ARG	CA-C	-5.47	1.45	1.52
3	I	263	ARG	CZ-NH2	5.46	1.40	1.33
1	D	212	GLY	C-N	5.46	1.40	1.33
1	e	57	LYS	C-N	5.46	1.41	1.33
2	j	165	VAL	N-CA	5.46	1.53	1.46
3	K	51	LEU	CA-C	-5.46	1.45	1.52
1	e	53	ARG	CD-NE	5.46	1.53	1.46
2	m	93	LEU	CA-CB	5.46	1.61	1.53
3	H	291	ASP	CA-CB	5.46	1.63	1.53
1	A	168	ARG	N-CA	-5.46	1.40	1.46
1	c	234	GLU	N-CA	-5.46	1.39	1.46
1	e	221	PHE	CA-CB	5.46	1.60	1.53
2	3	14	THR	C-N	5.46	1.40	1.33
2	l	96	ASN	CA-CB	5.46	1.61	1.53
3	H	53	SER	CA-C	-5.46	1.45	1.52
3	H	77	VAL	CA-CB	-5.46	1.47	1.54
3	M	376	THR	CA-CB	5.46	1.61	1.53
3	J	49	ARG	CZ-NH1	5.46	1.40	1.32
1	A	48	LEU	C-N	5.46	1.40	1.33
1	B	138	ILE	CA-CB	-5.45	1.47	1.54
1	g	114	LYS	CA-C	-5.45	1.45	1.52
2	n	202	GLU	C-N	5.45	1.40	1.33
3	H	41	ARG	NE-CZ	5.45	1.39	1.33
3	H	326	ARG	NE-CZ	5.45	1.39	1.33
3	I	81	SER	CA-CB	5.45	1.61	1.53
3	M	216	ILE	N-CA	-5.45	1.40	1.46
2	1	150	VAL	C-N	5.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	208	LEU	CA-C	-5.45	1.45	1.52
2	7	72	ILE	CA-C	5.45	1.59	1.52
3	J	97	GLU	CG-CD	5.45	1.65	1.52
1	b	99	ASN	CA-C	-5.45	1.45	1.52
1	E	195	ALA	N-CA	-5.45	1.39	1.46
2	6	83	ARG	CZ-NH1	5.45	1.40	1.32
2	m	212	ARG	CA-C	-5.45	1.46	1.52
2	4	171	ALA	C-N	5.45	1.40	1.33
2	n	87	VAL	CA-C	5.45	1.59	1.52
1	G	181	ASP	CA-C	-5.44	1.45	1.52
2	2	72	ILE	C-O	-5.44	1.17	1.24
1	B	130	ARG	CZ-NH1	5.44	1.40	1.32
2	5	108	VAL	N-CA	5.44	1.52	1.46
1	a	219	ARG	CA-C	-5.44	1.46	1.53
1	c	150	THR	CA-C	-5.44	1.46	1.52
1	d	96	ALA	N-CA	-5.44	1.39	1.46
1	E	22	PHE	N-CA	-5.44	1.38	1.46
2	m	62	ASP	CA-C	-5.44	1.45	1.52
1	c	246	LYS	CA-CB	5.44	1.64	1.53
2	2	140	THR	N-CA	-5.44	1.39	1.46
3	I	77	VAL	CA-C	-5.44	1.46	1.52
2	1	163	GLU	C-O	-5.43	1.17	1.24
2	5	79	ILE	CA-C	-5.43	1.45	1.52
3	H	16	LEU	CA-C	5.43	1.59	1.52
2	1	161	VAL	N-CA	-5.43	1.39	1.46
3	I	305	ARG	NE-CZ	5.43	1.39	1.33
2	1	88	ARG	NE-CZ	5.43	1.39	1.33
2	n	133	GLU	N-CA	-5.43	1.39	1.45
2	4	102	ARG	CZ-NH2	5.43	1.40	1.33
2	k	156	THR	C-N	-5.43	1.28	1.34
2	m	72	ILE	C-N	5.43	1.41	1.34
2	k	61	GLY	N-CA	-5.43	1.39	1.45
2	5	196	PHE	CA-CB	5.43	1.60	1.52
1	D	75	CYS	CA-C	-5.43	1.46	1.52
1	b	80	GLY	CA-C	-5.42	1.44	1.51
2	m	67	ALA	C-N	5.42	1.41	1.33
1	C	69	LYS	N-CA	-5.42	1.39	1.45
2	1	149	GLY	N-CA	5.42	1.53	1.45
2	1	198	GLN	CA-C	-5.42	1.46	1.52
3	M	78	VAL	C-O	-5.42	1.18	1.24
3	J	12	LYS	C-N	5.42	1.41	1.33
2	h	21	ASP	N-CA	-5.42	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	50	ASP	C-O	-5.42	1.16	1.24
1	A	149	GLU	CA-CB	5.42	1.63	1.53
1	A	219	ARG	CZ-NH1	5.42	1.40	1.32
2	m	154	ARG	NE-CZ	5.42	1.39	1.33
3	H	275	PHE	N-CA	5.42	1.52	1.45
1	e	241	ARG	NE-CZ	5.42	1.39	1.33
1	F	20	ARG	CZ-NH1	5.42	1.40	1.32
2	l	13	THR	C-N	5.42	1.41	1.33
1	F	140	GLY	N-CA	-5.41	1.39	1.45
1	G	21	LEU	CA-C	-5.41	1.46	1.52
1	G	122	GLN	CA-C	-5.41	1.45	1.52
1	A	161	ALA	CA-C	-5.41	1.45	1.52
1	A	91	ARG	CD-NE	5.41	1.53	1.46
1	C	173	GLU	C-N	5.41	1.40	1.33
1	c	10	ARG	NE-CZ	5.41	1.39	1.33
2	i	36	PHE	N-CA	5.41	1.53	1.45
2	3	125	ILE	CB-CG1	5.41	1.64	1.53
2	5	97	LEU	CA-C	-5.41	1.45	1.52
1	B	125	GLN	CA-C	-5.41	1.46	1.52
1	F	62	ASP	CA-C	5.41	1.60	1.52
3	M	44	TYR	CZ-OH	5.41	1.49	1.38
2	k	38	ALA	C-N	5.41	1.40	1.33
2	n	209	ALA	C-N	5.41	1.41	1.33
1	D	86	ARG	CA-CB	5.40	1.61	1.53
1	D	164	ILE	CA-C	-5.40	1.46	1.52
1	d	219	ARG	CZ-NH2	5.40	1.40	1.33
1	C	141	VAL	CA-CB	-5.40	1.47	1.54
1	G	14	VAL	N-CA	-5.40	1.40	1.46
1	d	100	ARG	CD-NE	5.40	1.53	1.46
2	2	211	PHE	C-N	5.40	1.39	1.32
3	M	319	GLN	C-N	5.40	1.40	1.33
1	C	225	SER	CA-CB	5.40	1.61	1.53
1	e	184	SER	C-N	5.40	1.40	1.33
2	m	207	ILE	C-N	5.40	1.41	1.33
1	f	154	GLY	N-CA	-5.40	1.37	1.45
3	K	299	ARG	NE-CZ	5.40	1.39	1.33
2	m	33	MET	CA-CB	5.40	1.61	1.52
2	3	113	GLY	CA-C	-5.39	1.45	1.51
2	7	115	ILE	C-N	5.39	1.40	1.33
3	L	195	VAL	CA-CB	-5.39	1.47	1.54
1	a	219	ARG	CZ-NH2	5.39	1.40	1.33
1	e	210	GLU	CA-C	-5.39	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	180	ARG	CD-NE	5.39	1.53	1.46
1	a	239	ARG	NE-CZ	5.39	1.39	1.33
1	c	134	VAL	N-CA	-5.39	1.40	1.46
1	F	204	LEU	CA-CB	-5.39	1.45	1.53
1	A	37	ALA	C-N	5.39	1.40	1.33
1	B	140	GLY	CA-C	-5.39	1.45	1.51
1	e	102	THR	N-CA	-5.39	1.38	1.46
2	4	189	VAL	CA-C	-5.39	1.46	1.52
1	a	46	VAL	C-O	-5.39	1.18	1.23
1	E	36	THR	C-N	5.39	1.40	1.33
1	F	84	ASP	CA-CB	5.39	1.61	1.53
2	h	149	GLY	C-N	5.39	1.40	1.33
1	c	100	ARG	C-N	5.38	1.41	1.33
2	6	116	ASP	CA-CB	5.38	1.62	1.53
2	n	88	ARG	CZ-NH2	5.38	1.40	1.33
3	L	317	ARG	NE-CZ	5.38	1.39	1.33
2	4	172	ILE	C-N	5.38	1.41	1.33
1	G	186	ASP	CA-C	-5.38	1.46	1.52
2	3	51	ARG	CZ-NH2	5.38	1.40	1.33
1	D	23	GLN	CA-C	-5.38	1.45	1.52
3	I	312	PRO	N-CA	-5.38	1.40	1.47
2	i	30	ARG	C-N	5.38	1.41	1.33
2	7	17	LEU	N-CA	-5.38	1.39	1.45
3	I	335	ASP	CA-CB	5.38	1.60	1.53
3	K	20	TYR	CA-C	-5.38	1.45	1.52
1	D	26	TYR	N-CA	-5.38	1.39	1.46
2	6	142	SER	CA-C	-5.38	1.45	1.52
3	L	167	PHE	CA-C	-5.38	1.45	1.52
1	d	199	SER	C-O	-5.38	1.17	1.24
1	b	44	GLU	C-N	5.37	1.38	1.32
1	C	88	LEU	C-N	5.37	1.40	1.33
1	F	97	GLN	C-O	-5.37	1.17	1.24
2	i	104	PHE	C-N	5.37	1.39	1.33
3	H	126	MET	C-N	5.37	1.38	1.33
2	i	175	ALA	N-CA	-5.37	1.39	1.46
3	H	364	ARG	CZ-NH2	5.37	1.40	1.33
1	c	169	ASN	N-CA	-5.37	1.39	1.46
2	i	205	GLU	CA-C	-5.37	1.45	1.52
1	d	77	ALA	C-N	5.37	1.41	1.33
1	d	108	THR	CA-C	-5.37	1.45	1.52
1	F	80	GLY	C-N	5.37	1.40	1.33
2	3	106	TYR	N-CA	-5.37	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	396	MET	CA-CB	5.37	1.62	1.53
3	M	368	ALA	C-N	5.37	1.41	1.33
1	C	209	ILE	CA-C	-5.37	1.46	1.52
2	m	38	ALA	C-N	5.37	1.40	1.33
3	I	44	TYR	CA-C	-5.37	1.45	1.52
1	F	76	ALA	N-CA	-5.37	1.39	1.46
2	j	30	ARG	CD-NE	5.37	1.53	1.46
1	A	241	ARG	C-N	5.36	1.41	1.33
1	e	235	ARG	CA-CB	5.36	1.62	1.53
3	J	317	ARG	C-N	5.36	1.40	1.34
3	H	305	ARG	NE-CZ	5.36	1.39	1.33
3	I	288	ASN	CA-CB	5.36	1.62	1.53
1	D	41	LYS	CA-C	-5.36	1.45	1.52
2	i	98	LEU	CA-C	-5.36	1.45	1.52
2	7	15	VAL	N-CA	-5.36	1.40	1.46
3	I	314	PHE	CA-C	-5.36	1.45	1.52
2	k	150	VAL	C-N	5.36	1.41	1.33
3	J	331	ALA	C-N	5.36	1.41	1.33
1	g	232	TYR	N-CA	-5.36	1.39	1.46
3	I	99	GLU	CA-CB	5.36	1.60	1.53
1	D	83	ALA	CA-C	-5.36	1.45	1.52
1	E	28	ARG	CD-NE	5.36	1.53	1.46
1	E	78	THR	C-N	5.36	1.40	1.33
3	I	317	ARG	CZ-NH1	5.36	1.40	1.32
1	e	33	ARG	C-N	5.35	1.41	1.33
2	5	153	ASP	CA-C	5.35	1.59	1.52
3	K	355	CYS	C-N	5.35	1.40	1.33
1	a	101	LEU	N-CA	-5.35	1.39	1.46
2	m	151	LEU	CA-C	-5.35	1.45	1.52
1	G	41	LYS	N-CA	-5.35	1.39	1.46
1	G	239	ARG	NE-CZ	5.35	1.39	1.33
3	K	387	THR	C-N	5.35	1.39	1.33
1	B	60	GLU	CA-C	-5.35	1.45	1.52
1	c	70	ILE	CA-CB	5.35	1.61	1.54
1	f	198	LEU	C-N	5.35	1.41	1.33
1	G	163	ALA	CA-C	-5.35	1.46	1.52
1	e	12	ILE	N-CA	-5.35	1.40	1.46
1	G	20	ARG	CA-C	-5.35	1.46	1.52
2	7	21	ASP	C-N	5.35	1.41	1.32
3	H	348	GLY	CA-C	-5.35	1.46	1.52
1	B	156	LEU	N-CA	5.34	1.52	1.46
1	F	155	ALA	C-N	5.34	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	47	GLN	CA-CB	5.34	1.60	1.53
2	2	122	ILE	CA-C	-5.34	1.46	1.52
2	6	132	ILE	N-CA	-5.34	1.39	1.46
3	L	236	SER	CA-C	-5.34	1.46	1.52
3	J	148	VAL	CA-CB	-5.34	1.47	1.54
3	K	211	PHE	CA-C	-5.34	1.46	1.52
2	6	204	VAL	N-CA	-5.34	1.40	1.46
3	J	321	PHE	CG-CD1	5.34	1.50	1.38
2	4	30	ARG	CD-NE	5.34	1.53	1.46
2	j	47	GLN	N-CA	-5.33	1.39	1.46
1	d	151	ASP	N-CA	5.33	1.50	1.45
2	h	29	LYS	N-CA	-5.33	1.39	1.46
2	7	106	TYR	CA-CB	5.33	1.62	1.53
1	e	180	ARG	CA-C	-5.33	1.46	1.52
1	E	84	ASP	CA-C	-5.33	1.45	1.52
1	E	122	GLN	C-N	5.33	1.41	1.33
1	E	139	ALA	CA-C	-5.33	1.46	1.52
1	F	171	VAL	CA-CB	-5.33	1.47	1.54
2	3	82	GLU	CA-CB	5.33	1.61	1.53
3	J	14	LYS	C-N	5.33	1.41	1.33
2	6	14	THR	CA-C	-5.33	1.46	1.52
3	I	386	THR	CA-CB	-5.33	1.44	1.53
3	H	129	GLY	C-O	5.33	1.31	1.23
1	d	142	ASP	CA-CB	5.32	1.62	1.53
1	g	10	ARG	C-N	5.32	1.41	1.33
2	5	124	SER	C-N	5.32	1.40	1.33
2	5	158	GLU	CA-CB	5.32	1.62	1.53
2	m	142	SER	CA-C	-5.32	1.45	1.52
3	M	29	ARG	CA-CB	5.32	1.61	1.53
3	M	157	VAL	CA-CB	5.32	1.60	1.55
3	M	302	ARG	N-CA	-5.32	1.39	1.46
3	H	235	PRO	N-CD	-5.32	1.40	1.47
1	C	208	ASN	N-CA	-5.32	1.41	1.46
2	i	178	ARG	CZ-NH2	5.32	1.40	1.33
2	i	33	MET	CA-C	-5.32	1.46	1.52
2	k	149	GLY	C-N	5.32	1.40	1.33
1	g	79	SER	CA-C	-5.32	1.45	1.52
2	2	184	ASP	N-CA	-5.32	1.39	1.46
3	L	221	ARG	NE-CZ	5.32	1.38	1.33
1	E	156	LEU	CA-C	-5.31	1.46	1.52
1	C	28	ARG	C-O	-5.31	1.16	1.24
1	f	180	ARG	NE-CZ	5.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	168	ARG	CZ-NH1	5.31	1.40	1.32
2	7	70	ILE	C-N	5.31	1.41	1.33
3	I	209	SER	N-CA	-5.31	1.39	1.46
3	K	105	ARG	CZ-NH2	5.31	1.40	1.33
3	M	38	GLU	C-N	5.31	1.40	1.33
2	3	25	MET	C-N	5.31	1.40	1.33
2	5	169	VAL	CA-CB	-5.31	1.47	1.54
2	n	60	VAL	CA-C	5.31	1.60	1.52
1	B	236	ALA	C-N	5.31	1.41	1.33
1	C	146	LYS	CA-C	-5.31	1.46	1.52
2	h	88	ARG	N-CA	-5.31	1.40	1.46
2	6	58	GLY	C-N	5.31	1.40	1.33
1	e	225	SER	CA-C	-5.31	1.45	1.52
1	G	183	LEU	CA-C	-5.31	1.46	1.53
2	h	83	ARG	CD-NE	5.31	1.53	1.46
3	J	366	GLU	CA-CB	5.31	1.61	1.53
1	B	20	ARG	CD-NE	5.30	1.53	1.46
1	G	130	ARG	CD-NE	5.30	1.53	1.46
1	G	235	ARG	N-CA	5.30	1.53	1.46
2	4	212	ARG	CD-NE	5.30	1.53	1.46
2	j	37	ILE	CA-CB	-5.30	1.47	1.53
1	F	20	ARG	CD-NE	5.30	1.53	1.46
3	K	341	ARG	CZ-NH2	5.30	1.40	1.33
2	1	155	PHE	N-CA	-5.30	1.39	1.46
2	6	47	GLN	CA-CB	5.30	1.60	1.53
2	k	102	ARG	NE-CZ	5.29	1.38	1.33
1	E	227	GLU	C-N	5.29	1.40	1.33
3	H	383	LEU	CA-CB	5.29	1.61	1.53
2	7	80	ARG	CA-CB	5.29	1.61	1.53
1	b	150	THR	C-N	5.29	1.40	1.33
2	3	14	THR	CA-C	-5.29	1.46	1.52
2	6	102	ARG	CZ-NH1	5.29	1.40	1.32
2	i	172	ILE	C-O	-5.29	1.17	1.24
2	n	140	THR	N-CA	5.29	1.53	1.46
3	L	274	GLY	N-CA	-5.29	1.35	1.45
1	a	125	GLN	CA-CB	5.29	1.62	1.53
2	3	124	SER	CA-C	-5.29	1.46	1.52
2	j	41	ALA	N-CA	-5.29	1.42	1.47
3	I	212	VAL	CA-CB	-5.29	1.47	1.54
3	I	269	LEU	C-O	-5.29	1.17	1.24
2	3	130	GLY	C-N	5.28	1.40	1.33
3	H	201	ALA	C-N	5.28	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	29	ARG	CD-NE	5.28	1.53	1.46
1	F	28	ARG	CZ-NH2	5.28	1.40	1.33
3	L	250	ARG	CA-CB	5.28	1.62	1.53
3	J	32	ASP	C-N	5.28	1.41	1.34
1	g	139	ALA	N-CA	-5.28	1.39	1.46
2	2	16	GLY	N-CA	5.28	1.53	1.45
3	M	242	GLU	N-CA	-5.28	1.39	1.46
2	h	24	VAL	CA-CB	5.28	1.60	1.54
2	4	127	PRO	CA-CB	-5.28	1.46	1.53
1	b	73	HIS	CA-C	-5.27	1.45	1.52
1	D	146	LYS	C-O	-5.27	1.17	1.23
1	d	26	TYR	N-CA	-5.27	1.40	1.46
1	f	211	VAL	N-CA	-5.27	1.40	1.46
1	g	233	VAL	N-CA	-5.27	1.39	1.46
2	h	94	THR	CB-OG1	-5.27	1.35	1.43
2	3	197	TYR	C-N	5.27	1.40	1.33
3	L	174	PRO	C-O	-5.27	1.20	1.24
1	B	158	GLU	C-N	5.27	1.40	1.33
1	e	211	VAL	C-N	5.27	1.40	1.33
2	n	21	ASP	CA-C	-5.27	1.45	1.52
1	g	68	TYR	N-CA	-5.27	1.39	1.45
2	2	207	ILE	C-N	5.27	1.40	1.33
2	k	52	MET	CA-C	-5.27	1.46	1.52
1	b	85	ALA	C-N	5.27	1.40	1.33
1	e	86	ARG	NE-CZ	5.27	1.38	1.33
2	h	117	SER	CA-CB	5.27	1.61	1.53
2	h	154	ARG	CZ-NH1	5.27	1.40	1.32
3	I	18	GLU	C-N	5.27	1.40	1.33
3	K	241	ASP	N-CA	-5.27	1.39	1.46
1	e	21	LEU	N-CA	-5.27	1.38	1.45
2	7	64	GLN	CA-C	-5.27	1.46	1.52
2	5	115	ILE	CA-CB	-5.26	1.47	1.55
3	K	28	ARG	C-O	-5.26	1.18	1.24
1	C	72	GLU	CA-C	-5.26	1.46	1.52
1	C	193	LEU	CA-CB	5.26	1.61	1.53
2	2	16	GLY	C-N	5.26	1.40	1.33
2	l	15	VAL	C-O	-5.26	1.18	1.24
1	C	86	ARG	CA-C	-5.26	1.45	1.52
2	h	14	THR	C-N	5.26	1.41	1.33
2	h	83	ARG	NE-CZ	5.26	1.38	1.33
2	6	12	THR	N-CA	5.26	1.56	1.46
3	K	346	ALA	CA-CB	5.26	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	213	GLN	C-N	5.26	1.40	1.33
1	e	185	PHE	N-CA	-5.26	1.40	1.46
2	2	89	ALA	C-N	5.26	1.40	1.33
3	H	317	ARG	CA-CB	5.26	1.61	1.53
3	K	310	PRO	C-N	5.26	1.41	1.33
1	C	42	CYS	C-N	5.25	1.41	1.33
1	E	95	GLU	C-N	5.25	1.41	1.33
1	C	24	VAL	N-CA	-5.25	1.40	1.46
1	D	131	PRO	C-N	5.25	1.41	1.33
2	h	87	VAL	CA-C	-5.25	1.45	1.52
2	3	138	VAL	CA-CB	-5.25	1.47	1.54
1	a	117	CYS	N-CA	-5.25	1.40	1.46
1	d	107	ILE	C-O	-5.25	1.17	1.24
3	M	205	ARG	CZ-NH1	5.25	1.40	1.32
2	3	202	GLU	CA-C	-5.25	1.46	1.52
2	n	97	LEU	N-CA	-5.25	1.40	1.46
1	d	91	ARG	CA-CB	5.25	1.61	1.53
1	e	158	GLU	N-CA	-5.25	1.39	1.46
1	G	79	SER	C-O	-5.25	1.17	1.23
3	L	211	PHE	CA-C	-5.25	1.46	1.52
1	G	176	GLU	CA-C	-5.25	1.45	1.52
2	1	114	GLY	N-CA	-5.25	1.39	1.45
3	M	205	ARG	CA-CB	5.25	1.60	1.53
1	E	5	GLN	C-N	5.25	1.40	1.33
2	3	51	ARG	C-O	-5.25	1.18	1.24
3	H	259	ARG	CZ-NH1	5.25	1.40	1.32
3	J	96	ASN	N-CA	-5.25	1.39	1.45
1	b	114	LYS	N-CA	-5.24	1.40	1.46
1	E	6	MET	N-CA	-5.24	1.39	1.46
1	F	139	ALA	N-CA	-5.24	1.40	1.46
1	F	239	ARG	C-O	-5.24	1.17	1.24
2	h	83	ARG	CA-C	-5.24	1.46	1.52
2	i	111	LEU	N-CA	-5.24	1.40	1.46
2	n	63	ALA	N-CA	-5.24	1.40	1.46
3	K	33	GLU	CA-C	-5.24	1.46	1.52
1	B	53	ARG	CD-NE	5.24	1.53	1.46
3	K	43	ARG	CA-CB	5.24	1.61	1.53
3	J	136	PRO	CA-C	-5.24	1.47	1.52
1	C	114	LYS	CA-C	-5.24	1.46	1.52
2	7	95	SER	CA-CB	-5.24	1.45	1.53
3	I	221	ARG	C-N	5.24	1.40	1.33
2	3	68	ARG	NE-CZ	5.24	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	163	ALA	C-N	5.24	1.40	1.33
2	2	49	ALA	C-O	-5.24	1.18	1.24
1	c	229	LEU	CA-C	-5.24	1.46	1.52
1	f	140	GLY	CA-C	-5.24	1.46	1.51
2	h	52	MET	CA-C	-5.24	1.46	1.52
2	l	155	PHE	C-N	5.24	1.39	1.32
2	7	75	ASN	CA-C	-5.24	1.46	1.52
2	7	204	VAL	CA-CB	-5.24	1.47	1.54
3	I	57	ARG	CA-CB	5.24	1.61	1.53
1	C	151	ASP	N-CA	-5.23	1.39	1.45
2	2	212	ARG	CD-NE	5.23	1.53	1.46
2	j	207	ILE	CA-C	5.23	1.59	1.52
3	H	354	ILE	N-CA	5.23	1.52	1.46
1	A	17	PRO	N-CA	-5.23	1.40	1.47
1	a	84	ASP	N-CA	-5.23	1.40	1.46
1	G	155	ALA	CA-C	-5.23	1.46	1.52
2	3	99	ASN	CA-C	-5.23	1.46	1.52
2	j	87	VAL	N-CA	5.23	1.53	1.46
3	H	120	PRO	CA-C	-5.23	1.46	1.52
1	d	81	LEU	CA-C	-5.23	1.45	1.52
1	e	242	GLU	CA-CB	5.23	1.61	1.53
2	m	106	TYR	CA-C	-5.23	1.45	1.52
3	M	82	SER	C-N	5.23	1.40	1.33
2	l	44	LYS	N-CA	-5.23	1.41	1.46
2	n	66	LEU	C-N	5.23	1.40	1.33
1	a	153	SER	N-CA	-5.22	1.39	1.46
1	G	100	ARG	NE-CZ	5.22	1.38	1.33
2	j	166	GLU	N-CA	5.22	1.52	1.46
1	e	184	SER	CA-C	-5.22	1.45	1.53
2	7	164	ALA	CA-CB	5.22	1.61	1.53
2	n	160	GLY	CA-C	-5.22	1.44	1.51
3	H	270	ALA	N-CA	-5.22	1.40	1.46
1	e	189	MET	C-N	5.22	1.40	1.33
2	6	169	VAL	N-CA	-5.22	1.40	1.46
3	H	381	LYS	N-CA	-5.22	1.40	1.46
1	f	120	LYS	N-CA	-5.22	1.40	1.46
2	6	106	TYR	C-N	5.22	1.41	1.33
3	I	68	VAL	N-CA	5.22	1.52	1.46
3	I	230	ALA	N-CA	-5.22	1.40	1.46
3	K	247	ALA	CA-CB	5.22	1.61	1.53
3	M	88	VAL	CA-C	-5.22	1.46	1.52
2	3	180	SER	C-N	5.22	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	208	LEU	C-O	-5.22	1.17	1.24
3	L	50	ARG	NE-CZ	5.22	1.38	1.33
2	m	170	ARG	N-CA	-5.22	1.40	1.46
2	7	70	ILE	CA-CB	-5.22	1.48	1.54
3	I	40	GLU	CA-C	-5.22	1.46	1.52
1	f	40	ILE	C-N	5.21	1.41	1.33
2	1	73	GLU	C-N	5.21	1.40	1.33
1	A	155	ALA	CA-C	-5.21	1.46	1.52
1	a	164	ILE	N-CA	-5.21	1.39	1.46
2	1	81	ARG	CZ-NH2	5.21	1.40	1.33
1	a	236	ALA	C-N	5.21	1.41	1.34
1	B	111	GLU	CA-C	-5.21	1.45	1.52
1	E	181	ASP	CA-CB	5.21	1.60	1.53
1	F	42	CYS	N-CA	-5.21	1.38	1.46
1	f	25	GLU	N-CA	-5.21	1.40	1.46
1	f	238	GLU	CA-C	-5.21	1.46	1.52
3	H	321	PHE	N-CA	5.21	1.52	1.46
3	L	119	LEU	CA-C	-5.21	1.46	1.52
1	a	111	GLU	CA-C	-5.21	1.46	1.52
1	C	225	SER	CA-C	-5.21	1.47	1.53
3	M	259	ARG	CD-NE	5.21	1.53	1.46
1	c	147	LEU	C-O	-5.20	1.18	1.24
1	D	9	ASP	N-CA	-5.20	1.39	1.46
2	5	102	ARG	CZ-NH2	5.20	1.40	1.33
1	B	77	ALA	CA-C	-5.20	1.45	1.53
1	c	93	ARG	CA-C	-5.20	1.46	1.52
1	G	53	ARG	NE-CZ	5.20	1.38	1.33
3	L	339	LEU	N-CA	-5.20	1.40	1.46
2	h	83	ARG	CZ-NH1	5.20	1.40	1.32
2	i	56	THR	C-O	5.20	1.30	1.24
2	m	134	GLU	N-CA	5.20	1.52	1.46
3	I	224	ARG	N-CA	-5.20	1.40	1.46
3	M	36	PHE	CA-CB	5.20	1.61	1.53
1	D	7	GLY	C-N	5.20	1.40	1.33
1	G	30	ALA	C-N	5.20	1.40	1.33
2	j	120	LYS	CA-CB	5.20	1.63	1.53
1	B	242	GLU	N-CA	5.20	1.52	1.46
1	C	223	GLU	CA-CB	5.20	1.61	1.53
2	m	115	ILE	CA-C	-5.20	1.46	1.52
3	H	358	ALA	C-N	5.20	1.40	1.33
1	D	79	SER	CA-C	-5.19	1.46	1.52
1	b	134	VAL	N-CA	-5.19	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	35	ASN	CA-CB	5.19	1.62	1.53
2	m	161	VAL	CA-CB	-5.19	1.48	1.54
1	A	111	GLU	C-N	5.19	1.41	1.33
1	b	74	ILE	C-N	5.19	1.40	1.33
2	4	82	GLU	N-CA	-5.19	1.38	1.46
3	H	164	PRO	C-O	-5.19	1.17	1.24
3	I	76	ARG	CZ-NH1	5.19	1.40	1.32
3	K	227	PHE	CA-CB	5.19	1.61	1.53
3	J	167	PHE	CA-C	-5.19	1.45	1.52
3	J	190	LEU	C-N	5.19	1.40	1.33
1	D	72	GLU	CG-CD	5.19	1.65	1.52
1	d	122	GLN	CA-C	-5.19	1.46	1.52
2	m	88	ARG	CZ-NH1	5.19	1.40	1.32
1	C	95	GLU	N-CA	5.19	1.52	1.46
1	D	175	PHE	C-N	5.19	1.40	1.33
1	g	209	ILE	CA-C	-5.19	1.46	1.52
2	m	35	ASN	C-N	5.19	1.40	1.33
1	B	194	VAL	CA-C	5.18	1.59	1.52
1	c	216	VAL	CA-C	-5.18	1.46	1.52
1	d	10	ARG	CD-NE	5.18	1.53	1.46
3	I	387	THR	CA-C	-5.18	1.46	1.52
3	K	36	PHE	CA-C	-5.18	1.46	1.52
3	J	83	THR	CA-C	-5.18	1.45	1.52
1	b	100	ARG	N-CA	5.18	1.52	1.46
1	c	200	ILE	C-N	5.18	1.41	1.33
1	g	180	ARG	NE-CZ	5.18	1.38	1.33
2	4	178	ARG	CD-NE	5.18	1.53	1.46
2	n	17	LEU	N-CA	-5.18	1.39	1.45
1	E	115	LYS	CA-CB	5.18	1.61	1.53
1	f	119	PHE	CA-C	-5.18	1.46	1.52
1	f	229	LEU	CA-C	-5.18	1.45	1.52
3	L	87	PHE	CA-CB	5.18	1.64	1.54
1	g	56	SER	CA-CB	5.18	1.61	1.53
2	l	187	ASP	N-CA	-5.18	1.39	1.45
1	a	241	ARG	CD-NE	5.18	1.53	1.46
1	C	112	LEU	C-O	-5.18	1.18	1.24
2	2	197	TYR	N-CA	-5.18	1.39	1.46
2	k	154	ARG	CA-CB	5.18	1.61	1.53
2	6	48	ILE	CA-C	-5.18	1.46	1.52
2	7	98	LEU	CA-CB	5.18	1.61	1.53
3	H	264	THR	N-CA	5.18	1.52	1.46
3	M	76	ARG	CZ-NH1	5.18	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	219	ARG	CZ-NH1	5.17	1.40	1.32
1	c	73	HIS	ND1-CE1	5.17	1.37	1.32
1	c	240	ILE	CA-C	5.17	1.59	1.52
2	k	137	ILE	C-N	5.17	1.39	1.33
2	k	168	ALA	CA-C	-5.17	1.46	1.52
3	J	46	ARG	NE-CZ	5.17	1.38	1.33
3	J	214	LYS	N-CA	5.17	1.52	1.46
1	c	219	ARG	CD-NE	5.17	1.53	1.46
2	n	44	LYS	N-CA	-5.17	1.38	1.46
1	C	47	ILE	CA-C	-5.17	1.46	1.52
1	g	15	PHE	CA-C	-5.17	1.46	1.53
2	1	91	ALA	CA-C	-5.17	1.46	1.52
2	1	175	ALA	CA-C	-5.17	1.46	1.52
3	H	99	GLU	N-CA	-5.17	1.39	1.46
3	L	126	MET	C-O	-5.17	1.17	1.24
3	J	41	ARG	N-CA	-5.17	1.40	1.46
1	G	137	LEU	CA-CB	5.17	1.61	1.53
2	7	80	ARG	NE-CZ	5.17	1.38	1.33
1	C	240	ILE	N-CA	-5.17	1.40	1.46
1	e	83	ALA	N-CA	-5.17	1.40	1.46
2	h	17	LEU	CA-C	-5.17	1.46	1.52
2	j	164	ALA	C-O	-5.17	1.17	1.24
2	m	26	ALA	N-CA	-5.17	1.39	1.46
2	n	159	ILE	C-N	5.17	1.41	1.33
1	A	244	LEU	CA-CB	5.17	1.60	1.53
2	k	23	VAL	CA-C	5.17	1.59	1.52
2	7	132	ILE	C-N	5.17	1.41	1.33
3	K	107	ALA	CA-CB	-5.17	1.46	1.53
3	M	268	LEU	C-N	5.17	1.40	1.33
1	a	161	ALA	CA-C	-5.17	1.45	1.52
1	E	25	GLU	CA-C	5.17	1.59	1.52
1	C	58	LEU	C-N	5.16	1.40	1.33
2	2	37	ILE	C-N	5.16	1.41	1.34
2	4	83	ARG	CZ-NH1	5.16	1.40	1.32
2	k	150	VAL	N-CA	-5.16	1.40	1.46
3	M	53	SER	CA-CB	5.16	1.61	1.53
3	M	256	SER	N-CA	5.16	1.52	1.46
1	A	77	ALA	CA-C	-5.16	1.46	1.52
1	E	127	GLY	CA-C	-5.16	1.44	1.51
2	4	67	ALA	C-N	5.16	1.41	1.33
3	H	143	ILE	N-CA	-5.16	1.39	1.46
1	C	98	ILE	CA-C	5.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	163	ALA	N-CA	-5.16	1.39	1.45
1	c	203	GLU	C-N	5.16	1.40	1.33
3	K	16	LEU	C-N	5.16	1.40	1.33
3	L	325	THR	N-CA	-5.16	1.39	1.46
1	F	97	GLN	CD-NE2	5.15	1.44	1.33
1	g	64	ILE	C-N	5.15	1.40	1.33
3	J	100	LEU	CA-CB	5.15	1.62	1.53
1	B	12	ILE	N-CA	-5.15	1.40	1.46
2	1	211	PHE	N-CA	5.15	1.52	1.46
2	n	53	ALA	N-CA	-5.15	1.39	1.45
3	J	277	PRO	N-CA	5.15	1.53	1.47
2	1	155	PHE	CA-CB	5.15	1.60	1.53
2	1	212	ARG	CD-NE	5.15	1.53	1.46
2	k	126	ASP	C-O	-5.15	1.16	1.23
2	7	94	THR	N-CA	-5.15	1.40	1.46
3	L	92	SER	CA-C	-5.15	1.46	1.52
2	h	185	GLY	CA-C	-5.15	1.44	1.51
2	j	30	ARG	CZ-NH2	5.15	1.40	1.33
3	I	360	MET	C-N	5.15	1.40	1.33
1	A	232	TYR	CA-C	-5.15	1.46	1.52
1	D	136	LEU	CA-CB	5.15	1.62	1.53
1	d	219	ARG	NE-CZ	5.15	1.38	1.33
2	7	161	VAL	CA-CB	-5.15	1.48	1.54
2	n	30	ARG	CD-NE	5.15	1.53	1.46
3	H	278	ARG	NE-CZ	5.15	1.38	1.33
3	H	315	GLU	N-CA	-5.15	1.40	1.46
3	M	270	ALA	N-CA	-5.15	1.40	1.46
3	J	118	VAL	C-O	5.15	1.30	1.24
1	B	132	PHE	CA-C	-5.15	1.46	1.52
1	C	238	GLU	C-O	5.15	1.30	1.24
1	e	200	ILE	C-N	5.14	1.41	1.33
1	F	141	VAL	N-CA	-5.14	1.40	1.46
3	K	357	GLU	CA-C	-5.14	1.45	1.52
3	M	159	LEU	C-O	-5.14	1.19	1.24
1	e	29	GLU	CA-C	5.14	1.59	1.52
3	I	317	ARG	CA-C	-5.14	1.46	1.52
3	M	138	VAL	C-O	-5.14	1.18	1.24
1	b	10	ARG	NE-CZ	5.14	1.38	1.33
2	k	62	ASP	CA-CB	5.14	1.61	1.53
2	5	129	GLY	N-CA	-5.14	1.39	1.45
1	c	241	ARG	CZ-NH2	5.14	1.40	1.33
2	5	174	SER	N-CA	-5.14	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	188	LYS	CA-C	-5.14	1.46	1.52
1	B	66	LYS	CA-C	-5.13	1.45	1.52
2	i	70	ILE	CA-C	-5.13	1.46	1.52
3	J	82	SER	C-N	5.13	1.41	1.33
1	e	43	LYS	CA-C	-5.13	1.45	1.52
2	i	83	ARG	NE-CZ	5.13	1.38	1.33
3	K	43	ARG	NE-CZ	5.13	1.38	1.33
1	A	42	CYS	C-O	5.13	1.29	1.24
1	F	172	THR	C-O	-5.13	1.18	1.24
2	1	125	ILE	CA-C	-5.13	1.46	1.52
2	3	23	VAL	C-O	5.13	1.29	1.24
3	J	257	GLY	CA-C	-5.13	1.44	1.51
1	C	226	PRO	N-CD	-5.13	1.40	1.47
1	G	173	GLU	CA-CB	5.13	1.61	1.53
2	1	193	GLU	CA-C	-5.13	1.45	1.52
3	H	52	ARG	CZ-NH1	5.13	1.40	1.32
1	e	244	LEU	CA-CB	5.13	1.61	1.53
1	F	49	ILE	CA-CB	5.13	1.61	1.54
1	g	161	ALA	C-N	5.13	1.40	1.33
2	5	174	SER	CA-C	-5.13	1.46	1.52
3	J	317	ARG	CZ-NH2	5.13	1.40	1.33
1	a	179	TYR	N-CA	-5.13	1.39	1.46
1	C	53	ARG	CZ-NH1	5.13	1.40	1.32
1	D	105	GLU	N-CA	-5.13	1.39	1.45
2	j	56	THR	CA-C	-5.13	1.46	1.52
2	l	37	ILE	C-N	5.13	1.41	1.33
3	M	206	VAL	C-N	5.13	1.39	1.33
2	n	159	ILE	CA-C	-5.12	1.47	1.52
2	h	115	ILE	CB-CG1	5.12	1.63	1.53
2	6	86	THR	C-N	5.12	1.40	1.33
1	c	89	ILE	CA-C	-5.12	1.45	1.52
1	f	233	VAL	N-CA	-5.12	1.40	1.46
3	H	171	GLY	C-N	5.12	1.39	1.33
3	I	92	SER	CA-C	-5.12	1.46	1.52
3	L	132	VAL	CA-CB	5.12	1.61	1.54
3	J	103	GLY	C-N	5.12	1.40	1.33
1	B	20	ARG	NE-CZ	5.12	1.38	1.33
2	m	150	VAL	C-N	5.12	1.40	1.33
1	g	215	LYS	CA-C	-5.12	1.46	1.52
2	h	139	ALA	CA-C	-5.12	1.46	1.52
2	i	128	ILE	CA-CB	-5.12	1.47	1.54
2	6	56	THR	N-CA	5.12	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	61	GLY	C-N	5.12	1.40	1.33
2	h	212	ARG	CD-NE	5.11	1.53	1.46
2	3	177	LYS	C-N	5.11	1.40	1.33
3	L	374	ASP	C-N	5.11	1.40	1.33
2	i	169	VAL	CA-C	-5.11	1.46	1.52
1	G	174	PHE	CA-CB	5.11	1.61	1.53
2	3	36	PHE	C-N	5.11	1.39	1.33
2	n	191	ILE	C-N	5.11	1.41	1.33
3	K	87	PHE	N-CA	-5.11	1.39	1.45
3	M	305	ARG	NE-CZ	5.11	1.38	1.33
1	a	72	GLU	CA-C	-5.11	1.45	1.52
1	a	205	VAL	CA-C	5.11	1.58	1.52
2	i	118	GLU	C-N	5.11	1.40	1.32
2	l	112	ILE	CA-CB	-5.11	1.47	1.53
2	7	122	ILE	C-O	-5.11	1.19	1.24
1	c	86	ARG	NE-CZ	5.11	1.38	1.33
1	f	48	LEU	CA-C	-5.11	1.46	1.52
2	1	82	GLU	N-CA	-5.11	1.39	1.46
2	1	69	ILE	CA-C	-5.11	1.46	1.52
2	6	80	ARG	CZ-NH1	5.11	1.39	1.32
2	7	142	SER	CA-CB	5.11	1.61	1.53
3	H	78	VAL	CA-CB	-5.11	1.47	1.53
3	L	184	PRO	N-CD	5.11	1.54	1.47
3	J	173	GLU	CA-CB	5.11	1.60	1.53
2	1	145	LEU	N-CA	5.10	1.52	1.46
1	a	69	LYS	N-CA	-5.10	1.39	1.46
1	b	104	ASP	C-N	5.10	1.39	1.33
2	2	30	ARG	C-N	5.10	1.41	1.33
3	L	181	TYR	C-N	5.10	1.41	1.33
3	M	100	LEU	N-CA	-5.10	1.39	1.45
3	J	341	ARG	CD-NE	5.10	1.53	1.46
1	a	22	PHE	C-O	-5.10	1.17	1.24
1	d	37	ALA	N-CA	-5.10	1.39	1.45
1	G	235	ARG	NE-CZ	5.10	1.38	1.33
2	j	77	TYR	C-N	5.10	1.40	1.33
1	E	52	LYS	CA-CB	5.10	1.60	1.53
2	2	21	ASP	CA-CB	5.10	1.61	1.53
2	2	154	ARG	NE-CZ	5.10	1.38	1.33
2	3	115	ILE	CA-CB	-5.10	1.48	1.54
2	3	132	ILE	CA-C	-5.10	1.46	1.52
2	3	211	PHE	CA-CB	5.10	1.61	1.53
2	1	120	LYS	CA-C	-5.10	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	191	ILE	CA-C	-5.10	1.46	1.52
3	H	258	ASP	CA-C	-5.10	1.46	1.52
3	H	350	ASP	CA-CB	5.10	1.61	1.53
3	K	302	ARG	NE-CZ	5.10	1.38	1.33
2	j	85	PRO	C-N	5.10	1.40	1.33
1	g	168	ARG	C-N	5.10	1.40	1.33
1	g	100	ARG	CZ-NH2	5.09	1.40	1.33
1	A	55	GLY	CA-C	-5.09	1.45	1.51
1	b	181	ASP	CG-OD1	5.09	1.35	1.25
1	F	233	VAL	C-N	5.09	1.40	1.33
2	2	135	LYS	C-N	5.09	1.40	1.33
2	j	146	THR	N-CA	-5.09	1.40	1.46
2	k	97	LEU	C-N	5.09	1.41	1.34
2	k	155	PHE	C-N	5.09	1.39	1.32
3	I	222	LEU	N-CA	-5.09	1.40	1.46
3	I	260	GLU	C-N	5.09	1.40	1.33
1	C	30	ALA	CA-CB	-5.09	1.44	1.53
1	c	241	ARG	CD-NE	5.09	1.53	1.46
2	n	121	SER	C-N	5.09	1.40	1.33
3	I	161	LEU	C-N	5.09	1.40	1.33
1	a	88	LEU	C-N	5.09	1.40	1.33
2	k	47	GLN	CA-CB	5.09	1.59	1.53
1	D	10	ARG	CZ-NH2	5.09	1.40	1.33
3	L	259	ARG	CZ-NH1	5.09	1.39	1.32
2	k	137	ILE	CA-C	-5.08	1.46	1.52
1	A	24	VAL	CA-CB	-5.08	1.47	1.54
1	d	236	ALA	N-CA	-5.08	1.40	1.46
2	3	182	SER	CA-CB	5.08	1.61	1.53
2	7	170	ARG	CZ-NH2	5.08	1.40	1.33
3	H	263	ARG	CD-NE	5.08	1.53	1.46
1	B	115	LYS	N-CA	-5.08	1.39	1.46
1	G	81	LEU	C-N	5.08	1.39	1.34
3	J	63	LEU	CA-C	-5.08	1.46	1.52
1	C	61	ALA	CA-C	-5.08	1.46	1.52
1	F	8	TYR	CA-C	-5.08	1.44	1.52
1	f	246	LYS	CA-CB	5.08	1.63	1.53
1	G	50	ALA	CA-C	5.08	1.59	1.52
2	1	91	ALA	CA-CB	5.08	1.61	1.53
2	h	190	LYS	CA-C	5.08	1.58	1.52
2	j	208	LEU	CA-CB	5.08	1.62	1.53
2	6	111	LEU	N-CA	-5.08	1.39	1.46
3	H	221	ARG	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	39	SER	CA-C	-5.08	1.46	1.52
3	I	306	ILE	CA-C	-5.08	1.46	1.52
3	K	204	ILE	C-N	5.08	1.42	1.33
3	M	380	GLU	C-N	5.08	1.40	1.33
3	J	307	ILE	N-CA	-5.08	1.40	1.46
1	A	244	LEU	N-CA	-5.07	1.40	1.46
1	b	103	TYR	CA-C	5.07	1.59	1.52
1	D	55	GLY	C-N	5.07	1.40	1.33
1	G	135	SER	CA-C	-5.07	1.46	1.52
3	L	281	VAL	C-O	-5.07	1.19	1.24
1	B	215	LYS	C-N	5.07	1.39	1.33
2	l	37	ILE	CA-CB	5.07	1.60	1.54
3	L	90	ASN	CA-CB	5.07	1.60	1.53
3	L	329	LYS	C-N	5.07	1.40	1.33
2	j	51	ARG	NE-CZ	5.07	1.38	1.33
2	l	177	LYS	C-N	5.07	1.40	1.33
1	g	33	ARG	CD-NE	5.07	1.53	1.46
3	L	147	ASP	CA-CB	5.07	1.61	1.53
1	a	86	ARG	N-CA	-5.07	1.40	1.46
2	h	66	LEU	C-O	-5.07	1.18	1.24
3	L	86	LYS	N-CA	-5.07	1.39	1.46
1	B	72	GLU	C-N	5.07	1.40	1.33
1	B	230	LYS	N-CA	-5.07	1.41	1.46
2	7	166	GLU	CA-C	-5.06	1.46	1.52
1	A	164	ILE	N-CA	-5.06	1.40	1.46
1	e	234	GLU	N-CA	-5.06	1.40	1.46
1	F	54	VAL	CA-C	5.06	1.58	1.52
1	G	33	ARG	NE-CZ	5.06	1.38	1.33
1	g	100	ARG	CA-C	-5.06	1.46	1.52
2	i	114	GLY	N-CA	-5.06	1.35	1.45
2	k	51	ARG	NE-CZ	5.06	1.38	1.33
2	n	68	ARG	N-CA	-5.06	1.40	1.46
3	I	133	GLU	CA-CB	5.06	1.61	1.53
3	I	267	GLN	CD-NE2	5.06	1.43	1.33
1	A	217	ASP	C-N	5.06	1.40	1.33
1	C	5	GLN	CA-CB	5.06	1.63	1.53
2	h	172	ILE	C-O	-5.06	1.17	1.24
2	6	104	PHE	CA-C	5.06	1.58	1.52
2	6	187	ASP	C-N	5.06	1.41	1.33
2	7	208	LEU	C-N	5.06	1.41	1.33
3	M	237	ILE	CA-C	-5.05	1.46	1.52
3	J	25	GLU	CA-C	5.05	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	ILE	CB-CG1	5.05	1.63	1.53
2	h	132	ILE	CA-C	-5.05	1.46	1.52
1	B	237	ASN	CA-C	5.05	1.59	1.52
1	D	185	PHE	CA-C	-5.05	1.46	1.52
3	I	137	GLU	N-CA	-5.05	1.40	1.46
2	1	23	VAL	C-N	5.05	1.40	1.33
1	a	125	GLN	C-N	5.05	1.40	1.33
1	b	65	GLU	CA-CB	5.05	1.61	1.53
1	c	148	TYR	C-N	5.05	1.40	1.33
1	d	120	LYS	CA-C	-5.05	1.46	1.52
1	e	89	ILE	C-N	5.05	1.40	1.33
1	e	232	TYR	N-CA	-5.05	1.40	1.46
1	f	241	ARG	C-O	-5.05	1.18	1.24
1	a	32	LYS	CA-C	-5.04	1.46	1.52
1	D	56	SER	N-CA	-5.04	1.39	1.46
3	K	131	GLU	CA-CB	5.04	1.59	1.53
3	J	52	ARG	NE-CZ	5.04	1.38	1.33
1	b	61	ALA	N-CA	-5.04	1.40	1.46
1	D	28	ARG	CZ-NH2	5.04	1.40	1.33
2	3	144	SER	CA-C	-5.04	1.46	1.52
2	7	80	ARG	C-O	5.04	1.29	1.24
3	I	119	LEU	N-CA	5.04	1.54	1.45
3	M	57	ARG	CD-NE	5.04	1.53	1.46
3	J	267	GLN	CA-C	-5.04	1.46	1.52
1	c	134	VAL	CA-C	-5.04	1.46	1.52
2	3	210	LYS	C-O	-5.04	1.17	1.24
2	m	155	PHE	CA-CB	5.04	1.61	1.53
3	K	308	GLU	N-CA	-5.04	1.39	1.46
1	d	44	GLU	C-N	5.04	1.38	1.32
2	l	187	ASP	CA-C	-5.04	1.46	1.52
1	D	61	ALA	CA-C	5.04	1.59	1.52
1	G	68	TYR	C-N	5.04	1.40	1.33
2	h	156	THR	C-N	-5.04	1.28	1.34
2	k	52	MET	N-CA	5.03	1.52	1.46
2	m	30	ARG	CD-NE	5.03	1.53	1.46
2	m	172	ILE	CA-C	-5.03	1.45	1.52
3	H	293	LEU	CA-C	-5.03	1.46	1.52
1	d	99	ASN	CA-CB	5.03	1.61	1.53
1	g	239	ARG	CA-C	-5.03	1.46	1.52
2	3	25	MET	CA-C	-5.03	1.46	1.52
3	L	346	ALA	CA-C	-5.03	1.46	1.52
2	2	111	LEU	CA-C	-5.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	110	LYS	CA-C	-5.03	1.46	1.52
1	f	108	THR	CA-C	-5.03	1.46	1.52
2	h	163	GLU	CA-C	-5.03	1.46	1.52
2	m	174	SER	C-O	5.03	1.30	1.24
2	m	184	ASP	CA-C	-5.03	1.46	1.53
3	I	351	ILE	C-N	5.03	1.40	1.33
3	L	178	VAL	N-CA	-5.03	1.40	1.46
1	B	10	ARG	CD-NE	5.03	1.53	1.46
1	f	138	ILE	CA-C	-5.03	1.46	1.52
1	d	150	THR	C-N	5.02	1.39	1.32
1	e	168	ARG	NE-CZ	5.02	1.38	1.33
1	e	189	MET	CA-C	-5.02	1.46	1.52
2	3	42	ALA	CA-C	-5.02	1.46	1.52
1	F	206	PRO	N-CD	-5.02	1.40	1.47
2	l	201	PRO	CA-C	-5.02	1.45	1.52
2	n	28	GLU	CA-CB	-5.02	1.45	1.53
3	I	61	PRO	N-CD	5.02	1.54	1.47
2	4	51	ARG	CD-NE	5.02	1.53	1.46
2	l	103	TYR	C-N	5.02	1.40	1.33
1	D	185	PHE	CG-CD2	5.02	1.49	1.38
2	4	66	LEU	C-N	5.02	1.40	1.33
2	k	17	LEU	CA-C	-5.02	1.46	1.52
1	c	29	GLU	C-N	5.02	1.40	1.33
3	H	119	LEU	CA-C	-5.02	1.47	1.52
1	B	213	TYR	CA-CB	5.01	1.62	1.53
1	F	118	ASP	CA-C	-5.01	1.45	1.52
1	F	237	ASN	CA-CB	5.01	1.61	1.53
2	m	81	ARG	NE-CZ	5.01	1.38	1.33
3	I	184	PRO	CA-C	-5.01	1.45	1.52
3	K	9	LEU	CB-CG	5.01	1.63	1.53
3	L	97	GLU	C-N	5.01	1.41	1.33
3	M	329	LYS	N-CA	-5.01	1.39	1.46
1	b	183	LEU	CB-CG	5.01	1.63	1.53
1	c	75	CYS	CA-C	-5.01	1.46	1.52
1	C	28	ARG	CZ-NH1	5.01	1.39	1.32
1	c	71	ASP	C-N	5.01	1.40	1.33
1	G	96	ALA	C-N	5.01	1.40	1.34
1	g	15	PHE	N-CA	-5.01	1.39	1.45
2	3	154	ARG	CD-NE	5.01	1.53	1.46
1	e	109	VAL	CA-CB	-5.01	1.48	1.54
1	F	65	GLU	CA-C	-5.01	1.46	1.52
2	1	54	MET	N-CA	5.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	166	GLU	CA-CB	5.01	1.61	1.53
2	k	171	ALA	C-N	5.01	1.39	1.33
1	c	201	GLU	CA-C	5.01	1.59	1.53
1	f	86	ARG	CA-C	-5.01	1.46	1.52
1	g	87	VAL	N-CA	5.01	1.53	1.46
1	F	91	ARG	CZ-NH2	5.01	1.40	1.33
1	F	132	PHE	CA-C	-5.01	1.46	1.52
2	h	65	PHE	C-N	5.01	1.40	1.33
2	3	158	GLU	CA-C	-5.01	1.45	1.52
3	J	74	ASP	N-CA	-5.01	1.41	1.46
1	c	107	ILE	CB-CG1	5.00	1.63	1.53
2	3	191	ILE	C-N	5.00	1.40	1.33
2	j	146	THR	C-N	5.00	1.40	1.33
1	B	121	GLN	C-N	5.00	1.40	1.33
1	F	168	ARG	CZ-NH2	5.00	1.40	1.33
1	G	28	ARG	CD-NE	5.00	1.53	1.46
2	1	17	LEU	C-N	5.00	1.40	1.33
2	1	141	GLY	C-N	5.00	1.40	1.33
3	K	238	ILE	CA-C	-5.00	1.47	1.52
3	L	326	ARG	CD-NE	5.00	1.53	1.46
1	B	208	ASN	C-N	-5.00	1.26	1.33
2	m	40	LYS	C-N	5.00	1.40	1.33
3	H	263	ARG	C-O	-5.00	1.17	1.24
3	J	107	ALA	N-CA	-5.00	1.39	1.46

All (4414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	170	ARG	NE-CZ-NH2	-22.14	99.28	119.20
2	l	170	ARG	NE-CZ-NH2	-21.50	99.85	119.20
3	M	383	LEU	N-CA-C	14.19	129.69	112.38
3	I	309	VAL	N-CA-C	-13.41	93.25	107.60
3	H	336	PHE	CA-CB-CG	-13.18	100.62	113.80
1	c	45	GLY	CA-C-O	12.57	129.59	120.91
1	G	230	LYS	CA-C-O	-12.54	106.79	118.33
3	L	167	PHE	CA-CB-CG	-12.43	101.37	113.80
1	G	151	ASP	CA-C-N	11.63	131.31	119.56
1	G	151	ASP	C-N-CA	11.63	131.31	119.56
2	5	33	MET	N-CA-C	-11.61	99.64	114.04
2	h	143	GLY	CA-C-N	11.59	135.81	120.28
2	h	143	GLY	C-N-CA	11.59	135.81	120.28
1	g	56	SER	N-CA-C	11.29	125.21	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	280	ASP	N-CA-C	-11.24	97.15	110.41
2	m	211	PHE	N-CA-C	-11.07	102.00	114.62
1	d	245	LYS	N-CA-C	-11.04	102.03	114.62
3	I	299	ARG	CA-C-O	-10.98	110.96	120.19
1	F	205	VAL	O-C-N	-10.94	114.80	121.69
3	J	61	PRO	CA-C-O	-10.88	112.13	120.73
2	m	201	PRO	CA-C-N	10.84	134.53	120.44
2	m	201	PRO	C-N-CA	10.84	134.53	120.44
1	g	56	SER	CA-C-N	10.79	134.47	120.44
1	g	56	SER	C-N-CA	10.79	134.47	120.44
2	6	194	ASP	N-CA-C	-10.77	100.88	114.56
3	I	60	SER	CA-C-N	10.61	131.31	120.38
3	I	60	SER	C-N-CA	10.61	131.31	120.38
3	K	303	PHE	CA-CB-CG	-10.61	103.19	113.80
2	i	146	THR	CA-C-N	10.57	134.44	120.28
2	i	146	THR	C-N-CA	10.57	134.44	120.28
3	J	124	ASP	CA-C-N	10.55	131.35	119.32
3	J	124	ASP	C-N-CA	10.55	131.35	119.32
3	J	276	ASP	CA-C-N	10.54	131.21	119.93
3	J	276	ASP	C-N-CA	10.54	131.21	119.93
1	b	160	LYS	N-CA-C	-10.51	100.46	113.28
1	F	146	LYS	CA-C-O	-10.48	108.90	121.06
1	D	65	GLU	N-CA-CB	10.48	128.31	110.50
1	F	205	VAL	N-CA-C	-10.47	100.61	109.19
3	I	188	LYS	N-CA-C	-10.45	100.27	113.43
2	6	143	GLY	CA-C-N	10.44	134.69	120.38
2	6	143	GLY	C-N-CA	10.44	134.69	120.38
3	J	266	MET	CA-C-N	10.36	135.00	120.29
3	J	266	MET	C-N-CA	10.36	135.00	120.29
3	K	99	GLU	N-CA-C	-10.28	101.50	114.56
3	L	174	PRO	O-C-N	-10.24	116.33	121.15
1	a	70	ILE	N-CA-C	-10.15	103.08	111.81
3	K	94	TYR	N-CA-C	-10.11	101.72	114.56
3	H	322	LYS	CA-C-N	10.09	134.28	120.46
3	H	322	LYS	C-N-CA	10.09	134.28	120.46
1	g	191	LEU	CA-C-N	10.07	131.16	119.98
1	g	191	LEU	C-N-CA	10.07	131.16	119.98
1	a	33	ARG	CA-C-N	10.01	129.61	120.10
1	a	33	ARG	C-N-CA	10.01	129.61	120.10
3	M	11	GLU	CA-C-O	9.91	131.05	120.55
1	C	143	GLU	N-CA-C	-9.87	101.58	114.31
3	H	52	ARG	CA-C-N	9.86	133.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	52	ARG	C-N-CA	9.86	133.26	120.44
1	E	205	VAL	O-C-N	-9.81	113.26	121.40
2	2	35	ASN	CA-CB-CG	9.75	122.35	112.60
1	E	144	VAL	CA-C-N	9.71	129.80	119.90
1	E	144	VAL	C-N-CA	9.71	129.80	119.90
3	M	290	ILE	N-CA-C	-9.70	103.69	113.10
2	i	104	PHE	O-C-N	-9.64	115.10	121.85
2	m	156	THR	O-C-N	-9.63	115.11	121.85
1	e	142	ASP	CA-CB-CG	-9.57	103.03	112.60
3	H	311	LEU	CA-C-O	-9.57	112.09	119.46
2	1	57	ALA	N-CA-C	-9.54	94.78	109.85
2	k	80	ARG	NE-CZ-NH1	-9.54	111.97	121.50
2	4	99	ASN	CA-CB-CG	-9.50	103.10	112.60
2	1	135	LYS	CA-C-O	-9.46	110.89	120.82
1	g	181	ASP	N-CA-C	-9.46	101.89	112.57
2	h	30	ARG	NE-CZ-NH2	9.45	127.70	119.20
1	E	152	PRO	CA-C-N	9.43	132.70	120.44
1	E	152	PRO	C-N-CA	9.43	132.70	120.44
1	D	132	PHE	CA-CB-CG	-9.43	104.37	113.80
1	g	33	ARG	NE-CZ-NH2	9.41	127.67	119.20
2	n	175	ALA	CA-C-N	9.41	132.89	120.28
2	n	175	ALA	C-N-CA	9.41	132.89	120.28
2	2	209	ALA	N-CA-C	-9.40	101.81	113.28
2	3	178	ARG	N-CA-C	-9.40	102.01	112.72
1	b	241	ARG	O-C-N	9.39	132.07	122.12
1	g	218	ASP	CA-CB-CG	9.38	121.98	112.60
3	M	43	ARG	CA-C-N	9.37	132.84	120.28
3	M	43	ARG	C-N-CA	9.37	132.84	120.28
3	I	382	VAL	CA-C-N	9.37	132.83	120.28
3	I	382	VAL	C-N-CA	9.37	132.83	120.28
2	2	104	PHE	CA-C-O	-9.36	110.64	120.28
2	h	122	ILE	O-C-N	-9.28	113.17	123.10
2	6	36	PHE	CA-CB-CG	9.26	123.06	113.80
3	M	30	LEU	CA-C-N	9.26	132.69	120.28
3	M	30	LEU	C-N-CA	9.26	132.69	120.28
1	E	191	LEU	CA-C-N	9.26	131.98	120.22
1	E	191	LEU	C-N-CA	9.26	131.98	120.22
2	6	161	VAL	CA-C-N	9.25	132.46	120.44
2	6	161	VAL	C-N-CA	9.25	132.46	120.44
3	K	366	GLU	CA-C-N	9.24	133.99	120.87
3	K	366	GLU	C-N-CA	9.24	133.99	120.87
1	F	167	GLY	CA-C-N	9.23	132.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	167	GLY	C-N-CA	9.23	132.45	120.44
3	M	128	TYR	N-CA-CB	9.23	123.69	110.12
2	3	165	VAL	CA-C-N	9.23	132.44	120.44
2	3	165	VAL	C-N-CA	9.23	132.44	120.44
1	F	106	PRO	CA-C-N	9.20	132.86	120.63
1	F	106	PRO	C-N-CA	9.20	132.86	120.63
1	g	225	SER	CA-C-N	9.20	129.26	119.05
1	g	225	SER	C-N-CA	9.20	129.26	119.05
2	n	182	SER	N-CA-C	-9.19	102.20	113.50
3	M	337	LYS	CA-C-N	9.19	132.38	120.44
3	M	337	LYS	C-N-CA	9.19	132.38	120.44
2	5	170	ARG	NH1-CZ-NH2	9.17	131.22	119.30
2	5	61	GLY	CA-C-N	9.15	132.88	120.44
2	5	61	GLY	C-N-CA	9.15	132.88	120.44
3	K	397	PHE	CA-CB-CG	-9.14	104.66	113.80
2	3	102	ARG	NE-CZ-NH2	9.14	127.42	119.20
3	K	179	LEU	CA-C-O	9.13	130.35	120.58
1	f	168	ARG	CA-C-N	9.11	132.82	120.44
1	f	168	ARG	C-N-CA	9.11	132.82	120.44
1	D	151	ASP	CA-CB-CG	-9.10	103.50	112.60
1	e	181	ASP	CA-C-O	9.09	130.21	119.48
1	g	185	PHE	CA-C-N	9.09	132.46	120.28
1	g	185	PHE	C-N-CA	9.09	132.46	120.28
2	7	128	ILE	N-CA-C	-9.09	103.53	113.43
2	i	199	TYR	N-CA-C	9.07	120.78	111.07
2	1	96	ASN	CA-C-N	9.07	132.44	120.28
2	1	96	ASN	C-N-CA	9.07	132.44	120.28
3	J	376	THR	CA-C-N	9.06	133.15	120.29
3	J	376	THR	C-N-CA	9.06	133.15	120.29
2	l	179	ASP	CA-CB-CG	-9.05	103.55	112.60
3	K	138	VAL	N-CA-CB	9.03	120.87	110.49
1	B	70	ILE	N-CA-C	-9.01	104.56	112.12
1	b	217	ASP	CA-CB-CG	-8.99	103.61	112.60
3	K	192	ALA	CA-C-O	-8.98	111.39	120.82
1	C	215	LYS	CA-C-N	8.98	131.88	120.56
1	C	215	LYS	C-N-CA	8.98	131.88	120.56
1	F	67	ILE	N-CA-CB	8.97	120.50	110.72
2	n	62	ASP	CA-CB-CG	-8.97	103.62	112.60
2	7	178	ARG	NE-CZ-NH2	-8.97	111.12	119.20
2	m	155	PHE	CA-CB-CG	8.96	122.77	113.80
3	J	281	VAL	O-C-N	-8.96	112.61	123.10
3	K	183	PRO	N-CA-C	8.91	121.57	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ARG	NE-CZ-NH1	-8.90	112.60	121.50
2	l	142	SER	CA-C-O	8.90	128.49	118.97
1	C	151	ASP	O-C-N	-8.88	113.80	121.35
3	I	342	ILE	CA-C-O	-8.87	111.45	120.85
3	M	387	THR	N-CA-CB	8.87	123.02	111.40
2	h	140	THR	N-CA-CB	8.86	125.46	110.49
3	L	23	LEU	CA-C-N	8.85	131.94	120.44
3	L	23	LEU	C-N-CA	8.85	131.94	120.44
1	D	64	ILE	CA-C-N	8.84	137.61	121.70
1	D	64	ILE	C-N-CA	8.84	137.61	121.70
1	a	114	LYS	CA-C-O	-8.80	111.22	120.55
1	c	80	GLY	CA-C-O	-8.80	112.74	122.24
1	b	69	LYS	N-CA-C	-8.76	96.36	110.20
1	A	185	PHE	CA-C-N	8.75	131.81	120.44
1	A	185	PHE	C-N-CA	8.75	131.81	120.44
1	A	189	MET	O-C-N	8.72	131.05	122.07
3	H	109	ASN	CA-CB-CG	-8.71	103.89	112.60
1	G	215	LYS	CA-C-N	8.71	131.53	120.56
1	G	215	LYS	C-N-CA	8.71	131.53	120.56
1	a	31	VAL	CA-C-N	8.71	132.28	120.44
1	a	31	VAL	C-N-CA	8.71	132.28	120.44
3	K	37	ILE	CA-C-N	8.71	132.28	120.44
3	K	37	ILE	C-N-CA	8.71	132.28	120.44
2	j	113	GLY	O-C-N	8.69	132.50	123.29
2	6	174	SER	CA-C-N	8.69	132.80	120.28
2	6	174	SER	C-N-CA	8.69	132.80	120.28
3	L	304	ASP	CA-CB-CG	-8.69	103.91	112.60
1	a	245	LYS	N-CA-C	-8.69	102.43	113.72
2	4	108	VAL	N-CA-C	-8.67	95.91	107.88
2	3	173	TYR	CA-C-N	8.67	132.60	120.29
2	3	173	TYR	C-N-CA	8.67	132.60	120.29
3	M	382	VAL	N-CA-C	8.67	119.23	110.82
3	K	64	LEU	CA-C-N	8.66	133.54	122.37
3	K	64	LEU	C-N-CA	8.66	133.54	122.37
1	C	82	VAL	CA-C-N	8.65	132.07	120.65
1	C	82	VAL	C-N-CA	8.65	132.07	120.65
1	G	70	ILE	N-CA-C	-8.64	104.90	111.90
3	I	228	GLN	CA-C-N	8.64	131.86	120.28
3	I	228	GLN	C-N-CA	8.64	131.86	120.28
1	c	112	LEU	CA-C-N	8.64	131.67	120.44
1	c	112	LEU	C-N-CA	8.64	131.67	120.44
2	7	81	ARG	N-CA-C	-8.63	102.75	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	165	GLY	N-CA-C	-8.63	102.84	111.56
3	H	269	LEU	CA-C-N	8.63	131.66	120.44
3	H	269	LEU	C-N-CA	8.63	131.66	120.44
1	A	136	LEU	N-CA-C	-8.62	96.25	109.95
3	K	303	PHE	N-CA-C	-8.61	94.87	108.30
3	K	368	ALA	N-CA-C	-8.60	102.10	112.59
3	M	291	ASP	CA-CB-CG	8.59	121.19	112.60
2	n	151	LEU	N-CA-C	8.59	120.26	111.07
3	J	361	PHE	CA-CB-CG	-8.58	105.22	113.80
3	K	61	PRO	N-CA-C	8.58	121.17	110.70
1	c	84	ASP	CA-C-N	8.57	131.59	120.44
1	c	84	ASP	C-N-CA	8.57	131.59	120.44
1	e	225	SER	CA-C-N	8.56	129.40	119.47
1	e	225	SER	C-N-CA	8.56	129.40	119.47
2	1	172	ILE	CA-C-N	8.56	132.44	120.29
2	1	172	ILE	C-N-CA	8.56	132.44	120.29
2	3	183	GLY	N-CA-C	-8.56	103.20	115.27
3	H	156	ALA	N-CA-C	8.56	120.23	111.07
1	E	13	THR	N-CA-C	-8.55	102.98	113.50
3	J	136	PRO	CA-C-N	8.55	131.73	120.28
3	J	136	PRO	C-N-CA	8.55	131.73	120.28
3	J	124	ASP	CA-C-O	-8.54	111.05	120.69
3	J	296	ALA	N-CA-C	8.53	120.20	111.07
1	e	101	LEU	CA-C-O	-8.52	111.92	120.70
1	E	140	GLY	CA-C-O	-8.52	113.34	121.60
3	J	96	ASN	OD1-CG-ND2	8.51	131.11	122.60
1	e	18	ASP	CA-CB-CG	-8.50	104.10	112.60
1	c	113	ALA	N-CA-C	8.49	120.16	111.07
3	M	137	GLU	N-CA-C	-8.49	103.04	112.72
1	e	33	ARG	NE-CZ-NH1	-8.48	113.02	121.50
1	B	142	ASP	N-CA-C	-8.47	101.41	112.68
1	f	166	MET	CA-C-O	8.47	129.67	120.10
1	B	144	VAL	CA-C-N	8.47	128.23	119.76
1	B	144	VAL	C-N-CA	8.47	128.23	119.76
2	6	44	LYS	CA-C-O	8.47	127.93	119.97
3	L	23	LEU	CA-C-O	-8.47	110.23	119.97
1	g	59	LEU	CA-C-N	8.46	132.72	120.71
1	g	59	LEU	C-N-CA	8.46	132.72	120.71
3	H	174	PRO	CA-C-N	8.46	128.98	119.93
3	H	174	PRO	C-N-CA	8.46	128.98	119.93
2	l	170	ARG	NE-CZ-NH1	8.46	129.96	121.50
1	E	245	LYS	N-CA-C	-8.45	102.37	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	108	VAL	O-C-N	8.43	130.31	122.97
1	A	73	HIS	CE1-NE2-CD2	-8.43	100.57	109.00
1	e	217	ASP	CA-CB-CG	8.43	121.03	112.60
3	H	93	GLN	CA-C-N	8.42	134.98	120.58
3	H	93	GLN	C-N-CA	8.42	134.98	120.58
1	G	112	LEU	CA-C-N	8.42	131.56	120.28
1	G	112	LEU	C-N-CA	8.42	131.56	120.28
3	K	249	ARG	CD-NE-CZ	-8.41	112.62	124.40
2	i	167	LEU	CA-C-N	8.40	131.37	120.44
2	i	167	LEU	C-N-CA	8.40	131.37	120.44
3	L	46	ARG	CA-C-N	8.39	131.52	120.28
3	L	46	ARG	C-N-CA	8.39	131.52	120.28
1	C	196	MET	N-CA-C	8.38	120.42	111.28
1	C	82	VAL	N-CA-CB	8.37	121.93	110.54
3	K	299	ARG	N-CA-C	8.37	121.62	110.08
3	K	393	LYS	N-CA-C	-8.35	102.28	114.39
1	B	208	ASN	CA-CB-CG	8.34	120.94	112.60
2	l	175	ALA	CA-C-N	8.34	132.98	120.31
2	l	175	ALA	C-N-CA	8.34	132.98	120.31
3	K	224	ARG	CA-C-N	8.34	131.28	120.44
3	K	224	ARG	C-N-CA	8.34	131.28	120.44
2	5	143	GLY	CA-C-N	8.34	132.28	120.28
2	5	143	GLY	C-N-CA	8.34	132.28	120.28
3	I	150	ILE	CA-C-N	8.34	132.28	120.28
3	I	150	ILE	C-N-CA	8.34	132.28	120.28
2	l	74	ALA	CA-C-N	8.32	131.44	120.28
2	l	74	ALA	C-N-CA	8.32	131.44	120.28
2	k	139	ALA	CA-C-N	8.32	136.67	121.70
2	k	139	ALA	C-N-CA	8.32	136.67	121.70
1	E	151	ASP	N-CA-C	-8.31	99.52	110.40
2	l	170	ARG	NH1-CZ-NH2	8.30	130.09	119.30
1	g	151	ASP	CA-C-N	8.29	129.09	119.47
1	g	151	ASP	C-N-CA	8.29	129.09	119.47
2	7	86	THR	CA-C-N	8.28	131.80	120.46
2	7	86	THR	C-N-CA	8.28	131.80	120.46
1	D	144	VAL	CA-C-N	8.26	128.77	119.93
1	D	144	VAL	C-N-CA	8.26	128.77	119.93
3	I	39	SER	CA-C-N	8.25	132.01	120.29
3	I	39	SER	C-N-CA	8.25	132.01	120.29
3	M	281	VAL	CA-C-N	8.25	136.56	121.70
3	M	281	VAL	C-N-CA	8.25	136.56	121.70
3	L	169	GLU	N-CA-C	8.25	120.35	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	16	SER	CA-C-N	8.22	127.86	119.56
1	b	16	SER	C-N-CA	8.22	127.86	119.56
2	j	171	ALA	N-CA-C	8.21	120.31	111.36
1	d	186	ASP	CA-CB-CG	-8.19	104.41	112.60
2	j	156	THR	CA-C-O	-8.19	112.97	120.50
3	H	174	PRO	N-CA-C	8.19	120.69	110.70
2	1	51	ARG	NE-CZ-NH1	-8.18	113.32	121.50
2	1	211	PHE	N-CA-C	-8.17	103.21	113.02
3	K	301	GLY	N-CA-C	-8.17	103.82	114.85
3	M	367	ARG	N-CA-CB	8.16	121.90	110.07
2	j	55	THR	N-CA-C	-8.15	96.68	109.72
2	j	166	GLU	CA-C-N	8.15	131.20	120.28
2	j	166	GLU	C-N-CA	8.15	131.20	120.28
2	4	103	TYR	N-CA-C	-8.15	102.90	112.92
1	D	8	TYR	N-CA-C	-8.14	102.66	112.59
2	1	129	GLY	N-CA-C	-8.14	103.73	112.04
1	G	211	VAL	CA-C-N	8.14	128.65	121.82
1	G	211	VAL	C-N-CA	8.14	128.65	121.82
1	E	211	VAL	N-CA-C	-8.13	96.72	108.11
3	H	12	LYS	CA-C-N	8.13	131.18	120.28
3	H	12	LYS	C-N-CA	8.13	131.18	120.28
3	J	254	ASP	CA-C-N	8.13	136.33	121.70
3	J	254	ASP	C-N-CA	8.13	136.33	121.70
2	h	13	THR	N-CA-C	-8.12	97.06	109.41
2	i	48	ILE	N-CA-C	-8.12	104.83	111.81
3	H	254	ASP	CA-CB-CG	-8.12	104.48	112.60
3	K	319	GLN	CA-C-N	8.11	131.94	120.42
3	K	319	GLN	C-N-CA	8.11	131.94	120.42
1	B	12	ILE	N-CA-C	-8.10	104.60	113.43
3	L	391	ASP	CA-C-N	8.09	136.26	121.70
3	L	391	ASP	C-N-CA	8.09	136.26	121.70
1	E	19	GLY	N-CA-C	-8.09	104.18	114.37
3	I	37	ILE	CA-C-N	8.09	131.77	120.29
3	I	37	ILE	C-N-CA	8.09	131.77	120.29
1	e	191	LEU	N-CA-C	8.08	120.09	111.28
3	H	233	LYS	CA-C-O	-8.08	112.80	121.20
1	d	187	ASP	CA-CB-CG	-8.07	104.53	112.60
1	g	12	ILE	CA-C-O	8.06	126.62	118.96
1	E	70	ILE	N-CA-C	-8.06	105.26	111.62
1	a	216	VAL	N-CA-C	-8.05	101.56	113.39
1	c	80	GLY	O-C-N	8.04	131.54	123.10
2	1	155	PHE	CA-CB-CG	-8.04	105.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	157	PRO	N-CA-C	-8.03	104.41	114.68
1	A	18	ASP	CA-CB-CG	-8.02	104.58	112.60
1	c	20	ARG	CA-C-N	8.02	132.10	120.71
1	c	20	ARG	C-N-CA	8.02	132.10	120.71
3	L	383	LEU	CA-C-N	8.02	131.02	120.28
3	L	383	LEU	C-N-CA	8.02	131.02	120.28
1	D	176	GLU	N-CA-CB	8.01	121.89	110.12
2	3	157	PRO	N-CA-C	-8.01	105.39	114.92
3	L	174	PRO	CA-C-O	-8.00	114.41	120.73
3	K	125	PRO	N-CA-C	-8.00	98.32	111.68
3	J	18	GLU	CB-CA-C	-8.00	97.51	110.79
2	m	112	ILE	N-CA-CB	8.00	122.45	111.41
1	d	96	ALA	CA-C-N	8.00	134.27	120.68
1	d	96	ALA	C-N-CA	8.00	134.27	120.68
2	5	170	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	D	208	ASN	CA-CB-CG	7.98	120.58	112.60
1	e	123	TYR	N-CA-C	-7.98	103.35	113.72
2	3	87	VAL	CA-C-N	7.98	130.97	120.28
2	3	87	VAL	C-N-CA	7.98	130.97	120.28
2	1	42	ALA	CA-C-N	7.97	132.19	120.87
2	1	42	ALA	C-N-CA	7.97	132.19	120.87
1	b	151	ASP	CA-CB-CG	-7.96	104.64	112.60
1	g	221	PHE	CA-CB-CG	-7.96	105.84	113.80
2	n	135	LYS	N-CA-C	-7.96	103.71	113.50
3	M	386	THR	O-C-N	-7.96	112.01	122.59
1	a	84	ASP	CA-C-N	7.95	130.94	120.28
1	a	84	ASP	C-N-CA	7.95	130.94	120.28
3	L	154	ARG	CA-C-N	7.95	130.94	120.28
3	L	154	ARG	C-N-CA	7.95	130.94	120.28
2	1	135	LYS	O-C-N	7.95	130.26	122.07
1	b	224	VAL	CA-C-N	7.95	132.76	120.60
1	b	224	VAL	C-N-CA	7.95	132.76	120.60
2	h	158	GLU	CA-C-N	7.94	131.39	120.35
2	h	158	GLU	C-N-CA	7.94	131.39	120.35
1	F	241	ARG	NE-CZ-NH1	-7.94	113.56	121.50
1	D	88	LEU	N-CA-C	7.94	119.94	111.28
2	h	139	ALA	N-CA-C	-7.94	97.26	109.24
2	4	33	MET	N-CA-C	-7.93	101.05	110.41
3	L	43	ARG	CA-C-N	7.93	130.91	120.28
3	L	43	ARG	C-N-CA	7.93	130.91	120.28
3	L	356	THR	CA-C-N	7.93	131.56	120.29
3	L	356	THR	C-N-CA	7.93	131.56	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	96	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	e	205	VAL	CA-C-N	7.92	128.10	119.87
1	e	205	VAL	C-N-CA	7.92	128.10	119.87
3	J	238	ILE	N-CA-C	-7.92	96.32	107.80
1	G	9	ASP	N-CA-C	-7.90	102.69	112.88
3	K	195	VAL	CA-C-N	7.90	130.87	120.28
3	K	195	VAL	C-N-CA	7.90	130.87	120.28
3	L	281	VAL	CA-C-N	7.89	135.91	121.70
3	L	281	VAL	C-N-CA	7.89	135.91	121.70
2	1	134	GLU	CA-C-N	7.89	130.70	120.44
2	1	134	GLU	C-N-CA	7.89	130.70	120.44
3	I	236	SER	CA-C-N	7.89	135.91	121.70
3	I	236	SER	C-N-CA	7.89	135.91	121.70
1	C	28	ARG	N-CA-C	-7.89	103.67	113.38
1	d	99	ASN	O-C-N	-7.89	113.16	122.15
1	c	137	LEU	N-CA-C	-7.88	95.41	108.34
3	K	257	GLY	CA-C-N	7.88	135.88	121.70
3	K	257	GLY	C-N-CA	7.88	135.88	121.70
2	h	211	PHE	CA-CB-CG	7.88	121.68	113.80
1	a	65	GLU	CA-C-O	7.87	128.86	120.36
1	g	245	LYS	N-CA-C	-7.87	101.80	113.61
2	l	148	TYR	CA-C-N	7.87	128.68	119.94
2	l	148	TYR	C-N-CA	7.87	128.68	119.94
3	J	220	ALA	CB-CA-C	-7.87	98.85	110.96
1	g	43	LYS	N-CA-C	-7.86	103.25	112.92
1	f	83	ALA	N-CA-C	-7.85	102.80	111.36
1	B	103	TYR	N-CA-C	-7.85	105.67	114.62
3	H	142	ASP	N-CA-C	-7.85	103.21	114.12
2	l	59	SER	CA-C-N	7.84	130.44	120.56
2	l	59	SER	C-N-CA	7.84	130.44	120.56
1	B	101	LEU	N-CA-C	7.83	119.45	111.07
3	J	25	GLU	CA-C-N	7.83	131.41	120.29
3	J	25	GLU	C-N-CA	7.83	131.41	120.29
1	g	29	GLU	CA-C-N	7.83	130.77	120.28
1	g	29	GLU	C-N-CA	7.83	130.77	120.28
1	D	99	ASN	CA-CB-CG	7.82	120.42	112.60
3	H	118	VAL	N-CA-C	-7.82	96.86	108.12
1	c	83	ALA	CA-C-N	7.82	130.76	120.28
1	c	83	ALA	C-N-CA	7.82	130.76	120.28
2	l	97	LEU	N-CA-C	7.82	119.44	111.07
3	I	19	ASP	CA-C-N	7.82	130.75	120.28
3	I	19	ASP	C-N-CA	7.82	130.75	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	24	VAL	CA-C-O	-7.81	112.36	120.71
2	n	144	SER	N-CA-C	7.80	119.78	111.28
3	H	98	GLU	CA-C-N	7.80	135.13	122.65
3	H	98	GLU	C-N-CA	7.80	135.13	122.65
3	K	341	ARG	O-C-N	7.80	130.39	122.12
2	4	46	TYR	N-CA-C	-7.80	95.32	108.26
3	I	266	MET	CA-C-N	7.79	131.50	120.28
3	I	266	MET	C-N-CA	7.79	131.50	120.28
3	I	141	GLU	N-CA-C	-7.79	103.35	113.17
1	E	184	SER	CA-C-N	7.79	131.35	120.29
1	E	184	SER	C-N-CA	7.79	131.35	120.29
1	d	69	LYS	CA-C-O	-7.79	112.44	120.54
3	H	317	ARG	CA-C-N	7.77	130.35	120.56
3	H	317	ARG	C-N-CA	7.77	130.35	120.56
2	2	97	LEU	CA-C-N	7.77	130.69	120.28
2	2	97	LEU	C-N-CA	7.77	130.69	120.28
2	2	66	LEU	CA-C-N	7.76	130.69	120.28
2	2	66	LEU	C-N-CA	7.76	130.69	120.28
2	k	166	GLU	CA-C-N	7.76	130.68	120.28
2	k	166	GLU	C-N-CA	7.76	130.68	120.28
2	m	33	MET	CA-C-N	7.76	129.19	120.42
2	m	33	MET	C-N-CA	7.76	129.19	120.42
3	J	254	ASP	CA-CB-CG	7.76	120.36	112.60
3	I	10	LEU	CA-C-N	7.75	130.98	120.44
3	I	10	LEU	C-N-CA	7.75	130.98	120.44
1	D	31	VAL	CA-C-N	7.75	130.66	120.28
1	D	31	VAL	C-N-CA	7.75	130.66	120.28
1	e	240	ILE	O-C-N	7.74	129.38	121.87
1	F	73	HIS	CA-CB-CG	7.74	121.54	113.80
1	G	232	TYR	CA-C-N	7.74	130.47	120.56
1	G	232	TYR	C-N-CA	7.74	130.47	120.56
3	I	303	PHE	CA-CB-CG	-7.74	106.06	113.80
1	F	158	GLU	CA-C-O	7.73	129.27	120.54
1	g	77	ALA	N-CA-C	-7.73	97.55	109.52
2	j	211	PHE	N-CA-C	-7.73	102.91	112.88
1	C	230	LYS	CA-C-N	7.72	127.62	119.05
1	C	230	LYS	C-N-CA	7.72	127.62	119.05
2	5	78	GLU	CA-C-N	7.72	131.38	120.42
2	5	78	GLU	C-N-CA	7.72	131.38	120.42
2	7	17	LEU	CA-C-N	7.72	133.16	123.12
2	7	17	LEU	C-N-CA	7.72	133.16	123.12
1	c	112	LEU	N-CA-C	-7.72	102.81	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	130	ARG	CA-C-O	-7.71	113.66	120.60
1	c	17	PRO	CA-C-N	7.71	131.38	120.28
1	c	17	PRO	C-N-CA	7.71	131.38	120.28
1	c	196	MET	N-CA-C	-7.71	102.95	111.36
2	j	194	ASP	N-CA-C	-7.71	104.77	114.56
1	b	240	ILE	N-CA-C	-7.71	103.02	110.42
1	C	233	VAL	O-C-N	-7.71	113.09	121.80
3	M	174	PRO	CA-C-O	-7.71	114.64	120.73
3	H	183	PRO	N-CA-C	7.70	120.09	110.70
1	e	109	VAL	N-CA-C	-7.70	102.94	110.72
2	5	157	PRO	N-CA-C	-7.70	105.76	114.92
2	k	65	PHE	CA-CB-CG	-7.69	106.11	113.80
2	l	76	LEU	CA-C-N	7.69	130.43	120.44
2	l	76	LEU	C-N-CA	7.69	130.43	120.44
1	a	43	LYS	N-CA-C	-7.68	103.80	113.02
3	M	373	LEU	CA-C-O	-7.68	112.28	120.42
1	b	188	ALA	O-C-N	7.68	130.26	122.12
1	c	98	ILE	CA-C-N	7.67	131.18	120.29
1	c	98	ILE	C-N-CA	7.67	131.18	120.29
2	7	17	LEU	N-CA-C	-7.66	96.96	108.99
1	D	239	ARG	CA-C-N	7.65	130.35	120.56
1	D	239	ARG	C-N-CA	7.65	130.35	120.56
1	b	239	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	d	217	ASP	N-CA-CB	7.63	121.46	110.16
2	1	168	ALA	CA-C-O	7.63	128.64	120.55
1	d	99	ASN	CA-C-O	7.63	128.51	120.42
2	3	23	VAL	O-C-N	-7.63	114.58	123.05
3	L	229	LEU	N-CA-C	-7.63	102.31	111.69
1	e	211	VAL	N-CA-CB	7.63	122.66	111.52
1	f	137	LEU	N-CA-CB	7.63	122.70	110.65
2	l	66	LEU	O-C-N	7.63	131.65	122.27
1	B	174	PHE	CA-C-O	-7.62	112.85	120.70
1	d	230	LYS	CA-C-O	-7.62	110.95	118.34
2	l	165	VAL	N-CA-CB	7.62	120.91	110.54
3	M	163	LYS	CA-C-N	7.62	127.51	119.05
3	M	163	LYS	C-N-CA	7.62	127.51	119.05
1	C	45	GLY	N-CA-C	-7.61	100.30	110.58
1	c	236	ALA	CA-C-N	7.61	130.48	120.28
1	c	236	ALA	C-N-CA	7.61	130.48	120.28
1	c	37	ALA	CA-C-O	-7.61	111.47	120.60
3	M	386	THR	CA-C-N	7.61	131.78	122.42
3	M	386	THR	C-N-CA	7.61	131.78	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	66	LYS	N-CA-C	-7.61	100.74	112.99
1	C	230	LYS	CA-C-O	-7.61	109.74	120.16
3	I	82	SER	CA-C-O	7.60	128.73	119.38
2	l	30	ARG	N-CA-CB	7.60	123.33	110.49
1	f	98	ILE	CA-C-N	7.59	130.31	120.44
1	f	98	ILE	C-N-CA	7.59	130.31	120.44
2	h	194	ASP	N-CA-C	-7.58	105.97	114.62
2	4	157	PRO	N-CA-C	-7.58	104.87	114.35
3	I	215	TYR	CB-CG-CD1	-7.58	109.43	120.80
1	b	66	LYS	N-CA-C	-7.58	102.94	114.16
1	E	218	ASP	N-CA-C	-7.58	104.17	113.41
1	f	29	GLU	CA-C-N	7.58	131.19	120.28
1	f	29	GLU	C-N-CA	7.58	131.19	120.28
1	G	15	PHE	O-C-N	-7.58	114.40	122.96
2	j	49	ALA	CA-C-N	7.58	130.76	120.38
2	j	49	ALA	C-N-CA	7.58	130.76	120.38
2	k	128	ILE	N-CA-C	-7.57	104.10	112.80
3	H	112	THR	N-CA-C	-7.57	101.15	110.61
1	c	67	ILE	N-CA-C	-7.56	97.52	108.11
2	1	66	LEU	O-C-N	7.56	130.77	122.15
1	b	61	ALA	CA-C-O	7.55	126.83	118.52
1	f	103	TYR	CA-C-N	7.55	133.08	122.36
1	f	103	TYR	C-N-CA	7.55	133.08	122.36
2	1	91	ALA	CA-C-N	7.55	131.01	120.29
2	1	91	ALA	C-N-CA	7.55	131.01	120.29
2	5	177	LYS	N-CA-C	-7.55	103.87	113.23
1	g	151	ASP	CA-C-O	-7.55	114.36	121.08
1	C	220	THR	N-CA-C	-7.54	95.74	108.26
1	E	188	ALA	N-CA-C	7.54	119.50	111.28
2	1	48	ILE	N-CA-C	-7.54	105.33	111.81
1	E	113	ALA	CA-C-N	7.54	130.24	120.44
1	E	113	ALA	C-N-CA	7.54	130.24	120.44
2	2	156	THR	O-C-N	-7.53	114.92	121.32
2	6	104	PHE	CA-C-O	-7.53	112.45	119.76
3	H	348	GLY	CA-C-N	7.53	131.76	120.31
3	H	348	GLY	C-N-CA	7.53	131.76	120.31
1	G	208	ASN	CA-CB-CG	7.53	120.13	112.60
2	k	88	ARG	NE-CZ-NH1	-7.52	113.98	121.50
3	M	319	GLN	CA-C-N	7.52	131.09	120.42
3	M	319	GLN	C-N-CA	7.52	131.09	120.42
1	D	165	GLY	CA-C-N	7.51	130.35	120.28
1	D	165	GLY	C-N-CA	7.51	130.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	32	THR	CA-C-O	-7.51	112.28	120.24
1	g	144	VAL	CA-C-N	7.51	127.94	119.83
1	g	144	VAL	C-N-CA	7.51	127.94	119.83
2	2	65	PHE	CA-CB-CG	-7.51	106.29	113.80
2	m	206	GLN	CB-CG-CD	-7.51	99.83	112.60
2	1	112	ILE	N-CA-CB	7.50	121.77	111.41
1	A	124	THR	N-CA-C	-7.50	102.03	112.45
1	d	132	PHE	CA-CB-CG	-7.50	106.30	113.80
3	L	37	ILE	CA-C-N	7.50	130.32	120.28
3	L	37	ILE	C-N-CA	7.50	130.32	120.28
1	A	42	CYS	CA-C-O	-7.49	112.48	121.32
2	2	142	SER	N-CA-CB	7.49	121.90	110.81
2	4	195	GLU	O-C-N	7.49	131.79	123.33
3	K	272	LEU	O-C-N	7.48	130.17	122.09
3	L	275	PHE	CA-CB-CG	-7.48	106.32	113.80
2	7	107	LEU	N-CA-CB	7.48	122.21	110.84
2	4	62	ASP	CA-CB-CG	-7.48	105.12	112.60
3	I	268	LEU	CA-C-N	7.48	130.91	120.29
3	I	268	LEU	C-N-CA	7.48	130.91	120.29
3	L	352	LYS	CA-C-O	-7.47	112.98	120.82
1	A	63	THR	N-CA-C	-7.46	97.23	109.40
2	k	51	ARG	NE-CZ-NH2	7.46	125.92	119.20
3	L	115	ILE	CA-CB-CG1	7.46	123.09	110.40
3	M	303	PHE	CA-C-N	7.46	130.13	120.44
3	M	303	PHE	C-N-CA	7.46	130.13	120.44
3	M	118	VAL	CA-C-O	-7.45	113.58	121.93
3	M	226	VAL	CA-C-N	7.45	130.87	120.29
3	M	226	VAL	C-N-CA	7.45	130.87	120.29
2	i	210	LYS	N-CA-C	-7.45	105.10	114.56
2	n	126	ASP	N-CA-C	-7.45	99.75	110.40
1	g	169	ASN	N-CA-C	7.44	119.03	111.07
1	g	187	ASP	N-CA-CB	7.44	120.80	110.01
2	k	29	LYS	O-C-N	7.44	133.13	122.94
3	I	149	GLN	N-CA-C	-7.44	103.67	112.89
1	e	116	ILE	CA-C-O	7.44	128.28	120.25
3	I	98	GLU	N-CA-C	-7.44	103.80	113.17
2	5	145	LEU	CA-C-O	7.43	128.30	120.42
1	d	170	ALA	CA-C-N	7.43	130.97	120.42
1	d	170	ALA	C-N-CA	7.43	130.97	120.42
1	a	28	ARG	CA-C-N	7.42	130.23	120.28
1	a	28	ARG	C-N-CA	7.42	130.23	120.28
1	a	80	GLY	N-CA-C	-7.42	103.50	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	131	ALA	O-C-N	-7.41	114.32	123.44
3	I	242	GLU	N-CA-C	-7.41	95.01	110.80
3	J	357	GLU	O-C-N	-7.41	113.70	122.15
3	M	371	THR	CA-C-N	7.41	130.20	120.28
3	M	371	THR	C-N-CA	7.41	130.20	120.28
2	k	54	MET	N-CA-C	-7.40	96.26	108.76
1	c	227	GLU	CA-C-N	7.39	130.79	120.29
1	c	227	GLU	C-N-CA	7.39	130.79	120.29
2	7	80	ARG	N-CA-C	7.39	118.98	111.07
3	M	228	GLN	CA-C-N	7.39	130.19	120.28
3	M	228	GLN	C-N-CA	7.39	130.19	120.28
1	G	136	LEU	CA-C-O	7.39	129.16	120.66
2	7	57	ALA	N-CA-C	-7.39	97.36	109.40
1	F	82	VAL	CB-CA-C	-7.39	102.03	112.22
2	l	128	ILE	N-CA-C	-7.39	105.94	113.10
2	i	60	VAL	N-CA-C	7.38	117.47	110.53
3	H	121	THR	N-CA-C	-7.38	101.11	112.99
2	l	48	ILE	CB-CA-C	-7.38	102.38	112.04
3	J	279	GLY	N-CA-C	-7.37	104.89	111.67
2	7	194	ASP	CA-CB-CG	-7.36	105.24	112.60
3	H	126	MET	CA-C-O	7.36	128.33	120.46
3	K	11	GLU	CA-C-N	7.36	130.44	120.44
3	K	11	GLU	C-N-CA	7.36	130.44	120.44
3	L	308	GLU	CA-C-N	7.36	129.25	122.85
3	L	308	GLU	C-N-CA	7.36	129.25	122.85
3	J	53	SER	CA-C-N	7.35	130.73	120.29
3	J	53	SER	C-N-CA	7.35	130.73	120.29
3	J	93	GLN	N-CA-C	-7.35	104.05	113.16
3	I	275	PHE	CA-CB-CG	7.35	121.15	113.80
2	j	58	GLY	N-CA-C	-7.34	104.14	111.56
3	K	211	PHE	CA-CB-CG	-7.34	106.45	113.80
3	L	146	LEU	CA-C-N	7.34	130.12	120.28
3	L	146	LEU	C-N-CA	7.34	130.12	120.28
3	L	268	LEU	N-CA-C	7.34	119.28	111.28
2	m	135	LYS	N-CA-C	-7.34	100.80	111.30
3	I	194	ALA	CA-C-N	7.34	130.52	120.46
3	I	194	ALA	C-N-CA	7.34	130.52	120.46
2	i	182	SER	N-CA-C	-7.34	101.43	111.56
1	e	57	LYS	CA-C-N	7.34	130.11	120.28
1	e	57	LYS	C-N-CA	7.34	130.11	120.28
3	I	325	THR	CA-C-O	-7.34	110.36	119.38
1	G	235	ARG	CD-NE-CZ	-7.33	114.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	73	GLU	CA-C-N	7.33	129.97	120.44
2	i	73	GLU	C-N-CA	7.33	129.97	120.44
1	B	230	LYS	CA-C-O	-7.32	111.89	118.63
2	j	113	GLY	CA-C-O	-7.32	113.05	121.46
1	F	44	GLU	N-CA-C	-7.31	103.95	114.12
1	F	226	PRO	CA-C-N	7.31	130.08	120.28
1	F	226	PRO	C-N-CA	7.31	130.08	120.28
2	2	198	GLN	N-CA-C	-7.31	95.22	108.02
3	I	73	GLU	O-C-N	-7.31	113.56	122.34
1	C	25	GLU	O-C-N	7.31	130.77	122.22
1	A	181	ASP	CA-CB-CG	-7.30	105.30	112.60
1	b	35	ALA	CA-C-N	7.30	131.08	120.71
1	b	35	ALA	C-N-CA	7.30	131.08	120.71
1	c	214	VAL	N-CA-CB	7.30	122.18	111.52
1	A	9	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	144	VAL	N-CA-C	-7.30	103.21	109.19
3	K	28	ARG	NE-CZ-NH1	7.29	128.79	121.50
2	2	47	GLN	CA-C-O	7.29	128.38	120.58
2	j	132	ILE	CA-C-O	7.29	128.05	120.39
2	m	83	ARG	CA-C-N	7.29	130.52	120.39
2	m	83	ARG	C-N-CA	7.29	130.52	120.39
1	A	65	GLU	CA-C-N	7.29	132.83	122.05
1	A	65	GLU	C-N-CA	7.29	132.83	122.05
1	F	21	LEU	N-CA-C	-7.28	95.06	108.02
2	6	116	ASP	CA-C-N	7.28	129.91	120.44
2	6	116	ASP	C-N-CA	7.28	129.91	120.44
1	b	172	THR	N-CA-CB	7.28	120.57	110.01
2	i	148	TYR	CB-CA-C	-7.28	98.71	110.79
3	J	322	LYS	CA-C-O	-7.28	112.84	120.55
3	K	206	VAL	CA-C-O	-7.27	114.25	121.67
2	k	212	ARG	CD-NE-CZ	-7.27	114.23	124.40
3	K	281	VAL	CA-C-N	7.26	134.78	121.70
3	K	281	VAL	C-N-CA	7.26	134.78	121.70
1	f	187	ASP	CA-C-N	7.26	130.01	120.28
1	f	187	ASP	C-N-CA	7.26	130.01	120.28
1	D	143	GLU	CA-C-O	7.26	126.99	118.79
1	G	91	ARG	NE-CZ-NH2	7.26	125.73	119.20
2	j	119	GLY	N-CA-C	-7.26	103.66	111.21
1	E	130	ARG	CA-C-N	7.26	127.18	120.21
1	E	130	ARG	C-N-CA	7.26	127.18	120.21
1	G	25	GLU	N-CA-C	-7.25	104.40	113.18
2	4	160	GLY	N-CA-C	-7.25	101.12	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	ALA	N-CA-C	-7.25	95.36	110.80
1	g	173	GLU	CA-C-N	7.25	129.99	120.28
1	g	173	GLU	C-N-CA	7.25	129.99	120.28
1	B	64	ILE	CA-C-N	7.25	134.75	121.70
1	B	64	ILE	C-N-CA	7.25	134.75	121.70
1	G	23	GLN	CB-CG-CD	-7.25	100.28	112.60
2	6	139	ALA	N-CA-C	-7.25	95.36	110.80
3	K	80	LYS	N-CA-C	-7.24	96.75	108.41
1	c	169	ASN	CA-CB-CG	-7.24	105.36	112.60
2	k	66	LEU	CA-C-N	7.23	129.97	120.28
2	k	66	LEU	C-N-CA	7.23	129.97	120.28
1	C	235	ARG	N-CA-C	7.23	120.03	111.71
2	5	148	TYR	CA-C-N	7.23	128.16	119.99
2	5	148	TYR	C-N-CA	7.23	128.16	119.99
1	B	36	THR	N-CA-C	7.22	120.46	110.35
1	G	137	LEU	CA-C-O	-7.22	112.51	120.38
1	B	168	ARG	N-CA-C	7.22	118.80	111.07
1	E	224	VAL	O-C-N	-7.22	114.72	122.95
2	3	158	GLU	CA-C-N	7.22	130.94	120.91
2	3	158	GLU	C-N-CA	7.22	130.94	120.91
1	c	123	TYR	N-CA-C	-7.21	104.47	113.20
1	E	151	ASP	CA-CB-CG	-7.21	105.39	112.60
2	j	74	ALA	CA-C-N	7.21	129.94	120.28
2	j	74	ALA	C-N-CA	7.21	129.94	120.28
1	b	110	LYS	CA-C-N	7.21	130.25	120.44
1	b	110	LYS	C-N-CA	7.21	130.25	120.44
3	J	31	GLU	CA-C-N	7.21	130.66	120.28
3	J	31	GLU	C-N-CA	7.21	130.66	120.28
2	5	190	LYS	N-CA-C	-7.21	98.35	109.52
2	6	126	ASP	CA-C-N	7.21	127.36	119.87
2	6	126	ASP	C-N-CA	7.21	127.36	119.87
3	H	60	SER	O-C-N	7.21	129.60	121.32
1	F	64	ILE	CA-C-N	7.20	132.25	120.94
1	F	64	ILE	C-N-CA	7.20	132.25	120.94
3	I	116	VAL	N-CA-CB	-7.20	104.44	111.57
1	A	163	ALA	N-CA-C	-7.20	98.37	109.24
3	J	252	ASN	N-CA-C	-7.20	98.73	108.24
3	L	144	GLY	N-CA-C	-7.20	101.52	111.09
1	g	91	ARG	CA-C-O	7.19	128.18	120.55
1	B	135	SER	N-CA-C	-7.19	97.68	109.40
3	J	335	ASP	CA-CB-CG	-7.19	105.41	112.60
2	i	126	ASP	CA-CB-CG	-7.19	105.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	266	MET	O-C-N	7.19	129.74	122.12
1	A	73	HIS	ND1-CE1-NE2	7.19	115.59	108.40
2	1	160	GLY	CA-C-N	7.18	130.62	120.42
2	1	160	GLY	C-N-CA	7.18	130.62	120.42
1	g	62	ASP	N-CA-C	-7.18	103.16	113.21
3	K	248	ALA	CA-C-O	-7.18	113.63	121.31
2	l	156	THR	CA-C-O	-7.17	113.69	120.94
2	n	116	ASP	CA-CB-CG	-7.17	105.42	112.60
1	D	143	GLU	N-CA-C	-7.17	102.98	114.09
2	k	136	ASP	CA-CB-CG	7.16	119.76	112.60
3	I	164	PRO	CA-C-N	7.16	130.46	120.29
3	I	164	PRO	C-N-CA	7.16	130.46	120.29
3	I	229	LEU	N-CA-C	-7.16	103.47	111.28
3	K	112	THR	N-CA-C	-7.16	97.45	108.76
1	e	63	THR	N-CA-C	-7.16	103.00	114.09
2	7	212	ARG	N-CA-C	-7.16	100.26	108.49
1	d	106	PRO	CA-C-N	7.15	131.19	120.75
1	d	106	PRO	C-N-CA	7.15	131.19	120.75
2	2	143	GLY	CA-C-N	7.15	129.86	120.28
2	2	143	GLY	C-N-CA	7.15	129.86	120.28
3	L	297	ILE	CA-C-N	7.15	129.86	120.28
3	L	297	ILE	C-N-CA	7.15	129.86	120.28
1	d	105	GLU	CA-C-N	7.15	127.19	119.90
1	d	105	GLU	C-N-CA	7.15	127.19	119.90
2	3	106	TYR	N-CA-C	-7.15	97.25	108.90
1	a	168	ARG	CD-NE-CZ	-7.15	114.39	124.40
1	d	145	PRO	CA-C-O	-7.14	113.43	121.43
2	h	149	GLY	CA-C-N	7.13	130.24	120.46
2	h	149	GLY	C-N-CA	7.13	130.24	120.46
2	n	70	ILE	CA-C-N	7.13	129.84	120.28
2	n	70	ILE	C-N-CA	7.13	129.84	120.28
2	n	68	ARG	CA-C-O	-7.13	113.33	120.82
1	g	174	PHE	CA-C-O	7.13	128.11	120.55
2	l	154	ARG	NE-CZ-NH1	-7.13	114.37	121.50
3	H	51	LEU	O-C-N	7.12	129.67	122.12
3	K	281	VAL	N-CA-C	-7.12	97.77	108.17
3	K	19	ASP	N-CA-C	7.12	119.12	111.36
1	D	105	GLU	O-C-N	-7.12	115.68	121.80
2	4	78	GLU	O-C-N	7.12	130.27	122.15
2	k	104	PHE	CA-C-N	7.12	127.16	119.90
2	k	104	PHE	C-N-CA	7.12	127.16	119.90
2	i	165	VAL	N-CA-CB	7.12	121.25	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	33	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	g	189	MET	CA-C-N	7.11	130.20	120.46
1	g	189	MET	C-N-CA	7.11	130.20	120.46
3	I	266	MET	CA-C-O	-7.11	113.01	120.55
3	L	387	THR	O-C-N	7.11	127.38	121.83
3	H	57	ARG	N-CA-C	7.11	119.11	111.36
1	b	20	ARG	NE-CZ-NH2	-7.10	112.81	119.20
2	h	88	ARG	N-CA-C	-7.10	103.47	111.14
3	M	384	LYS	N-CA-C	7.10	118.67	111.07
1	B	9	ASP	N-CA-C	-7.09	104.66	113.38
3	H	393	LYS	N-CA-C	-7.09	102.66	112.30
3	J	315	GLU	O-C-N	7.09	130.23	122.15
2	l	51	ARG	NE-CZ-NH2	7.08	125.58	119.20
2	n	40	LYS	O-C-N	7.08	130.23	122.15
1	g	153	SER	N-CA-C	-7.08	104.11	112.89
2	7	157	PRO	CA-C-O	7.08	125.09	118.29
3	L	366	GLU	CA-C-O	-7.08	113.10	122.44
1	B	217	ASP	N-CA-CB	7.08	120.48	109.94
1	c	239	ARG	CA-C-O	7.07	127.92	120.42
2	n	59	SER	CA-C-N	7.07	131.86	120.55
2	n	59	SER	C-N-CA	7.07	131.86	120.55
1	D	189	MET	N-CA-C	7.07	118.63	111.07
1	E	25	GLU	CA-C-O	7.07	128.10	119.97
3	K	207	VAL	N-CA-C	-7.07	98.31	108.42
3	J	21	TYR	O-C-N	7.07	130.20	122.15
1	d	161	ALA	N-CA-CB	7.06	122.43	110.49
2	6	53	ALA	N-CA-C	-7.06	98.58	109.24
3	I	324	HIS	CE1-NE2-CD2	-7.06	101.94	109.00
1	b	124	THR	N-CA-C	-7.06	102.79	111.40
1	A	209	ILE	CA-C-O	7.05	128.45	120.90
3	L	318	ILE	N-CA-C	-7.05	103.59	110.72
3	M	221	ARG	CA-C-N	7.05	129.73	120.28
3	M	221	ARG	C-N-CA	7.05	129.73	120.28
2	l	119	GLY	N-CA-C	-7.05	104.44	111.56
1	A	243	LEU	N-CA-C	7.05	118.96	111.28
2	1	163	GLU	CA-C-N	7.05	130.30	120.29
2	1	163	GLU	C-N-CA	7.05	130.30	120.29
1	F	113	ALA	CB-CA-C	7.04	122.48	110.79
3	L	383	LEU	N-CA-C	7.04	118.95	111.28
1	a	95	GLU	N-CA-CB	7.04	121.19	110.28
3	K	213	GLN	OE1-CD-NE2	7.04	129.64	122.60
1	d	240	ILE	O-C-N	-7.04	115.04	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	325	THR	CA-C-N	7.03	129.59	120.44
3	K	325	THR	C-N-CA	7.03	129.59	120.44
3	M	310	PRO	N-CA-C	-7.03	97.98	112.47
2	3	184	ASP	CA-C-N	7.03	135.19	121.41
2	3	184	ASP	C-N-CA	7.03	135.19	121.41
3	H	164	PRO	N-CA-C	-7.03	104.82	114.80
2	4	122	ILE	N-CA-CB	7.03	121.78	111.52
1	a	48	LEU	CA-C-O	7.03	127.69	120.24
1	D	104	ASP	CA-CB-CG	7.03	119.63	112.60
3	M	378	ALA	N-CA-C	7.03	118.94	111.28
3	J	357	GLU	CA-C-N	7.02	129.99	120.44
3	J	357	GLU	C-N-CA	7.02	129.99	120.44
1	d	212	GLY	O-C-N	-7.02	117.48	123.59
3	I	81	SER	CA-C-O	7.02	129.54	121.47
3	L	36	PHE	CA-C-N	7.02	129.41	120.56
3	L	36	PHE	C-N-CA	7.02	129.41	120.56
3	L	197	ASN	OD1-CG-ND2	7.02	129.62	122.60
1	a	152	PRO	CA-C-N	7.02	130.38	120.28
1	a	152	PRO	C-N-CA	7.02	130.38	120.28
2	5	15	VAL	CA-C-N	7.02	130.53	121.27
2	5	15	VAL	C-N-CA	7.02	130.53	121.27
3	K	205	ARG	CD-NE-CZ	-7.02	114.58	124.40
3	M	396	MET	N-CA-C	-7.01	104.60	113.72
1	D	95	GLU	CA-C-N	7.01	129.98	120.44
1	D	95	GLU	C-N-CA	7.01	129.98	120.44
1	D	61	ALA	N-CA-C	-7.01	103.84	112.88
3	K	209	SER	N-CA-C	-7.01	95.87	110.80
1	G	89	ILE	CA-C-O	-7.01	112.90	120.47
2	l	193	GLU	CA-C-O	-7.01	110.41	119.59
1	E	103	TYR	N-CA-C	-7.00	105.93	114.75
2	h	103	TYR	N-CA-C	-7.00	103.92	113.30
3	H	324	HIS	CG-CD2-NE2	7.00	114.20	107.20
3	L	148	VAL	CA-C-N	7.00	130.23	120.29
3	L	148	VAL	C-N-CA	7.00	130.23	120.29
1	a	182	ASP	N-CA-CB	7.00	122.32	110.49
2	6	100	SER	O-C-N	7.00	129.28	122.07
3	L	148	VAL	CB-CA-C	-7.00	102.85	112.02
1	F	18	ASP	CA-CB-CG	-7.00	105.60	112.60
2	4	144	SER	CA-C-N	6.99	129.53	120.44
2	4	144	SER	C-N-CA	6.99	129.53	120.44
1	D	120	LYS	CA-C-N	6.99	129.65	120.28
1	D	120	LYS	C-N-CA	6.99	129.65	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	205	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	b	212	GLY	N-CA-C	-6.99	101.50	111.42
1	C	202	SER	CA-C-N	6.99	132.99	121.39
1	C	202	SER	C-N-CA	6.99	132.99	121.39
1	e	62	ASP	N-CA-C	-6.99	103.26	114.09
3	L	341	ARG	CA-C-N	6.99	130.03	120.46
3	L	341	ARG	C-N-CA	6.99	130.03	120.46
1	b	31	VAL	CA-C-N	6.98	130.21	120.29
1	b	31	VAL	C-N-CA	6.98	130.21	120.29
2	1	83	ARG	NE-CZ-NH2	6.98	125.48	119.20
3	L	27	TYR	CA-C-N	6.98	129.51	120.44
3	L	27	TYR	C-N-CA	6.98	129.51	120.44
2	2	152	GLU	N-CA-C	-6.98	104.03	112.54
1	A	241	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	3	75	ASN	CA-C-N	6.98	129.96	120.54
2	3	75	ASN	C-N-CA	6.98	129.96	120.54
1	a	53	ARG	CA-C-N	6.97	134.52	121.97
1	a	53	ARG	C-N-CA	6.97	134.52	121.97
2	4	51	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	g	89	ILE	CA-C-N	6.96	130.18	120.29
1	g	89	ILE	C-N-CA	6.96	130.18	120.29
2	l	187	ASP	CA-CB-CG	6.96	119.56	112.60
2	h	62	ASP	CA-CB-CG	-6.96	105.64	112.60
2	7	84	LYS	CA-C-N	6.96	126.99	119.89
2	7	84	LYS	C-N-CA	6.96	126.99	119.89
3	I	137	GLU	N-CA-C	6.96	118.95	111.36
3	L	166	LEU	CA-C-N	6.96	129.60	120.28
3	L	166	LEU	C-N-CA	6.96	129.60	120.28
3	M	264	THR	CA-C-N	6.96	129.90	120.44
3	M	264	THR	C-N-CA	6.96	129.90	120.44
2	m	91	ALA	N-CA-C	6.96	120.25	111.69
3	H	275	PHE	N-CA-CB	6.96	120.19	110.17
1	f	165	GLY	CA-C-N	6.95	130.29	120.28
1	f	165	GLY	C-N-CA	6.95	130.29	120.28
1	G	61	ALA	N-CA-C	-6.95	104.54	113.16
2	l	166	GLU	CA-C-N	6.95	130.16	120.29
2	l	166	GLU	C-N-CA	6.95	130.16	120.29
1	G	56	SER	CA-C-O	6.95	123.73	119.77
2	i	150	VAL	N-CA-C	-6.95	104.00	110.53
2	4	44	LYS	N-CA-C	-6.94	103.88	114.16
3	I	37	ILE	CA-C-O	6.94	127.97	120.47
3	J	248	ALA	N-CA-CB	6.94	120.24	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	126	ASP	CA-C-N	6.94	126.64	119.56
2	m	126	ASP	C-N-CA	6.94	126.64	119.56
3	K	180	LEU	N-CA-CB	6.94	121.47	110.23
1	a	103	TYR	CA-C-O	6.93	126.45	118.55
3	I	198	GLN	N-CA-CB	6.93	120.31	110.67
3	L	85	PRO	CA-C-N	6.93	130.55	120.71
3	L	85	PRO	C-N-CA	6.93	130.55	120.71
3	L	386	THR	N-CA-C	-6.93	105.45	114.04
1	D	132	PHE	CB-CG-CD2	6.93	132.48	120.70
1	g	195	ALA	CA-C-N	6.93	130.12	120.29
1	g	195	ALA	C-N-CA	6.93	130.12	120.29
2	k	51	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	C	9	ASP	N-CA-CB	6.92	122.19	110.49
1	b	212	GLY	O-C-N	-6.92	118.62	123.95
3	J	363	ILE	O-C-N	6.92	128.59	121.87
1	A	137	LEU	CB-CA-C	-6.92	98.33	109.75
2	4	194	ASP	CA-CB-CG	-6.92	105.68	112.60
2	k	211	PHE	N-CA-CB	6.92	119.86	110.38
3	M	127	VAL	CA-C-O	-6.92	112.14	120.78
1	A	151	ASP	CA-CB-CG	-6.91	105.69	112.60
3	H	37	ILE	CA-C-N	6.91	129.54	120.28
3	H	37	ILE	C-N-CA	6.91	129.54	120.28
1	C	55	GLY	N-CA-C	6.91	122.52	114.16
1	f	144	VAL	N-CA-CB	6.91	120.88	111.21
3	K	376	THR	CA-C-N	6.91	129.42	120.44
3	K	376	THR	C-N-CA	6.91	129.42	120.44
3	J	204	ILE	N-CA-C	-6.91	97.67	108.23
2	k	165	VAL	N-CA-CB	6.90	119.93	110.54
3	H	97	GLU	CB-CG-CD	-6.90	100.86	112.60
1	b	26	TYR	CA-C-N	6.90	129.53	120.28
1	b	26	TYR	C-N-CA	6.90	129.53	120.28
3	K	110	GLN	CA-C-N	6.90	129.84	120.38
3	K	110	GLN	C-N-CA	6.90	129.84	120.38
3	K	56	GLU	N-CA-CB	6.90	120.48	110.20
1	F	109	VAL	CA-C-N	6.90	129.41	120.44
1	F	109	VAL	C-N-CA	6.90	129.41	120.44
1	E	172	THR	CA-C-N	6.90	130.08	120.29
1	E	172	THR	C-N-CA	6.90	130.08	120.29
1	A	112	LEU	N-CA-C	-6.89	103.85	111.36
3	M	269	LEU	CA-C-N	6.89	129.52	120.28
3	M	269	LEU	C-N-CA	6.89	129.52	120.28
1	A	237	ASN	N-CA-C	6.89	119.64	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	187	ASP	CA-CB-CG	6.89	119.49	112.60
2	k	139	ALA	O-C-N	-6.89	115.34	123.41
2	5	19	CYS	N-CA-C	-6.89	98.96	109.85
1	b	18	ASP	N-CA-C	-6.89	105.02	113.50
1	g	141	VAL	N-CA-C	-6.89	97.51	107.78
3	I	179	LEU	N-CA-CB	6.89	121.78	110.69
1	e	212	GLY	N-CA-C	-6.89	100.57	111.18
3	I	220	ALA	CA-C-N	6.89	129.82	120.38
3	I	220	ALA	C-N-CA	6.89	129.82	120.38
1	A	144	VAL	N-CA-C	-6.89	94.00	108.88
2	i	129	GLY	N-CA-C	-6.89	104.15	112.48
1	B	53	ARG	N-CA-C	-6.88	104.45	112.92
3	K	241	ASP	CA-CB-CG	-6.88	105.72	112.60
1	C	56	SER	N-CA-CB	6.88	122.06	111.46
2	6	158	GLU	N-CA-C	-6.88	101.98	110.65
2	6	93	LEU	CA-C-N	6.88	129.50	120.28
2	6	93	LEU	C-N-CA	6.88	129.50	120.28
2	2	198	GLN	CA-C-N	6.88	129.50	120.28
2	2	198	GLN	C-N-CA	6.88	129.50	120.28
2	1	92	THR	O-C-N	6.88	129.99	122.15
3	K	324	HIS	CA-C-N	6.88	129.50	120.28
3	K	324	HIS	C-N-CA	6.88	129.50	120.28
3	J	142	ASP	CA-CB-CG	-6.88	105.72	112.60
3	M	206	VAL	N-CA-C	-6.88	98.22	108.12
3	M	375	PHE	CA-CB-CG	-6.87	106.93	113.80
3	L	50	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	d	112	LEU	N-CA-C	-6.87	103.88	111.36
1	A	22	PHE	CA-C-N	6.86	129.48	120.28
1	A	22	PHE	C-N-CA	6.86	129.48	120.28
2	j	210	LYS	N-CA-C	-6.86	103.20	112.26
3	K	304	ASP	CA-CB-CG	6.86	119.46	112.60
3	I	257	GLY	CA-C-N	6.86	129.36	120.44
3	I	257	GLY	C-N-CA	6.86	129.36	120.44
2	k	122	ILE	N-CA-C	-6.86	98.30	108.45
3	M	294	ASP	CA-CB-CG	-6.86	105.74	112.60
3	I	156	ALA	N-CA-C	6.86	120.12	111.69
1	b	105	GLU	CA-C-N	6.85	126.61	119.76
1	b	105	GLU	C-N-CA	6.85	126.61	119.76
3	J	313	THR	CA-C-N	6.85	129.76	120.44
3	J	313	THR	C-N-CA	6.85	129.76	120.44
3	H	330	LEU	CA-C-N	6.85	132.37	122.44
3	H	330	LEU	C-N-CA	6.85	132.37	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	TYR	CB-CG-CD1	-6.85	110.53	120.80
2	i	27	THR	N-CA-C	-6.85	98.66	109.07
2	l	45	ILE	CB-CA-C	6.85	120.33	110.33
2	j	21	ASP	CA-CB-CG	6.85	119.45	112.60
1	G	141	VAL	N-CA-CB	6.84	121.13	111.82
2	3	211	PHE	CA-C-O	-6.84	111.10	119.18
3	H	32	ASP	CA-CB-CG	-6.84	105.75	112.60
2	3	88	ARG	CA-C-N	6.84	132.13	120.71
2	3	88	ARG	C-N-CA	6.84	132.13	120.71
1	A	109	VAL	O-C-N	-6.84	115.23	121.87
1	G	228	GLU	N-CA-C	-6.84	104.75	113.23
3	L	129	GLY	CA-C-O	6.84	127.82	120.30
2	3	204	VAL	CA-C-N	6.84	130.13	120.28
2	3	204	VAL	C-N-CA	6.84	130.13	120.28
3	L	88	VAL	CA-C-N	6.84	129.59	122.27
3	L	88	VAL	C-N-CA	6.84	129.59	122.27
3	J	219	GLY	O-C-N	6.83	128.80	122.17
2	3	139	ALA	CA-C-N	6.83	134.00	121.70
2	3	139	ALA	C-N-CA	6.83	134.00	121.70
2	m	39	SER	N-CA-C	-6.83	98.27	108.99
1	E	10	ARG	N-CA-C	-6.83	104.98	113.38
1	e	86	ARG	N-CA-C	-6.83	103.92	111.36
1	f	57	LYS	N-CA-C	-6.83	104.69	113.16
2	4	65	PHE	N-CA-C	6.83	118.72	111.28
2	h	40	LYS	CA-C-O	6.82	126.41	118.90
2	j	168	ALA	CA-C-O	6.82	127.65	120.42
3	I	211	PHE	N-CA-C	-6.82	103.77	111.14
1	a	15	PHE	O-C-N	6.82	130.62	122.85
1	D	119	PHE	CA-CB-CG	-6.82	106.98	113.80
1	E	73	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
2	h	77	TYR	CD1-CG-CD2	6.82	128.33	118.10
2	5	116	ASP	N-CA-C	-6.82	99.24	108.24
3	K	282	LYS	N-CA-CB	6.82	122.09	110.50
3	L	82	SER	CA-C-N	6.82	129.30	120.44
3	L	82	SER	C-N-CA	6.82	129.30	120.44
1	f	73	HIS	ND1-CE1-NE2	6.81	115.21	108.40
2	h	64	GLN	CA-C-O	-6.81	113.20	120.42
2	7	182	SER	N-CA-C	-6.81	99.86	110.42
2	k	204	VAL	N-CA-CB	6.81	119.29	110.57
3	K	333	ASP	N-CA-CB	6.81	122.00	110.49
3	K	163	LYS	CA-C-N	6.81	126.50	119.56
3	K	163	LYS	C-N-CA	6.81	126.50	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	150	VAL	CA-C-N	6.81	129.40	120.28
2	j	150	VAL	C-N-CA	6.81	129.40	120.28
2	n	147	ALA	N-CA-CB	6.81	120.12	110.12
1	G	14	VAL	O-C-N	6.80	130.10	122.68
1	g	190	VAL	N-CA-C	-6.80	103.68	110.62
2	k	174	SER	CA-C-N	6.80	130.65	120.31
2	k	174	SER	C-N-CA	6.80	130.65	120.31
3	L	276	ASP	N-CA-C	-6.80	101.21	109.72
2	n	62	ASP	N-CA-C	-6.80	103.94	111.36
1	A	152	PRO	CA-C-N	6.80	129.39	120.28
1	A	152	PRO	C-N-CA	6.80	129.39	120.28
2	6	156	THR	O-C-N	-6.80	116.24	121.55
3	J	40	GLU	CA-C-N	6.80	129.28	120.44
3	J	40	GLU	C-N-CA	6.80	129.28	120.44
3	H	316	GLY	CA-C-O	-6.80	113.28	120.90
3	I	387	THR	N-CA-CB	6.80	122.47	110.37
1	B	128	GLY	CA-C-N	6.79	132.27	123.03
1	B	128	GLY	C-N-CA	6.79	132.27	123.03
2	k	208	LEU	N-CA-C	-6.79	104.25	112.54
1	e	101	LEU	N-CA-C	6.78	118.47	111.14
2	n	207	ILE	CB-CA-C	-6.78	102.86	112.22
3	J	49	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	e	92	ALA	CA-C-N	6.78	129.69	120.54
1	e	92	ALA	C-N-CA	6.78	129.69	120.54
2	l	174	SER	CA-C-N	6.78	129.36	120.28
2	l	174	SER	C-N-CA	6.78	129.36	120.28
3	H	11	GLU	CA-C-N	6.78	129.25	120.44
3	H	11	GLU	C-N-CA	6.78	129.25	120.44
1	c	188	ALA	CA-C-O	-6.77	113.37	120.55
3	M	169	GLU	CA-CB-CG	-6.77	100.56	114.10
1	A	171	VAL	CA-C-O	6.77	127.56	120.25
1	f	193	LEU	CA-C-N	6.77	129.74	120.46
1	f	193	LEU	C-N-CA	6.77	129.74	120.46
2	h	153	ASP	N-CA-C	6.77	118.31	111.07
3	I	224	ARG	CA-C-N	6.77	129.35	120.28
3	I	224	ARG	C-N-CA	6.77	129.35	120.28
3	J	141	GLU	N-CA-C	-6.77	104.57	114.39
2	h	36	PHE	CA-CB-CG	-6.76	107.03	113.80
1	g	85	ALA	N-CA-C	6.76	118.31	111.07
2	5	135	LYS	N-CA-C	6.76	119.49	111.71
2	l	29	LYS	CA-C-N	6.76	134.46	121.54
2	l	29	LYS	C-N-CA	6.76	134.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	133	GLU	CA-C-N	6.76	133.08	122.94
2	n	133	GLU	C-N-CA	6.76	133.08	122.94
3	I	183	PRO	CA-C-N	6.76	126.52	119.76
3	I	183	PRO	C-N-CA	6.76	126.52	119.76
1	B	235	ARG	NE-CZ-NH2	6.76	125.28	119.20
2	3	129	GLY	O-C-N	6.76	129.33	122.91
3	L	397	PHE	CA-CB-CG	-6.76	107.04	113.80
2	3	144	SER	N-CA-C	6.76	118.65	111.28
1	C	134	VAL	CB-CA-C	-6.76	101.93	111.19
1	g	229	LEU	CB-CA-C	-6.76	99.57	110.79
3	J	241	ASP	N-CA-CB	-6.76	100.16	110.16
1	B	12	ILE	N-CA-CB	-6.75	104.78	112.21
2	l	162	ASP	CA-CB-CG	-6.75	105.85	112.60
1	C	52	LYS	CA-C-N	6.75	130.29	120.71
1	C	52	LYS	C-N-CA	6.75	130.29	120.71
1	C	221	PHE	CA-CB-CG	-6.75	107.05	113.80
2	n	35	ASN	CA-CB-CG	6.75	119.34	112.60
1	b	214	VAL	N-CA-CB	6.74	120.37	112.35
3	L	303	PHE	CA-CB-CG	6.74	120.54	113.80
1	d	168	ARG	CB-CA-C	-6.74	100.03	110.81
2	h	44	LYS	N-CA-C	-6.74	106.00	114.56
3	J	282	LYS	N-CA-CB	6.74	121.95	110.50
3	J	336	PHE	O-C-N	6.74	129.26	122.12
1	B	240	ILE	O-C-N	6.73	128.51	121.91
3	J	233	LYS	CA-C-N	6.73	129.69	120.67
3	J	233	LYS	C-N-CA	6.73	129.69	120.67
2	6	62	ASP	CA-CB-CG	-6.73	105.87	112.60
1	d	229	LEU	CA-C-N	6.73	128.50	120.09
1	d	229	LEU	C-N-CA	6.73	128.50	120.09
2	4	202	GLU	N-CA-C	6.73	119.18	111.11
2	n	27	THR	N-CA-C	-6.72	98.85	109.07
1	A	212	GLY	N-CA-C	-6.72	101.33	111.14
3	M	157	VAL	CB-CA-C	-6.72	105.06	111.44
1	C	112	LEU	CA-C-N	6.72	129.28	120.28
1	C	112	LEU	C-N-CA	6.72	129.28	120.28
2	k	57	ALA	N-CA-C	-6.72	99.11	109.52
1	D	48	LEU	N-CA-C	-6.71	97.47	108.41
3	M	301	GLY	CA-C-O	6.71	126.58	119.06
1	G	93	ARG	NE-CZ-NH2	-6.71	113.16	119.20
3	H	281	VAL	N-CA-C	-6.71	96.61	107.28
1	B	31	VAL	CB-CA-C	-6.70	102.97	112.22
2	k	166	GLU	N-CA-C	-6.70	103.91	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	THR	N-CA-CB	6.70	120.66	110.28
2	4	195	GLU	CA-C-O	-6.70	113.49	120.99
1	B	144	VAL	CA-C-O	-6.69	113.83	121.59
2	3	125	ILE	CA-C-O	6.69	127.45	120.36
2	h	177	LYS	N-CA-C	-6.69	104.13	112.90
1	e	216	VAL	O-C-N	6.69	128.47	121.91
1	f	14	VAL	CA-C-N	6.69	130.21	120.71
1	f	14	VAL	C-N-CA	6.69	130.21	120.71
1	G	196	MET	CA-C-N	6.69	127.55	119.99
1	G	196	MET	C-N-CA	6.69	127.55	119.99
1	B	159	TYR	CA-CB-CG	-6.69	101.86	113.90
3	M	336	PHE	N-CA-C	-6.69	105.12	113.28
2	h	88	ARG	CA-C-O	-6.69	113.81	120.70
1	C	119	PHE	N-CA-CB	6.68	119.95	110.12
2	l	169	VAL	CA-C-N	6.68	129.23	120.28
2	l	169	VAL	C-N-CA	6.68	129.23	120.28
3	H	381	LYS	O-C-N	6.68	128.95	122.07
1	B	62	ASP	CA-CB-CG	-6.68	105.92	112.60
2	6	137	ILE	N-CA-C	-6.67	99.13	108.27
2	1	182	SER	N-CA-C	-6.67	99.27	109.41
3	I	106	VAL	CA-C-N	6.67	130.29	120.95
3	I	106	VAL	C-N-CA	6.67	130.29	120.95
3	H	231	LYS	CA-C-N	6.67	131.86	120.72
3	H	231	LYS	C-N-CA	6.67	131.86	120.72
1	D	180	ARG	N-CA-C	-6.67	98.90	109.23
1	E	46	VAL	N-CA-C	-6.67	98.44	108.17
2	m	28	GLU	N-CA-C	-6.67	99.81	110.14
3	I	272	LEU	O-C-N	-6.67	115.06	122.12
2	m	212	ARG	N-CA-C	-6.66	98.54	109.40
3	H	115	ILE	N-CA-CB	6.66	118.15	110.49
3	M	103	GLY	CA-C-O	6.66	126.36	119.10
1	a	172	THR	N-CA-CB	6.66	119.91	110.12
3	I	32	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	68	TYR	N-CA-CB	6.66	121.51	110.52
3	M	105	ARG	NE-CZ-NH2	-6.66	113.21	119.20
1	D	118	ASP	CA-C-N	6.65	129.09	120.44
1	D	118	ASP	C-N-CA	6.65	129.09	120.44
1	G	182	ASP	CA-C-N	6.65	132.11	120.87
1	G	182	ASP	C-N-CA	6.65	132.11	120.87
1	E	61	ALA	N-CA-C	6.65	118.53	111.28
3	L	41	ARG	CA-C-N	6.65	129.57	120.46
3	L	41	ARG	C-N-CA	6.65	129.57	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	163	GLU	CB-CG-CD	-6.64	101.31	112.60
2	i	177	LYS	CA-C-O	6.64	127.59	120.55
1	C	105	GLU	CA-C-N	6.64	127.04	119.93
1	C	105	GLU	C-N-CA	6.64	127.04	119.93
1	c	63	THR	N-CA-C	-6.64	104.76	114.39
2	h	66	LEU	CA-C-N	6.64	129.18	120.28
2	h	66	LEU	C-N-CA	6.64	129.18	120.28
2	2	113	GLY	CA-C-N	6.64	131.68	121.12
2	2	113	GLY	C-N-CA	6.64	131.68	121.12
1	f	216	VAL	N-CA-CB	6.64	118.32	110.55
1	d	63	THR	N-CA-C	-6.64	107.06	114.62
1	F	51	ASP	CA-CB-CG	-6.64	105.96	112.60
2	1	77	TYR	CB-CG-CD1	6.63	130.75	120.80
3	H	374	ASP	CA-C-N	6.63	129.17	120.28
3	H	374	ASP	C-N-CA	6.63	129.17	120.28
3	K	389	ILE	CA-C-O	-6.63	111.06	119.95
1	E	123	TYR	CB-CG-CD2	-6.63	110.85	120.80
1	e	86	ARG	NE-CZ-NH1	-6.63	114.87	121.50
2	i	45	ILE	N-CA-C	-6.63	98.82	108.11
2	5	102	ARG	N-CA-C	-6.63	105.22	113.38
3	H	84	GLY	CA-C-N	6.63	128.13	119.84
3	H	84	GLY	C-N-CA	6.63	128.13	119.84
1	f	230	LYS	CA-C-N	6.63	126.14	119.24
1	f	230	LYS	C-N-CA	6.63	126.14	119.24
3	H	249	ARG	N-CA-C	-6.63	99.26	109.14
3	I	288	ASN	N-CA-C	-6.63	103.23	112.45
2	h	186	ILE	N-CA-C	-6.63	98.58	108.12
1	C	64	ILE	CB-CA-C	6.63	118.83	111.08
1	D	224	VAL	CB-CA-C	-6.63	102.94	110.96
2	i	150	VAL	N-CA-CB	6.63	119.05	110.57
1	B	16	SER	CA-C-O	-6.62	113.19	120.87
1	A	12	ILE	N-CA-C	-6.62	106.54	112.90
2	i	39	SER	CA-C-N	6.62	129.45	120.44
2	i	39	SER	C-N-CA	6.62	129.45	120.44
3	L	32	ASP	CA-C-N	6.62	129.81	120.28
3	L	32	ASP	C-N-CA	6.62	129.81	120.28
1	d	144	VAL	CA-C-N	6.62	126.64	119.89
1	d	144	VAL	C-N-CA	6.62	126.64	119.89
3	H	62	PRO	CA-C-N	6.62	132.32	122.99
3	H	62	PRO	C-N-CA	6.62	132.32	122.99
2	m	99	ASN	O-C-N	-6.61	115.26	122.07
3	I	51	LEU	N-CA-C	6.61	118.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	CA-CB-CG2	6.61	121.74	110.50
2	2	50	ASP	CA-CB-CG	-6.61	105.99	112.60
2	j	174	SER	N-CA-C	-6.61	104.16	111.36
3	H	219	GLY	N-CA-C	-6.61	104.51	113.37
1	a	73	HIS	ND1-CE1-NE2	6.61	115.01	108.40
1	E	210	GLU	CA-C-O	-6.61	112.99	120.32
2	i	159	ILE	CA-C-O	-6.61	114.97	121.58
3	J	50	ARG	CA-C-N	6.60	130.35	120.31
3	J	50	ARG	C-N-CA	6.60	130.35	120.31
3	H	347	SER	CA-C-N	6.60	127.26	120.00
3	H	347	SER	C-N-CA	6.60	127.26	120.00
3	K	328	MET	N-CA-C	-6.60	105.98	112.97
2	l	201	PRO	CA-C-N	6.60	129.96	120.79
2	l	201	PRO	C-N-CA	6.60	129.96	120.79
1	B	223	GLU	CB-CG-CD	-6.59	101.39	112.60
1	D	145	PRO	N-CA-CB	6.59	109.12	103.19
2	2	159	ILE	CA-C-N	6.59	131.10	121.67
2	2	159	ILE	C-N-CA	6.59	131.10	121.67
3	H	302	ARG	O-C-N	6.59	131.36	122.59
1	g	24	VAL	CA-C-O	-6.59	114.09	120.95
2	7	75	ASN	CA-CB-CG	-6.59	106.01	112.60
2	5	40	LYS	O-C-N	6.59	128.94	122.09
3	K	132	VAL	N-CA-CB	6.59	120.53	112.10
1	E	211	VAL	N-CA-CB	6.59	120.50	111.41
1	e	200	ILE	CA-C-N	6.59	131.48	122.19
1	e	200	ILE	C-N-CA	6.59	131.48	122.19
2	n	166	GLU	O-C-N	6.59	129.66	122.15
1	b	225	SER	CA-C-O	-6.58	113.25	120.69
1	g	237	ASN	N-CA-CB	6.58	120.36	110.22
3	J	379	ILE	O-C-N	-6.58	115.48	121.87
1	a	228	GLU	N-CA-C	-6.58	104.48	113.30
1	G	73	HIS	CA-CB-CG	-6.58	107.22	113.80
1	D	116	ILE	CA-C-N	6.58	129.64	120.29
1	D	116	ILE	C-N-CA	6.58	129.64	120.29
3	I	93	GLN	CA-C-N	6.58	129.39	120.44
3	I	93	GLN	C-N-CA	6.58	129.39	120.44
1	A	21	LEU	N-CA-C	-6.58	97.69	108.41
1	B	119	PHE	N-CA-C	-6.58	104.19	111.36
1	E	159	TYR	CA-C-N	6.58	131.70	120.71
1	E	159	TYR	C-N-CA	6.58	131.70	120.71
2	1	96	ASN	CA-CB-CG	-6.58	106.02	112.60
2	5	182	SER	N-CA-C	-6.58	104.57	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	25	MET	O-C-N	-6.58	115.35	123.44
3	J	383	LEU	N-CA-CB	6.58	120.35	110.22
2	k	96	ASN	OD1-CG-ND2	6.57	129.17	122.60
3	K	74	ASP	N-CA-C	-6.57	104.84	112.92
1	B	73	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
1	d	132	PHE	O-C-N	6.57	130.28	122.79
3	I	55	VAL	CB-CA-C	-6.57	103.27	112.14
3	M	243	LEU	N-CA-C	-6.57	102.56	110.44
1	a	92	ALA	CA-C-N	6.57	129.08	120.28
1	a	92	ALA	C-N-CA	6.57	129.08	120.28
2	i	62	ASP	CA-C-N	6.57	129.08	120.28
2	i	62	ASP	C-N-CA	6.57	129.08	120.28
2	1	122	ILE	N-CA-C	-6.56	98.59	108.17
2	1	191	ILE	N-CA-CB	6.56	122.06	111.23
2	3	112	ILE	N-CA-C	-6.56	98.92	108.11
1	d	217	ASP	CA-CB-CG	6.56	119.16	112.60
2	5	40	LYS	CA-C-O	-6.56	113.88	120.90
3	J	186	THR	N-CA-C	-6.56	105.10	113.23
2	h	87	VAL	CA-C-N	6.56	129.36	120.44
2	h	87	VAL	C-N-CA	6.56	129.36	120.44
2	7	120	LYS	CB-CG-CD	6.56	126.38	111.30
2	k	77	TYR	CA-C-O	-6.55	113.47	120.42
2	l	169	VAL	CA-CB-CG2	-6.55	99.26	110.40
3	K	311	LEU	CA-C-N	6.55	126.53	119.78
3	K	311	LEU	C-N-CA	6.55	126.53	119.78
1	F	102	THR	CA-C-O	6.55	127.02	119.35
1	A	59	LEU	CA-C-N	6.55	130.45	120.82
1	A	59	LEU	C-N-CA	6.55	130.45	120.82
1	b	168	ARG	N-CA-C	6.55	118.42	111.28
2	i	185	GLY	N-CA-C	-6.55	97.65	113.18
2	7	160	GLY	O-C-N	-6.55	117.17	122.81
3	I	27	TYR	CA-C-N	6.55	129.06	120.28
3	I	27	TYR	C-N-CA	6.55	129.06	120.28
2	n	33	MET	N-CA-C	-6.55	103.71	112.94
3	L	65	VAL	N-CA-C	-6.55	99.05	108.48
2	2	32	THR	N-CA-C	-6.55	99.24	109.72
2	4	186	ILE	CA-C-O	-6.55	113.34	120.67
2	2	48	ILE	N-CA-C	-6.54	104.47	110.82
1	g	145	PRO	N-CA-CB	6.54	109.16	103.27
2	1	40	LYS	N-CA-C	-6.54	104.61	112.59
2	n	211	PHE	CA-CB-CG	-6.54	107.26	113.80
1	D	204	LEU	CB-CA-C	-6.54	98.47	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	135	LYS	N-CA-C	6.54	119.24	111.33
3	L	361	PHE	N-CA-C	6.54	118.49	111.36
3	H	356	THR	O-C-N	-6.54	115.19	122.12
3	I	50	ARG	NE-CZ-NH2	6.54	125.08	119.20
3	K	322	LYS	CA-C-N	6.54	128.79	120.56
3	K	322	LYS	C-N-CA	6.54	128.79	120.56
1	C	208	ASN	O-C-N	6.53	129.55	121.84
3	M	132	VAL	CA-CB-CG1	6.53	121.50	110.40
1	c	46	VAL	N-CA-C	-6.53	99.70	108.06
1	e	64	ILE	N-CA-C	-6.53	101.15	109.58
2	j	143	GLY	CA-C-N	6.53	129.92	120.38
2	j	143	GLY	C-N-CA	6.53	129.92	120.38
1	d	188	ALA	CA-C-N	6.53	128.93	120.44
1	d	188	ALA	C-N-CA	6.53	128.93	120.44
3	J	390	PRO	CA-C-N	6.53	130.14	120.87
3	J	390	PRO	C-N-CA	6.53	130.14	120.87
1	F	112	LEU	O-C-N	-6.53	115.20	122.12
2	l	147	ALA	CA-C-N	6.53	129.03	120.28
2	l	147	ALA	C-N-CA	6.53	129.03	120.28
3	H	369	LYS	O-C-N	6.53	130.66	123.22
3	J	61	PRO	N-CA-C	6.53	117.56	110.58
1	D	14	VAL	CA-C-O	6.52	128.94	120.78
2	i	212	ARG	N-CA-C	-6.52	105.45	113.41
1	A	44	GLU	N-CA-C	-6.52	104.96	113.17
1	D	182	ASP	CA-CB-CG	-6.52	106.08	112.60
3	H	175	PRO	CB-CA-C	6.52	119.92	111.64
3	L	244	ASP	CA-C-O	6.52	127.33	120.42
2	m	148	TYR	CA-C-N	6.52	127.33	120.03
2	m	148	TYR	C-N-CA	6.52	127.33	120.03
3	M	333	ASP	N-CA-CB	6.52	120.77	111.19
1	D	87	VAL	N-CA-CB	6.51	119.90	110.52
3	H	227	PHE	CA-C-N	6.51	128.91	120.44
3	H	227	PHE	C-N-CA	6.51	128.91	120.44
3	H	297	ILE	N-CA-C	-6.51	106.17	112.29
3	J	66	GLY	O-C-N	-6.51	118.93	123.95
2	j	131	ALA	N-CA-C	-6.51	96.76	108.48
2	5	69	ILE	N-CA-CB	6.51	118.17	110.55
3	L	168	ALA	O-C-N	6.51	128.78	122.07
1	E	143	GLU	N-CA-C	-6.51	105.64	113.97
2	6	31	ALA	N-CA-C	-6.51	98.79	109.40
1	A	105	GLU	CA-C-N	6.51	127.97	119.84
1	A	105	GLU	C-N-CA	6.51	127.97	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	211	PHE	N-CA-CB	6.51	119.66	109.83
3	M	23	LEU	CA-C-N	6.50	129.32	120.54
3	M	23	LEU	C-N-CA	6.50	129.32	120.54
1	A	143	GLU	N-CA-CB	6.50	121.47	110.49
1	f	99	ASN	CA-C-N	6.50	129.64	120.28
1	f	99	ASN	C-N-CA	6.50	129.64	120.28
2	2	88	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	C	122	GLN	CB-CG-CD	-6.50	101.56	112.60
1	E	13	THR	N-CA-CB	6.50	120.08	110.53
3	H	288	ASN	CA-CB-CG	-6.50	106.10	112.60
1	g	93	ARG	NE-CZ-NH2	6.50	125.05	119.20
3	I	353	ALA	CA-C-O	6.49	127.43	120.55
2	3	167	LEU	N-CA-C	6.49	118.44	111.36
2	7	87	VAL	O-C-N	6.49	128.17	121.87
1	b	237	ASN	OD1-CG-ND2	6.49	129.09	122.60
1	C	71	ASP	CA-C-O	-6.49	111.23	120.51
3	H	114	ALA	N-CA-CB	6.49	121.46	110.49
2	5	157	PRO	N-CA-CB	6.48	108.98	102.17
1	A	24	VAL	N-CA-C	-6.48	103.93	111.00
1	D	113	ALA	CB-CA-C	-6.48	99.83	110.85
2	n	137	ILE	CA-C-O	6.48	128.88	120.78
3	L	89	VAL	CA-C-N	6.48	131.68	122.09
3	L	89	VAL	C-N-CA	6.48	131.68	122.09
3	J	149	GLN	N-CA-CB	6.48	121.15	110.39
1	C	191	LEU	CA-C-N	6.48	127.13	120.00
1	C	191	LEU	C-N-CA	6.48	127.13	120.00
2	m	112	ILE	CA-CB-CG2	6.48	121.52	110.50
3	J	395	VAL	CA-C-N	6.48	128.97	120.28
3	J	395	VAL	C-N-CA	6.48	128.97	120.28
2	l	133	GLU	N-CA-CB	6.48	119.75	109.51
2	1	138	VAL	N-CA-CB	6.48	119.94	111.19
3	I	30	LEU	N-CA-C	6.48	119.16	111.71
1	G	109	VAL	CB-CA-C	-6.48	103.59	111.88
1	B	185	PHE	CA-CB-CG	-6.47	107.33	113.80
1	C	142	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	221	PHE	O-C-N	6.47	131.20	122.59
1	c	63	THR	CA-C-N	6.47	129.24	120.63
1	c	63	THR	C-N-CA	6.47	129.24	120.63
2	h	202	GLU	N-CA-CB	6.47	119.40	110.01
2	k	98	LEU	CA-C-O	-6.47	112.53	119.97
3	I	84	GLY	CA-C-N	6.47	126.49	119.89
3	I	84	GLY	C-N-CA	6.47	126.49	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	VAL	CA-CB-CG2	6.46	121.39	110.40
2	j	47	GLN	CA-C-N	6.46	129.60	120.42
2	j	47	GLN	C-N-CA	6.46	129.60	120.42
2	k	186	ILE	CB-CA-C	6.46	121.89	111.29
1	A	170	ALA	N-CA-C	6.46	118.32	111.28
3	K	116	VAL	N-CA-C	-6.46	107.20	113.53
1	E	132	PHE	CA-CB-CG	-6.46	107.34	113.80
2	l	112	ILE	N-CA-C	-6.46	97.01	107.28
2	2	60	VAL	CB-CA-C	-6.46	103.71	111.97
3	I	291	ASP	CA-C-N	6.45	131.44	122.28
3	I	291	ASP	C-N-CA	6.45	131.44	122.28
3	L	304	ASP	CB-CA-C	-6.45	98.28	110.67
1	e	116	ILE	CA-CB-CG2	-6.45	99.53	110.50
1	f	228	GLU	N-CA-C	-6.45	105.71	113.97
3	K	56	GLU	CA-C-N	6.45	130.12	120.31
3	K	56	GLU	C-N-CA	6.45	130.12	120.31
3	J	252	ASN	OD1-CG-ND2	6.45	129.05	122.60
2	m	109	GLN	CA-C-O	6.45	127.33	120.36
3	L	41	ARG	NH1-CZ-NH2	6.45	127.68	119.30
3	L	199	THR	N-CA-CB	6.45	119.78	110.88
1	C	224	VAL	N-CA-CB	6.45	118.36	111.46
1	e	90	ASP	N-CA-CB	6.45	119.60	110.12
3	M	283	VAL	N-CA-C	-6.45	99.14	108.17
1	b	26	TYR	CB-CG-CD1	6.45	130.47	120.80
3	M	249	ARG	NE-CZ-NH2	-6.45	113.40	119.20
2	i	148	TYR	N-CA-CB	6.44	119.59	110.12
3	L	285	GLY	CA-C-O	-6.44	114.27	121.23
1	B	81	LEU	CB-CA-C	-6.44	100.60	110.26
1	c	151	ASP	CA-CB-CG	-6.44	106.16	112.60
2	3	175	ALA	N-CA-C	6.44	119.12	111.71
3	J	91	THR	N-CA-C	-6.44	101.85	110.55
1	D	41	LYS	N-CA-C	-6.44	100.44	110.42
2	k	80	ARG	CA-C-O	6.44	127.38	120.55
2	6	28	GLU	CA-CB-CG	6.44	126.97	114.10
2	k	191	ILE	N-CA-C	-6.44	98.25	107.77
1	g	124	THR	N-CA-CB	6.43	119.85	110.26
3	K	206	VAL	O-C-N	6.43	130.08	123.00
3	L	112	THR	N-CA-C	6.43	119.28	111.82
1	c	230	LYS	CA-C-O	-6.43	112.71	118.63
3	H	101	LYS	O-C-N	-6.43	113.92	121.32
3	M	309	VAL	N-CA-C	-6.43	97.55	107.71
1	B	103	TYR	CB-CA-C	-6.43	100.73	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	80	ARG	CD-NE-CZ	-6.43	115.40	124.40
1	E	174	PHE	N-CA-C	6.43	117.94	111.07
2	3	140	THR	N-CA-CB	6.42	122.42	111.50
2	4	152	GLU	N-CA-CB	6.42	120.19	110.30
1	F	144	VAL	O-C-N	-6.42	115.86	121.57
1	G	142	ASP	N-CA-C	-6.42	104.14	112.68
3	I	83	THR	O-C-N	6.42	130.17	122.27
1	E	63	THR	N-CA-C	-6.42	99.24	109.76
1	E	171	VAL	CA-C-O	-6.42	111.82	119.58
1	c	205	VAL	CA-C-N	6.42	126.04	119.56
1	c	205	VAL	C-N-CA	6.42	126.04	119.56
2	4	125	ILE	N-CA-CB	6.42	120.26	111.41
3	I	254	ASP	O-C-N	-6.42	113.99	122.20
1	g	71	ASP	N-CA-C	-6.41	99.89	108.74
2	h	121	SER	CA-C-N	6.41	131.85	122.94
2	h	121	SER	C-N-CA	6.41	131.85	122.94
3	K	382	VAL	N-CA-C	6.41	116.58	110.42
3	I	157	VAL	CA-C-N	6.41	128.78	120.44
3	I	157	VAL	C-N-CA	6.41	128.78	120.44
1	F	46	VAL	CA-C-N	6.41	131.85	122.94
1	F	46	VAL	C-N-CA	6.41	131.85	122.94
1	g	57	LYS	O-C-N	6.41	128.67	122.07
1	D	93	ARG	CA-C-N	6.41	128.63	120.56
1	D	93	ARG	C-N-CA	6.41	128.63	120.56
1	G	137	LEU	N-CA-C	-6.41	98.76	109.07
2	j	157	PRO	N-CA-C	-6.41	103.86	114.75
2	3	156	THR	O-C-N	-6.40	117.34	121.88
3	K	329	LYS	N-CA-C	6.40	118.04	108.31
1	b	55	GLY	CA-C-N	6.40	133.28	122.15
1	b	55	GLY	C-N-CA	6.40	133.28	122.15
2	l	19	CYS	N-CA-C	-6.40	100.99	110.46
3	I	165	GLU	N-CA-C	6.40	118.33	111.36
3	L	362	ALA	CA-C-N	6.40	128.75	120.56
3	L	362	ALA	C-N-CA	6.40	128.75	120.56
1	D	100	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	a	135	SER	N-CA-C	-6.39	98.98	109.40
1	e	83	ALA	CB-CA-C	-6.39	99.98	110.85
1	g	200	ILE	CA-C-N	6.39	131.23	122.34
1	g	200	ILE	C-N-CA	6.39	131.23	122.34
2	6	165	VAL	N-CA-C	-6.39	104.26	110.72
2	n	158	GLU	N-CA-CB	6.39	119.18	110.42
1	c	111	GLU	CA-C-N	6.39	129.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	111	GLU	C-N-CA	6.39	129.13	120.44
3	K	25	GLU	CB-CG-CD	-6.39	101.74	112.60
2	5	36	PHE	N-CA-C	-6.39	99.70	109.41
2	j	161	VAL	CA-C-O	6.39	127.62	120.85
2	5	80	ARG	O-C-N	6.39	129.43	122.15
2	7	32	THR	CA-C-O	-6.39	113.46	120.36
1	e	14	VAL	N-CA-CB	6.38	121.77	111.23
2	7	137	ILE	CA-CB-CG2	6.38	121.35	110.50
2	n	147	ALA	N-CA-C	-6.38	104.32	111.28
1	a	225	SER	CA-C-O	-6.38	114.01	120.96
1	B	49	ILE	O-C-N	-6.38	116.28	123.10
3	I	283	VAL	O-C-N	-6.38	116.48	123.18
1	e	128	GLY	N-CA-C	-6.38	106.75	114.66
1	a	67	ILE	N-CA-CB	6.38	120.49	111.82
1	G	176	GLU	N-CA-C	-6.37	104.38	111.71
2	i	85	PRO	N-CA-C	6.37	120.44	111.33
3	I	57	ARG	NE-CZ-NH1	6.37	127.87	121.50
2	3	201	PRO	N-CA-CB	6.37	109.94	103.25
3	J	216	ILE	CA-C-O	-6.37	113.96	121.80
3	H	392	LEU	N-CA-C	-6.37	97.69	108.26
2	j	155	PHE	CA-C-O	-6.37	114.03	121.16
3	I	108	LEU	N-CA-C	-6.37	99.02	109.40
3	J	174	PRO	CA-C-N	6.37	126.38	119.89
3	J	174	PRO	C-N-CA	6.37	126.38	119.89
2	6	157	PRO	N-CA-C	-6.36	105.76	114.80
3	K	178	VAL	N-CA-CB	-6.36	103.37	111.64
1	b	60	GLU	N-CA-C	-6.36	101.07	110.48
3	I	214	LYS	N-CA-CB	6.36	119.60	110.06
1	C	150	THR	N-CA-C	-6.36	99.94	110.17
1	f	21	LEU	CA-C-O	-6.36	114.20	121.19
1	G	94	ILE	CA-C-O	-6.36	114.11	120.85
3	M	150	ILE	N-CA-CB	6.35	119.18	110.54
1	C	148	TYR	N-CA-C	-6.35	99.81	109.85
1	d	73	HIS	N-CA-C	-6.35	104.69	112.88
1	c	37	ALA	O-C-N	6.35	131.01	123.33
2	1	171	ALA	N-CA-C	6.35	118.20	111.28
2	5	61	GLY	CA-C-O	-6.35	114.51	121.05
1	a	98	ILE	N-CA-C	-6.35	104.56	110.53
1	D	26	TYR	CB-CG-CD2	6.35	130.32	120.80
3	I	215	TYR	CB-CG-CD2	6.35	130.32	120.80
3	H	367	ARG	CA-C-O	6.35	128.02	121.23
2	m	210	LYS	N-CA-C	-6.35	104.33	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	93	GLN	N-CA-C	-6.35	105.36	113.23
2	h	195	GLU	N-CA-C	-6.34	99.08	108.79
1	a	82	VAL	CA-C-N	6.34	129.10	120.54
1	a	82	VAL	C-N-CA	6.34	129.10	120.54
2	k	201	PRO	CA-C-N	6.34	129.10	120.54
2	k	201	PRO	C-N-CA	6.34	129.10	120.54
2	5	87	VAL	CA-C-N	6.34	128.78	120.28
2	5	87	VAL	C-N-CA	6.34	128.78	120.28
1	f	103	TYR	N-CA-C	-6.34	107.39	114.62
3	H	29	ARG	CD-NE-CZ	-6.34	115.52	124.40
1	B	188	ALA	CA-C-N	6.34	129.29	120.29
1	B	188	ALA	C-N-CA	6.34	129.29	120.29
2	k	55	THR	CA-C-O	-6.34	113.99	120.71
2	k	62	ASP	CA-C-O	6.33	127.27	119.79
1	e	19	GLY	O-C-N	6.33	129.65	122.62
1	f	173	GLU	O-C-N	-6.33	115.41	122.12
2	j	66	LEU	N-CA-CB	6.33	119.43	110.12
3	I	296	ALA	CA-C-N	6.33	130.89	121.77
3	I	296	ALA	C-N-CA	6.33	130.89	121.77
3	K	19	ASP	CA-C-N	6.33	129.28	120.29
3	K	19	ASP	C-N-CA	6.33	129.28	120.29
1	a	220	THR	CA-C-O	-6.33	113.38	120.66
2	i	189	VAL	CA-C-O	-6.33	113.77	120.48
3	K	44	TYR	CA-C-N	6.33	128.76	120.28
3	K	44	TYR	C-N-CA	6.33	128.76	120.28
2	5	85	PRO	O-C-N	-6.33	115.44	123.04
1	e	178	GLU	CB-CA-C	-6.33	100.87	109.28
2	l	168	ALA	N-CA-C	6.33	118.18	111.28
2	m	73	GLU	CA-C-N	6.33	129.28	120.29
2	m	73	GLU	C-N-CA	6.33	129.28	120.29
3	K	156	ALA	N-CA-C	6.33	118.26	111.36
1	F	113	ALA	CA-C-N	6.33	129.27	120.29
1	F	113	ALA	C-N-CA	6.33	129.27	120.29
2	m	188	VAL	N-CA-C	-6.33	99.03	108.46
3	J	45	GLU	N-CA-C	6.33	118.17	111.28
1	F	100	ARG	N-CA-CB	6.32	119.96	110.22
1	f	180	ARG	NE-CZ-NH1	-6.32	115.18	121.50
3	H	341	ARG	CA-C-N	6.32	129.12	120.46
3	H	341	ARG	C-N-CA	6.32	129.12	120.46
1	D	67	ILE	N-CA-CB	6.32	119.31	111.41
1	f	105	GLU	CB-CG-CD	-6.32	101.86	112.60
2	2	202	GLU	N-CA-C	6.32	117.83	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	103	TYR	CA-C-N	6.32	129.60	122.59
2	k	103	TYR	C-N-CA	6.32	129.60	122.59
3	J	207	VAL	O-C-N	-6.32	116.34	123.10
1	f	108	THR	CA-C-N	6.32	129.11	120.46
1	f	108	THR	C-N-CA	6.32	129.11	120.46
2	7	96	ASN	CA-C-O	-6.31	113.73	120.42
2	7	64	GLN	OE1-CD-NE2	-6.31	116.29	122.60
3	M	227	PHE	CA-CB-CG	-6.31	107.49	113.80
1	D	194	VAL	CA-C-N	6.31	128.64	120.44
1	D	194	VAL	C-N-CA	6.31	128.64	120.44
1	f	70	ILE	N-CA-C	-6.31	106.39	111.81
1	B	200	ILE	N-CA-C	-6.31	105.55	112.80
1	a	186	ASP	CA-CB-CG	6.30	118.90	112.60
2	6	33	MET	N-CA-CB	6.30	120.67	110.77
1	E	189	MET	CA-C-N	6.30	129.09	120.46
1	E	189	MET	C-N-CA	6.30	129.09	120.46
1	e	130	ARG	N-CA-C	-6.30	100.46	110.10
2	i	135	LYS	N-CA-C	-6.30	105.17	112.92
2	i	191	ILE	N-CA-CB	6.30	119.16	111.60
1	A	164	ILE	CA-C-O	-6.30	115.15	121.45
1	a	67	ILE	N-CA-C	-6.30	98.45	107.77
1	B	242	GLU	CB-CA-C	-6.30	100.34	110.79
1	G	9	ASP	N-CA-CB	6.30	120.49	110.73
1	e	134	VAL	CA-C-O	6.29	126.25	121.09
2	3	15	VAL	N-CA-C	-6.29	99.61	108.80
3	K	375	PHE	N-CA-CB	6.29	119.14	110.01
1	e	117	CYS	N-CA-CB	6.29	119.37	110.12
2	h	38	ALA	N-CA-CB	-6.29	101.93	110.67
1	G	109	VAL	CA-C-N	6.29	128.71	120.28
1	G	109	VAL	C-N-CA	6.29	128.71	120.28
2	7	100	SER	CA-C-N	6.29	132.51	122.83
2	7	100	SER	C-N-CA	6.29	132.51	122.83
3	H	256	SER	CA-C-N	6.29	126.96	119.98
3	H	256	SER	C-N-CA	6.29	126.96	119.98
3	J	173	GLU	CA-C-N	6.29	126.86	120.38
3	J	173	GLU	C-N-CA	6.29	126.86	120.38
1	F	145	PRO	N-CA-CB	6.29	109.18	103.33
1	D	73	HIS	CE1-NE2-CD2	-6.29	102.71	109.00
3	J	38	GLU	CA-C-N	6.29	129.86	120.31
3	J	38	GLU	C-N-CA	6.29	129.86	120.31
1	A	23	GLN	O-C-N	6.28	128.78	122.12
3	L	380	GLU	CA-C-N	6.28	128.94	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	380	GLU	C-N-CA	6.28	128.94	120.65
1	f	109	VAL	CA-C-O	6.28	127.48	120.95
1	D	238	GLU	CA-C-N	6.28	128.60	120.44
1	D	238	GLU	C-N-CA	6.28	128.60	120.44
3	J	10	LEU	N-CA-C	-6.28	104.36	111.14
2	2	212	ARG	N-CA-C	6.28	120.87	109.32
3	K	234	ALA	N-CA-C	6.28	117.80	109.83
3	J	315	GLU	CA-C-O	-6.28	113.77	120.42
1	E	204	LEU	CA-C-N	6.28	131.46	122.24
1	E	204	LEU	C-N-CA	6.28	131.46	122.24
1	F	155	ALA	N-CA-CB	6.28	119.99	110.45
2	k	124	SER	N-CA-C	-6.28	99.47	109.76
3	L	113	LEU	N-CA-CB	6.27	121.09	110.49
1	B	28	ARG	N-CA-CB	6.27	119.44	110.16
3	K	184	PRO	N-CA-C	-6.27	100.59	111.32
1	e	235	ARG	N-CA-CB	6.27	119.96	110.30
2	h	126	ASP	N-CA-C	-6.27	100.97	110.50
3	I	119	LEU	CA-C-N	6.27	126.73	120.52
3	I	119	LEU	C-N-CA	6.27	126.73	120.52
3	K	204	ILE	N-CA-C	-6.27	98.64	108.23
3	K	367	ARG	NE-CZ-NH2	6.27	124.84	119.20
2	l	110	LEU	N-CA-C	-6.27	99.98	109.95
3	J	31	GLU	CA-C-O	-6.27	114.24	120.82
1	D	26	TYR	CB-CG-CD1	-6.27	111.40	120.80
1	f	145	PRO	N-CA-CB	6.27	109.83	103.25
3	L	269	LEU	N-CA-C	6.27	124.15	110.80
1	d	10	ARG	NE-CZ-NH1	-6.26	115.24	121.50
2	2	33	MET	N-CA-C	-6.26	97.60	108.69
2	6	60	VAL	N-CA-C	6.26	117.01	110.62
3	I	269	LEU	CA-C-O	6.26	127.06	120.42
2	n	198	GLN	CA-C-N	6.26	128.96	120.38
2	n	198	GLN	C-N-CA	6.26	128.96	120.38
2	h	74	ALA	N-CA-CB	6.26	119.53	110.20
2	n	83	ARG	NE-CZ-NH2	6.26	124.83	119.20
3	J	298	LEU	N-CA-C	6.26	118.10	111.28
3	M	42	ILE	CA-C-N	6.26	129.18	120.29
3	M	42	ILE	C-N-CA	6.26	129.18	120.29
1	g	68	TYR	CA-CB-CG	-6.26	102.64	113.90
2	h	106	TYR	N-CA-CB	6.26	120.50	110.86
2	l	170	ARG	O-C-N	6.26	128.75	122.12
1	F	151	ASP	CA-CB-CG	-6.25	106.34	112.60
3	H	395	VAL	CA-C-O	6.25	125.92	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	209	ALA	CA-C-N	6.25	131.31	120.68
2	1	209	ALA	C-N-CA	6.25	131.31	120.68
3	L	393	LYS	N-CA-C	-6.25	99.17	108.99
1	B	190	VAL	CA-C-N	6.25	128.66	120.28
1	B	190	VAL	C-N-CA	6.25	128.66	120.28
1	E	28	ARG	CB-CA-C	-6.25	97.10	109.67
2	7	12	THR	CA-CB-OG1	6.25	118.98	109.60
3	J	182	GLY	N-CA-C	-6.25	99.59	112.34
1	A	13	THR	N-CA-C	-6.25	105.66	113.28
1	A	242	GLU	CA-C-N	6.25	128.65	120.28
1	A	242	GLU	C-N-CA	6.25	128.65	120.28
1	e	16	SER	CA-C-O	-6.25	114.46	119.71
2	h	96	ASN	CB-CG-ND2	-6.25	107.03	116.40
2	j	116	ASP	CA-CB-CG	6.25	118.85	112.60
3	M	161	LEU	N-CA-CB	6.25	119.51	110.20
1	g	77	ALA	N-CA-CB	6.25	122.42	111.55
2	4	45	ILE	O-C-N	-6.25	116.51	123.26
2	5	31	ALA	N-CA-CB	6.25	119.29	110.36
2	7	174	SER	CA-C-N	6.24	129.27	120.28
2	7	174	SER	C-N-CA	6.24	129.27	120.28
3	K	78	VAL	N-CA-CB	6.24	117.53	110.72
3	J	220	ALA	N-CA-C	6.24	117.78	110.97
1	b	54	VAL	CA-C-O	-6.24	114.76	121.19
1	f	112	LEU	CA-C-O	6.24	127.16	120.55
3	L	114	ALA	N-CA-C	-6.24	98.45	109.06
3	K	362	ALA	O-C-N	6.24	128.49	122.07
3	K	44	TYR	CA-C-O	-6.24	112.80	119.97
3	J	337	LYS	CB-CG-CD	6.24	125.64	111.30
1	f	143	GLU	CA-C-N	6.23	133.66	122.13
1	f	143	GLU	C-N-CA	6.23	133.66	122.13
2	1	184	ASP	N-CA-C	-6.23	105.71	113.38
2	l	170	ARG	CA-C-O	-6.23	113.94	120.55
1	C	223	GLU	CA-C-O	-6.23	113.59	120.38
2	7	175	ALA	CA-C-N	6.23	129.78	120.31
2	7	175	ALA	C-N-CA	6.23	129.78	120.31
1	f	113	ALA	N-CA-C	6.23	118.07	111.28
2	k	95	SER	CA-C-N	6.23	129.13	120.29
2	k	95	SER	C-N-CA	6.23	129.13	120.29
1	a	22	PHE	CA-C-N	6.23	128.62	120.28
1	a	22	PHE	C-N-CA	6.23	128.62	120.28
1	d	118	ASP	CA-C-N	6.23	128.53	120.44
1	d	118	ASP	C-N-CA	6.23	128.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	GLU	N-CA-C	-6.22	104.16	112.94
2	5	75	ASN	O-C-N	6.22	128.72	122.12
3	H	245	ALA	N-CA-C	-6.22	104.16	112.94
3	H	257	GLY	O-C-N	6.22	128.16	122.19
1	f	77	ALA	N-CA-C	-6.22	99.88	109.52
3	K	381	LYS	CA-C-O	-6.22	114.29	120.70
2	3	120	LYS	N-CA-C	-6.22	98.48	109.06
3	H	287	THR	CA-C-N	6.22	131.60	122.08
3	H	287	THR	C-N-CA	6.22	131.60	122.08
2	4	76	LEU	N-CA-C	6.22	118.14	111.36
1	D	205	VAL	O-C-N	-6.22	115.81	121.41
2	7	83	ARG	CA-C-N	6.22	129.72	120.83
2	7	83	ARG	C-N-CA	6.22	129.72	120.83
1	D	189	MET	CA-C-N	6.21	128.97	120.46
1	D	189	MET	C-N-CA	6.21	128.97	120.46
1	G	15	PHE	CA-C-N	6.21	130.97	121.03
1	G	15	PHE	C-N-CA	6.21	130.97	121.03
2	l	204	VAL	CA-C-N	6.21	130.54	120.60
2	l	204	VAL	C-N-CA	6.21	130.54	120.60
1	F	168	ARG	N-CA-C	-6.21	104.43	111.07
2	i	79	ILE	CA-C-N	6.21	129.11	120.29
2	i	79	ILE	C-N-CA	6.21	129.11	120.29
2	h	90	ILE	CA-C-O	-6.21	114.27	120.85
1	E	237	ASN	CA-CB-CG	6.21	118.81	112.60
3	H	28	ARG	N-CA-C	6.20	118.84	111.71
3	M	286	ALA	CA-C-N	6.20	132.52	122.53
3	M	286	ALA	C-N-CA	6.20	132.52	122.53
2	7	138	VAL	N-CA-C	-6.20	100.17	108.35
3	H	222	LEU	CA-C-O	-6.20	112.48	119.79
3	L	302	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	D	186	ASP	O-C-N	6.20	129.22	122.15
1	d	230	LYS	CB-CG-CD	6.20	125.55	111.30
3	J	356	THR	CA-C-N	6.20	129.09	120.29
3	J	356	THR	C-N-CA	6.20	129.09	120.29
1	a	16	SER	CA-C-O	-6.20	115.02	120.60
1	a	24	VAL	CB-CA-C	-6.20	103.78	112.14
3	K	104	ALA	N-CA-C	-6.20	99.30	109.40
1	G	51	ASP	N-CA-C	6.19	118.97	110.24
1	F	94	ILE	CA-C-N	6.19	128.58	120.28
1	F	94	ILE	C-N-CA	6.19	128.58	120.28
2	3	37	ILE	CA-C-O	-6.19	113.90	120.53
3	J	77	VAL	N-CA-C	-6.19	99.20	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	80	ARG	NE-CZ-NH1	-6.19	115.31	121.50
3	M	18	GLU	CA-C-O	-6.19	114.32	120.70
1	c	36	THR	N-CA-C	6.19	118.76	110.35
2	1	76	LEU	CA-C-N	6.19	128.49	120.44
2	1	76	LEU	C-N-CA	6.19	128.49	120.44
1	d	204	LEU	N-CA-CB	6.19	120.36	110.46
2	4	188	VAL	N-CA-C	-6.18	98.63	108.90
2	i	120	LYS	CA-C-O	-6.18	112.94	120.54
2	j	29	LYS	N-CA-C	-6.18	105.74	113.28
2	k	60	VAL	CA-C-N	6.18	126.97	119.99
2	k	60	VAL	C-N-CA	6.18	126.97	119.99
2	k	140	THR	CA-CB-OG1	6.18	118.87	109.60
2	6	77	TYR	CB-CA-C	-6.18	101.18	110.88
3	M	283	VAL	O-C-N	-6.18	116.69	123.18
1	B	105	GLU	CA-C-N	6.18	125.94	119.76
1	B	105	GLU	C-N-CA	6.18	125.94	119.76
1	A	220	THR	N-CA-C	-6.18	97.36	108.48
3	K	134	GLU	CA-C-N	6.18	130.74	120.86
3	K	134	GLU	C-N-CA	6.18	130.74	120.86
1	f	166	MET	O-C-N	-6.17	115.00	122.22
1	B	165	GLY	N-CA-C	-6.17	102.93	111.76
1	A	48	LEU	CA-C-N	6.17	131.22	123.14
1	A	48	LEU	C-N-CA	6.17	131.22	123.14
3	I	298	LEU	N-CA-C	-6.17	103.17	111.87
1	a	234	GLU	N-CA-CB	6.17	119.19	110.12
3	I	183	PRO	CA-C-O	-6.17	111.61	120.56
3	L	152	GLU	N-CA-C	6.17	118.08	111.36
3	K	390	PRO	CA-C-O	-6.16	114.48	122.12
1	E	94	ILE	O-C-N	-6.16	115.89	121.87
1	f	186	ASP	CA-CB-CG	-6.16	106.44	112.60
1	g	74	ILE	CA-CB-CG1	6.16	120.87	110.40
2	l	97	LEU	CA-C-N	6.16	128.53	120.28
2	l	97	LEU	C-N-CA	6.16	128.53	120.28
2	n	48	ILE	N-CA-C	-6.16	105.72	111.45
3	L	142	ASP	N-CA-C	-6.16	104.25	112.94
3	K	128	TYR	CA-C-N	6.16	131.57	120.79
3	K	128	TYR	C-N-CA	6.16	131.57	120.79
3	J	128	TYR	N-CA-C	6.16	118.78	111.33
1	D	205	VAL	CB-CA-C	6.16	116.96	110.37
1	E	78	THR	CA-CB-OG1	6.16	118.83	109.60
3	I	324	HIS	CB-CG-CD2	-6.16	123.20	131.20
2	3	150	VAL	CA-C-N	6.15	128.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	150	VAL	C-N-CA	6.15	128.53	120.28
1	E	238	GLU	CA-C-N	6.15	129.03	120.29
1	E	238	GLU	C-N-CA	6.15	129.03	120.29
3	H	90	ASN	CA-CB-CG	-6.15	106.45	112.60
1	E	64	ILE	CA-C-N	6.15	132.77	121.70
1	E	64	ILE	C-N-CA	6.15	132.77	121.70
1	E	99	ASN	CA-CB-CG	6.15	118.75	112.60
1	b	228	GLU	N-CA-CB	6.15	119.69	110.65
2	j	72	ILE	N-CA-C	-6.15	104.35	110.62
2	l	104	PHE	CA-C-N	6.15	126.17	119.90
2	l	104	PHE	C-N-CA	6.15	126.17	119.90
3	H	127	VAL	N-CA-C	-6.15	100.98	109.46
1	B	185	PHE	CA-C-N	6.14	128.51	120.28
1	B	185	PHE	C-N-CA	6.14	128.51	120.28
3	L	81	SER	N-CA-CB	6.14	119.15	110.36
1	c	71	ASP	N-CA-C	-6.14	100.13	108.24
2	h	191	ILE	CA-C-O	6.14	128.46	120.78
3	K	99	GLU	CA-C-O	6.14	125.55	118.55
3	L	173	GLU	CA-C-N	6.14	124.08	119.66
3	L	173	GLU	C-N-CA	6.14	124.08	119.66
3	J	286	ALA	CB-CA-C	6.14	121.40	110.16
1	F	216	VAL	N-CA-C	-6.14	106.82	112.96
1	A	115	LYS	CA-C-O	6.14	126.92	119.31
1	f	144	VAL	CA-C-N	6.14	127.51	119.84
1	f	144	VAL	C-N-CA	6.14	127.51	119.84
3	L	146	LEU	N-CA-C	-6.14	95.84	108.18
2	n	104	PHE	CA-CB-CG	-6.14	107.66	113.80
3	I	352	LYS	O-C-N	-6.14	115.62	122.12
3	M	383	LEU	CA-C-O	-6.14	112.06	119.49
1	F	26	TYR	O-C-N	-6.13	115.16	122.15
3	H	209	SER	CA-C-N	6.13	128.50	120.28
3	H	209	SER	C-N-CA	6.13	128.50	120.28
3	I	44	TYR	N-CA-CB	6.13	119.24	110.16
3	M	11	GLU	CA-C-N	6.13	128.42	120.44
3	M	11	GLU	C-N-CA	6.13	128.42	120.44
1	E	73	HIS	CG-CD2-NE2	6.13	113.33	107.20
2	n	36	PHE	CA-C-O	-6.13	114.47	121.40
1	D	80	GLY	O-C-N	-6.13	116.66	123.10
1	a	85	ALA	O-C-N	6.13	128.62	122.12
1	C	77	ALA	CA-C-O	-6.13	114.29	121.46
2	2	91	ALA	O-C-N	-6.13	115.76	122.07
3	K	10	LEU	CA-C-N	6.13	128.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	10	LEU	C-N-CA	6.13	128.41	120.44
1	d	238	GLU	N-CA-C	6.13	117.62	111.07
3	L	371	THR	CA-C-N	6.13	128.49	120.28
3	L	371	THR	C-N-CA	6.13	128.49	120.28
1	c	27	ALA	N-CA-C	6.12	118.04	111.36
1	G	93	ARG	CB-CA-C	-6.12	100.44	110.85
1	G	14	VAL	CA-C-O	-6.12	113.23	120.76
2	1	150	VAL	CA-C-N	6.12	128.77	120.44
2	1	150	VAL	C-N-CA	6.12	128.77	120.44
2	h	126	ASP	CA-CB-CG	-6.12	106.48	112.60
2	3	40	LYS	N-CA-C	-6.12	103.52	113.19
3	K	304	ASP	N-CA-CB	6.12	120.84	110.49
1	C	108	THR	N-CA-C	-6.12	99.68	109.96
1	g	190	VAL	CA-CB-CG2	-6.12	100.00	110.40
2	i	179	ASP	CA-CB-CG	-6.12	106.48	112.60
2	4	65	PHE	CA-CB-CG	-6.12	107.68	113.80
3	H	24	ARG	CA-C-N	6.12	128.48	120.28
3	H	24	ARG	C-N-CA	6.12	128.48	120.28
1	G	161	ALA	CA-C-O	6.12	127.62	120.89
2	i	55	THR	CA-CB-OG1	6.12	118.78	109.60
1	E	104	ASP	CA-CB-CG	6.12	118.72	112.60
1	F	190	VAL	CA-CB-CG2	-6.12	100.00	110.40
1	f	32	LYS	CA-C-O	6.12	127.00	119.05
1	f	85	ALA	N-CA-C	6.12	117.95	111.28
1	E	15	PHE	CA-C-O	-6.12	114.31	121.16
2	4	179	ASP	CA-C-O	6.12	128.02	121.11
3	J	218	GLU	N-CA-C	6.12	118.03	111.36
1	a	78	THR	N-CA-C	-6.11	99.44	109.40
1	e	34	GLY	CA-C-N	6.11	129.50	120.95
1	e	34	GLY	C-N-CA	6.11	129.50	120.95
2	2	104	PHE	O-C-N	6.11	126.22	121.88
2	j	204	VAL	N-CA-C	6.11	116.89	110.72
3	J	327	LYS	N-CA-C	-6.11	105.66	113.23
2	5	78	GLU	CA-C-O	-6.11	112.95	119.97
3	L	199	THR	N-CA-C	-6.11	105.63	114.12
1	C	34	GLY	O-C-N	6.10	129.00	122.96
1	b	194	VAL	CA-C-N	6.10	128.37	120.44
1	b	194	VAL	C-N-CA	6.10	128.37	120.44
1	d	169	ASN	CA-C-N	6.10	128.74	120.44
1	d	169	ASN	C-N-CA	6.10	128.74	120.44
2	m	128	ILE	CA-CB-CG1	6.10	120.77	110.40
3	I	22	LYS	CA-C-N	6.10	128.45	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	22	LYS	C-N-CA	6.10	128.45	120.28
3	L	10	LEU	CA-C-O	-6.10	114.08	120.55
2	i	172	ILE	CA-C-N	6.10	128.45	120.28
2	i	172	ILE	C-N-CA	6.10	128.45	120.28
2	3	175	ALA	O-C-N	6.10	129.35	122.22
2	4	130	GLY	O-C-N	6.10	128.06	122.81
2	m	111	LEU	N-CA-C	-6.10	97.35	108.02
1	G	30	ALA	N-CA-CB	6.10	119.61	110.22
1	e	246	LYS	CA-CB-CG	6.09	126.29	114.10
1	g	212	GLY	N-CA-C	-6.09	100.38	110.80
2	2	129	GLY	O-C-N	-6.09	117.52	122.64
2	k	153	ASP	CA-CB-CG	6.09	118.69	112.60
2	5	49	ALA	CA-C-O	6.09	127.45	121.05
1	C	148	TYR	CA-CB-CG	-6.09	102.94	113.90
1	g	67	ILE	O-C-N	6.09	129.66	123.20
2	i	37	ILE	N-CA-C	-6.09	98.43	107.51
2	l	199	TYR	N-CA-CB	6.09	119.60	110.22
1	C	60	GLU	CA-C-N	6.09	128.44	120.28
1	C	60	GLU	C-N-CA	6.09	128.44	120.28
1	g	115	LYS	CA-C-N	6.09	128.23	120.56
1	g	115	LYS	C-N-CA	6.09	128.23	120.56
2	j	118	GLU	CB-CG-CD	-6.09	102.25	112.60
2	6	97	LEU	CA-C-O	-6.09	114.09	120.55
1	D	92	ALA	CB-CA-C	-6.09	100.50	110.85
1	f	86	ARG	CA-C-O	-6.09	113.97	120.42
2	l	33	MET	N-CA-C	-6.09	99.08	109.24
2	l	74	ALA	CA-C-O	6.09	126.87	120.42
2	n	14	THR	O-C-N	-6.09	115.81	123.17
3	K	203	PHE	CA-CB-CG	-6.09	107.71	113.80
3	K	269	LEU	CA-C-O	-6.09	114.43	120.82
1	d	183	LEU	CA-C-O	-6.08	115.10	121.55
3	L	10	LEU	CA-C-N	6.08	129.56	120.31
3	L	10	LEU	C-N-CA	6.08	129.56	120.31
1	a	111	GLU	CA-C-N	6.08	128.43	120.28
1	a	111	GLU	C-N-CA	6.08	128.43	120.28
1	B	93	ARG	NE-CZ-NH2	-6.08	113.72	119.20
3	J	127	VAL	CA-C-N	6.08	128.71	120.38
3	J	127	VAL	C-N-CA	6.08	128.71	120.38
1	e	70	ILE	N-CA-C	-6.08	105.79	111.45
2	7	102	ARG	NH1-CZ-NH2	-6.08	111.39	119.30
3	I	106	VAL	N-CA-C	-6.08	99.45	108.45
1	e	47	ILE	O-C-N	-6.08	116.69	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	221	PHE	CA-CB-CG	-6.08	107.72	113.80
2	l	148	TYR	O-C-N	-6.08	115.68	122.12
3	J	304	ASP	N-CA-C	-6.08	104.94	112.90
2	5	192	THR	CA-C-N	6.08	131.49	122.74
2	5	192	THR	C-N-CA	6.08	131.49	122.74
1	d	224	VAL	CA-C-N	6.08	128.83	120.39
1	d	224	VAL	C-N-CA	6.08	128.83	120.39
2	k	206	GLN	CB-CG-CD	-6.08	102.27	112.60
1	e	62	ASP	CA-CB-CG	6.07	118.67	112.60
1	f	19	GLY	O-C-N	6.07	128.83	122.51
2	n	98	LEU	O-C-N	-6.07	115.68	122.12
3	K	285	GLY	N-CA-C	-6.07	103.36	113.02
1	D	228	GLU	CA-C-O	6.07	126.85	119.38
1	e	38	ILE	CB-CA-C	6.07	119.19	110.33
3	J	362	ALA	N-CA-C	6.07	117.90	111.28
3	M	112	THR	N-CA-C	-6.07	107.11	114.75
3	M	367	ARG	N-CA-C	-6.06	104.59	111.14
2	6	69	ILE	CA-C-N	6.06	128.77	120.46
2	6	69	ILE	C-N-CA	6.06	128.77	120.46
1	a	246	LYS	CB-CG-CD	6.06	125.24	111.30
1	a	93	ARG	CB-CA-C	-6.06	100.73	110.79
1	E	167	GLY	CA-C-N	6.06	128.72	120.54
1	E	167	GLY	C-N-CA	6.06	128.72	120.54
2	i	94	THR	N-CA-C	-6.06	104.75	111.36
3	I	361	PHE	CA-C-N	6.06	128.40	120.28
3	I	361	PHE	C-N-CA	6.06	128.40	120.28
3	L	198	GLN	CA-C-O	-6.06	112.33	119.48
3	L	297	ILE	CA-C-O	-6.06	114.65	120.95
1	G	208	ASN	O-C-N	6.06	129.46	122.25
2	2	30	ARG	N-CA-CB	6.06	120.72	110.49
2	m	68	ARG	CA-C-N	6.06	128.19	120.56
2	m	68	ARG	C-N-CA	6.06	128.19	120.56
1	B	18	ASP	CA-CB-CG	-6.05	106.55	112.60
3	K	397	PHE	N-CA-CB	6.05	120.01	110.87
3	J	190	LEU	CA-C-N	6.05	128.39	120.28
3	J	190	LEU	C-N-CA	6.05	128.39	120.28
3	M	317	ARG	O-C-N	6.05	128.30	122.07
1	e	216	VAL	CB-CA-C	-6.05	104.22	111.97
2	i	109	GLN	OE1-CD-NE2	6.05	128.65	122.60
2	j	78	GLU	CA-C-N	6.05	128.75	120.46
2	j	78	GLU	C-N-CA	6.05	128.75	120.46
2	k	209	ALA	N-CA-C	-6.05	104.25	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	147	ALA	N-CA-C	6.05	118.67	111.71
1	d	79	SER	N-CA-C	-6.05	97.59	108.48
2	7	134	GLU	N-CA-CB	6.05	121.96	111.13
2	n	53	ALA	CA-C-O	-6.05	114.03	121.11
3	K	136	PRO	CA-C-O	-6.05	114.54	121.56
2	l	84	LYS	CA-C-N	6.05	125.96	119.85
2	l	84	LYS	C-N-CA	6.05	125.96	119.85
1	A	58	LEU	N-CA-CB	6.05	119.13	110.06
2	k	178	ARG	CA-C-O	6.05	126.95	120.24
2	6	195	GLU	O-C-N	6.05	129.89	123.42
1	a	200	ILE	N-CA-C	-6.04	106.84	112.83
3	L	138	VAL	CB-CA-C	-6.04	102.67	111.68
1	d	94	ILE	N-CA-CB	6.04	119.65	110.58
1	f	163	ALA	N-CA-CB	6.04	120.93	111.56
3	L	71	ILE	O-C-N	-6.04	116.73	123.26
1	c	108	THR	N-CA-C	-6.04	99.81	109.96
1	f	92	ALA	CB-CA-C	-6.04	99.07	110.67
2	h	141	GLY	CA-C-O	-6.04	116.34	122.56
2	5	173	TYR	CA-C-N	6.04	128.37	120.28
2	5	173	TYR	C-N-CA	6.04	128.37	120.28
2	6	99	ASN	N-CA-C	6.04	117.86	111.28
1	A	221	PHE	N-CA-C	6.04	119.24	110.42
1	b	205	VAL	O-C-N	-6.04	114.21	121.10
1	D	81	LEU	N-CA-CB	6.04	118.92	110.04
1	E	20	ARG	NE-CZ-NH2	-6.04	113.77	119.20
2	4	140	THR	N-CA-CB	6.04	120.69	110.49
3	J	290	ILE	N-CA-C	-6.04	104.62	110.72
1	B	78	THR	CA-C-N	6.03	132.56	121.94
1	B	78	THR	C-N-CA	6.03	132.56	121.94
1	d	89	ILE	CA-C-O	6.03	126.98	120.47
1	G	144	VAL	N-CA-C	-6.03	102.19	109.01
2	h	96	ASN	CA-C-N	6.03	128.86	120.29
2	h	96	ASN	C-N-CA	6.03	128.86	120.29
2	3	35	ASN	CA-CB-CG	-6.03	106.57	112.60
2	n	112	ILE	N-CA-C	-6.03	98.94	107.75
2	m	83	ARG	N-CA-CB	6.03	120.69	110.49
3	J	149	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	d	149	GLU	N-CA-CB	6.03	121.23	110.80
3	I	41	ARG	CD-NE-CZ	-6.03	115.96	124.40
3	I	219	GLY	N-CA-C	-6.03	95.81	113.30
3	M	168	ALA	CA-C-N	6.03	128.36	120.28
3	M	168	ALA	C-N-CA	6.03	128.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ILE	N-CA-CB	6.03	120.02	111.82
1	e	203	GLU	N-CA-CB	6.03	118.93	109.83
1	e	202	SER	CA-C-N	6.03	129.27	120.71
1	e	202	SER	C-N-CA	6.03	129.27	120.71
2	4	77	TYR	O-C-N	6.03	128.51	122.12
2	k	163	GLU	CB-CA-C	-6.03	98.15	109.72
2	n	103	TYR	N-CA-C	-6.03	105.10	112.88
3	H	228	GLN	OE1-CD-NE2	6.03	128.63	122.60
3	K	161	LEU	CA-C-O	6.03	126.91	120.70
3	L	40	GLU	CA-C-O	6.03	126.90	119.97
3	K	198	GLN	CA-C-O	6.03	126.93	120.24
3	J	81	SER	N-CA-CB	6.03	119.06	110.44
1	F	207	GLU	N-CA-C	-6.02	105.23	113.30
3	K	339	LEU	CA-C-N	6.02	128.35	120.28
3	K	339	LEU	C-N-CA	6.02	128.35	120.28
2	5	174	SER	N-CA-CB	6.02	118.97	110.12
2	m	85	PRO	CA-C-N	6.02	132.57	122.87
2	m	85	PRO	C-N-CA	6.02	132.57	122.87
1	A	167	GLY	CA-C-N	6.02	129.16	120.79
1	A	167	GLY	C-N-CA	6.02	129.16	120.79
1	C	174	PHE	CA-CB-CG	-6.02	107.78	113.80
3	J	66	GLY	CA-C-O	6.02	126.95	121.47
1	c	48	LEU	CA-C-O	6.02	127.00	120.32
1	D	213	TYR	CA-CB-CG	6.02	124.73	113.90
1	F	204	LEU	CA-C-O	6.02	129.48	121.78
1	A	92	ALA	CA-C-N	6.02	128.34	120.28
1	A	92	ALA	C-N-CA	6.02	128.34	120.28
3	H	151	GLU	N-CA-CB	6.02	119.49	110.22
3	L	296	ALA	CA-C-N	6.02	128.70	120.46
3	L	296	ALA	C-N-CA	6.02	128.70	120.46
1	E	86	ARG	N-CA-CB	6.02	118.73	110.01
1	g	140	GLY	CA-C-O	-6.02	114.64	121.68
2	l	175	ALA	N-CA-C	6.02	117.84	111.28
1	a	170	ALA	CA-C-N	6.01	128.96	120.42
1	a	170	ALA	C-N-CA	6.01	128.96	120.42
1	F	195	ALA	CB-CA-C	-6.01	100.62	110.85
2	j	192	THR	CB-CA-C	6.01	120.84	110.01
2	m	151	LEU	N-CA-C	6.01	117.84	111.28
2	7	67	ALA	N-CA-C	6.01	117.84	111.28
2	l	156	THR	O-C-N	-6.01	116.21	121.32
1	G	15	PHE	CA-C-O	6.01	128.38	121.47
2	l	47	GLN	CA-C-N	6.01	129.33	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	47	GLN	C-N-CA	6.01	129.33	120.74
3	J	11	GLU	N-CA-C	6.01	117.83	111.28
2	j	164	ALA	CA-C-N	6.00	128.69	120.46
2	j	164	ALA	C-N-CA	6.00	128.69	120.46
3	H	329	LYS	N-CA-C	-6.00	99.61	109.40
1	A	186	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	201	GLU	N-CA-CB	6.00	121.89	112.46
1	F	12	ILE	CA-C-O	6.00	125.56	119.20
2	h	131	ALA	N-CA-CB	6.00	119.25	109.95
2	3	187	ASP	CA-C-N	6.00	132.75	122.67
2	3	187	ASP	C-N-CA	6.00	132.75	122.67
1	e	151	ASP	CA-C-O	-6.00	114.48	120.66
2	l	18	VAL	N-CA-C	-6.00	99.94	108.58
1	a	65	GLU	N-CA-C	-6.00	99.12	108.90
1	d	38	ILE	N-CA-C	-6.00	100.43	108.35
1	G	13	THR	N-CA-C	-6.00	104.86	111.82
1	g	81	LEU	N-CA-C	6.00	118.93	110.23
2	3	36	PHE	CA-CB-CG	6.00	119.80	113.80
1	E	69	LYS	N-CA-C	-6.00	99.93	109.76
2	k	96	ASN	CA-C-N	6.00	128.24	120.44
2	k	96	ASN	C-N-CA	6.00	128.24	120.44
3	H	50	ARG	CA-C-N	6.00	128.32	120.28
3	H	50	ARG	C-N-CA	6.00	128.32	120.28
1	b	126	TYR	N-CA-CB	6.00	118.78	109.97
1	b	115	LYS	CA-C-O	-5.99	114.53	120.82
2	2	164	ALA	N-CA-C	-5.99	105.05	112.90
2	n	75	ASN	OD1-CG-ND2	-5.99	116.61	122.60
3	H	68	VAL	CA-C-O	-5.99	113.29	120.78
1	c	197	GLY	O-C-N	5.99	130.49	122.70
2	6	148	TYR	N-CA-C	-5.99	104.75	111.28
2	7	90	ILE	CA-C-N	5.99	128.22	120.44
2	7	90	ILE	C-N-CA	5.99	128.22	120.44
3	H	32	ASP	CA-C-N	5.99	128.59	120.38
3	H	32	ASP	C-N-CA	5.99	128.59	120.38
3	M	313	THR	CA-C-N	5.99	128.23	120.44
3	M	313	THR	C-N-CA	5.99	128.23	120.44
3	J	394	GLY	CA-C-N	5.99	130.06	121.55
3	J	394	GLY	C-N-CA	5.99	130.06	121.55
1	a	188	ALA	CA-C-N	5.99	128.79	120.29
1	a	188	ALA	C-N-CA	5.99	128.79	120.29
2	2	125	ILE	N-CA-C	-5.99	99.01	107.75
3	M	44	TYR	N-CA-C	-5.99	104.76	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	GLU	CA-C-N	5.98	128.58	120.44
1	C	238	GLU	C-N-CA	5.98	128.58	120.44
3	M	11	GLU	O-C-N	-5.98	115.78	122.12
1	B	186	ASP	CA-C-N	5.98	128.78	120.29
1	B	186	ASP	C-N-CA	5.98	128.78	120.29
2	m	163	GLU	N-CA-C	-5.98	105.06	112.90
2	n	153	ASP	CA-C-O	-5.98	114.54	120.70
1	C	144	VAL	N-CA-CB	5.98	118.04	111.64
2	k	24	VAL	CA-CB-CG2	-5.98	100.23	110.40
3	M	113	LEU	N-CA-CB	5.98	121.00	111.91
3	M	304	ASP	N-CA-CB	-5.98	101.34	110.01
3	L	220	ALA	CB-CA-C	-5.98	101.46	110.90
1	d	115	LYS	CA-C-N	5.97	130.57	120.29
1	d	115	LYS	C-N-CA	5.97	130.57	120.29
2	6	99	ASN	CA-CB-CG	-5.97	106.62	112.60
2	6	106	TYR	N-CA-C	-5.97	103.37	112.99
2	7	35	ASN	N-CA-C	-5.97	105.32	114.16
3	L	66	GLY	O-C-N	-5.97	116.96	123.29
1	B	221	PHE	N-CA-C	5.97	123.52	110.80
1	E	134	VAL	CA-CB-CG2	5.97	120.55	110.40
1	G	235	ARG	CA-C-N	5.97	128.77	120.29
1	G	235	ARG	C-N-CA	5.97	128.77	120.29
3	I	282	LYS	CA-C-O	5.97	127.79	120.92
1	f	229	LEU	CA-C-O	-5.97	113.11	119.97
2	j	146	THR	CA-C-N	5.97	128.20	120.44
2	j	146	THR	C-N-CA	5.97	128.20	120.44
3	H	352	LYS	N-CA-CB	5.97	118.67	110.01
3	M	172	ILE	O-C-N	5.97	129.50	122.69
1	A	151	ASP	CA-C-N	5.97	125.84	119.28
1	A	151	ASP	C-N-CA	5.97	125.84	119.28
2	n	160	GLY	CA-C-N	5.97	130.55	120.29
2	n	160	GLY	C-N-CA	5.97	130.55	120.29
3	L	122	SER	N-CA-C	-5.97	99.28	109.24
3	L	253	SER	CA-C-N	5.97	131.94	122.93
3	L	253	SER	C-N-CA	5.97	131.94	122.93
1	g	229	LEU	N-CA-CB	5.96	118.89	110.12
3	K	223	VAL	CA-C-O	-5.96	114.53	120.85
3	K	367	ARG	NE-CZ-NH1	-5.96	115.54	121.50
3	L	337	LYS	CA-C-N	5.96	128.76	120.29
3	L	337	LYS	C-N-CA	5.96	128.76	120.29
2	h	102	ARG	CA-C-O	5.96	126.92	119.59
3	K	397	PHE	N-CA-C	-5.96	101.10	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	187	ASP	CB-CA-C	-5.96	101.52	110.88
3	J	298	LEU	CA-C-N	5.96	129.15	120.51
3	J	298	LEU	C-N-CA	5.96	129.15	120.51
1	D	66	LYS	N-CA-C	-5.96	107.24	114.75
1	d	114	LYS	CA-C-N	5.96	128.26	120.28
1	d	114	LYS	C-N-CA	5.96	128.26	120.28
2	l	38	ALA	N-CA-C	-5.96	107.24	114.75
3	K	314	PHE	CA-C-N	5.96	129.37	120.31
3	K	314	PHE	C-N-CA	5.96	129.37	120.31
1	c	207	GLU	CA-C-O	5.96	125.69	119.14
2	l	71	LYS	CB-CA-C	-5.96	101.53	110.88
1	B	104	ASP	N-CA-CB	5.96	120.96	111.91
1	A	97	GLN	CA-C-N	5.95	130.06	120.30
1	A	97	GLN	C-N-CA	5.95	130.06	120.30
1	B	240	ILE	CA-C-N	5.95	128.18	120.44
1	B	240	ILE	C-N-CA	5.95	128.18	120.44
1	f	127	GLY	CA-C-N	5.95	126.55	120.00
1	f	127	GLY	C-N-CA	5.95	126.55	120.00
2	i	189	VAL	O-C-N	5.95	129.43	123.18
1	a	82	VAL	CA-C-O	5.95	127.16	120.85
2	7	99	ASN	CA-CB-CG	5.95	118.55	112.60
3	I	249	ARG	CA-C-O	5.95	128.25	122.01
1	b	91	ARG	NE-CZ-NH2	5.95	124.55	119.20
1	F	49	ILE	N-CA-C	-5.95	99.56	108.12
1	G	93	ARG	NE-CZ-NH1	5.94	127.44	121.50
2	h	103	TYR	CB-CG-CD1	5.94	129.72	120.80
1	D	232	TYR	CA-C-N	5.94	128.60	120.46
1	D	232	TYR	C-N-CA	5.94	128.60	120.46
2	3	78	GLU	CA-C-N	5.94	130.04	120.30
2	3	78	GLU	C-N-CA	5.94	130.04	120.30
3	J	71	ILE	CB-CA-C	5.94	118.44	110.42
1	B	187	ASP	CA-C-N	5.94	128.24	120.28
1	B	187	ASP	C-N-CA	5.94	128.24	120.28
2	l	90	ILE	N-CA-C	-5.94	103.72	112.04
2	6	54	MET	CA-CB-CG	5.94	125.98	114.10
3	H	311	LEU	N-CA-CB	5.94	119.17	109.90
1	c	141	VAL	N-CA-C	-5.94	99.50	108.17
1	G	174	PHE	N-CA-C	5.94	117.83	111.36
1	a	46	VAL	N-CA-C	-5.94	100.14	108.27
1	C	37	ALA	N-CA-CB	5.94	120.57	110.71
1	D	82	VAL	CA-C-N	5.94	128.24	120.28
1	D	82	VAL	C-N-CA	5.94	128.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	ARG	N-CA-C	-5.94	98.16	110.80
3	J	170	VAL	CA-C-N	5.94	130.01	122.00
3	J	170	VAL	C-N-CA	5.94	130.01	122.00
1	a	106	PRO	CA-C-N	5.93	129.16	120.91
1	a	106	PRO	C-N-CA	5.93	129.16	120.91
2	4	72	ILE	CA-C-O	-5.93	114.78	120.95
1	E	244	LEU	N-CA-C	-5.93	105.96	112.72
3	L	376	THR	CA-C-N	5.93	128.72	120.29
3	L	376	THR	C-N-CA	5.93	128.72	120.29
3	J	124	ASP	CA-CB-CG	-5.93	106.67	112.60
1	G	194	VAL	N-CA-C	-5.93	104.57	110.62
2	i	56	THR	O-C-N	5.93	130.74	123.21
2	k	58	GLY	CA-C-N	5.93	129.25	120.95
2	k	58	GLY	C-N-CA	5.93	129.25	120.95
3	L	130	PHE	CA-C-N	5.93	132.86	121.54
3	L	130	PHE	C-N-CA	5.93	132.86	121.54
1	G	241	ARG	CA-C-N	5.93	128.22	120.28
1	G	241	ARG	C-N-CA	5.93	128.22	120.28
2	4	197	TYR	CB-CG-CD2	-5.93	111.91	120.80
1	a	156	LEU	CB-CA-C	-5.92	101.67	110.62
1	e	173	GLU	CA-C-N	5.92	128.22	120.28
1	e	173	GLU	C-N-CA	5.92	128.22	120.28
2	j	202	GLU	N-CA-C	5.92	118.22	111.11
3	M	298	LEU	CA-C-N	5.92	130.34	120.86
3	M	298	LEU	C-N-CA	5.92	130.34	120.86
1	e	32	LYS	CA-C-N	5.92	128.70	120.29
1	e	32	LYS	C-N-CA	5.92	128.70	120.29
1	G	46	VAL	O-C-N	5.92	129.75	123.00
1	A	42	CYS	N-CA-C	-5.92	100.58	108.34
1	b	65	GLU	CB-CG-CD	-5.92	102.54	112.60
1	g	39	GLY	N-CA-C	-5.92	99.15	113.18
2	j	115	ILE	N-CA-C	-5.92	99.11	107.75
3	I	165	GLU	CA-C-O	5.92	126.69	120.42
3	J	290	ILE	O-C-N	5.92	127.93	121.83
1	b	181	ASP	N-CA-C	-5.92	105.72	113.17
1	f	19	GLY	N-CA-C	-5.92	106.31	116.01
2	k	59	SER	CA-C-N	5.92	128.82	120.42
2	k	59	SER	C-N-CA	5.92	128.82	120.42
2	6	149	GLY	CA-C-O	5.92	127.39	121.00
3	H	79	VAL	N-CA-CB	5.92	119.12	111.67
3	K	264	THR	CA-C-N	5.92	128.21	120.28
3	K	264	THR	C-N-CA	5.92	128.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	187	ASP	N-CA-C	5.91	117.73	111.28
2	3	49	ALA	CA-C-N	5.91	129.01	120.38
2	3	49	ALA	C-N-CA	5.91	129.01	120.38
1	g	239	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	B	242	GLU	N-CA-CB	5.91	118.81	110.12
1	b	135	SER	N-CA-CB	5.91	122.12	111.37
1	f	28	ARG	N-CA-CB	5.91	118.81	110.12
3	K	169	GLU	N-CA-C	-5.91	104.92	111.36
1	B	204	LEU	CA-C-O	5.91	128.69	121.72
2	7	59	SER	O-C-N	-5.91	115.89	122.86
1	F	113	ALA	N-CA-CB	-5.90	101.44	110.12
2	1	19	CYS	O-C-N	-5.90	116.33	122.94
3	I	283	VAL	CA-C-O	5.90	126.74	120.48
3	J	357	GLU	CA-C-O	5.90	126.68	120.42
1	e	151	ASP	CA-C-N	5.90	125.77	119.28
1	e	151	ASP	C-N-CA	5.90	125.77	119.28
2	4	45	ILE	CA-C-O	5.90	126.59	120.39
3	H	111	GLN	OE1-CD-NE2	-5.90	116.70	122.60
3	K	178	VAL	CA-C-N	5.90	130.27	122.42
3	K	178	VAL	C-N-CA	5.90	130.27	122.42
1	e	241	ARG	NE-CZ-NH2	5.90	124.51	119.20
2	h	152	GLU	CB-CG-CD	-5.90	102.57	112.60
3	M	124	ASP	CA-C-N	5.90	125.58	119.56
3	M	124	ASP	C-N-CA	5.90	125.58	119.56
2	k	77	TYR	O-C-N	5.90	128.87	122.15
1	c	87	VAL	CB-CA-C	-5.90	104.18	112.14
1	f	202	SER	O-C-N	5.90	130.39	122.96
2	k	84	LYS	CG-CD-CE	5.90	124.86	111.30
3	K	133	GLU	N-CA-C	-5.90	98.67	108.75
1	C	189	MET	CA-C-O	-5.89	114.30	120.55
1	e	47	ILE	N-CA-CB	5.89	119.54	111.41
2	2	47	GLN	O-C-N	-5.89	115.86	122.93
3	L	101	LYS	N-CA-C	-5.89	101.41	108.25
3	M	240	ILE	CA-C-O	5.89	127.56	120.66
1	C	241	ARG	CA-C-O	-5.89	114.17	120.42
2	j	23	VAL	N-CA-C	-5.89	100.20	108.27
3	I	97	GLU	N-CA-C	-5.89	106.07	113.20
1	A	116	ILE	N-CA-CB	5.89	118.11	110.57
1	b	218	ASP	N-CA-C	-5.89	106.64	113.88
1	f	67	ILE	N-CA-C	-5.89	99.86	108.11
3	K	154	ARG	N-CA-C	5.89	118.46	111.33
1	d	214	VAL	N-CA-C	-5.89	99.06	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	297	ILE	CA-C-N	5.88	128.17	120.28
3	J	297	ILE	C-N-CA	5.88	128.17	120.28
1	b	181	ASP	CA-C-O	5.88	126.23	119.35
1	c	53	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	E	214	VAL	N-CA-C	-5.88	99.65	108.12
2	j	148	TYR	O-C-N	-5.88	115.88	122.12
1	f	37	ALA	N-CA-CB	5.88	121.78	111.13
3	H	208	GLY	CA-C-N	5.88	128.09	120.44
3	H	208	GLY	C-N-CA	5.88	128.09	120.44
1	F	197	GLY	CA-C-N	5.88	128.44	120.44
1	F	197	GLY	C-N-CA	5.88	128.44	120.44
3	K	192	ALA	O-C-N	5.88	128.12	122.07
1	B	43	LYS	CA-C-N	5.88	131.60	122.49
1	B	43	LYS	C-N-CA	5.88	131.60	122.49
1	C	196	MET	CA-C-N	5.88	126.50	119.98
1	C	196	MET	C-N-CA	5.88	126.50	119.98
1	D	17	PRO	CA-C-N	5.87	128.08	120.44
1	D	17	PRO	C-N-CA	5.87	128.08	120.44
2	l	104	PHE	N-CA-C	-5.87	100.30	108.76
3	H	260	GLU	N-CA-CB	5.87	118.69	109.94
1	D	224	VAL	N-CA-CB	5.87	117.69	111.00
1	f	121	GLN	O-C-N	5.87	129.09	122.22
1	g	142	ASP	CA-C-N	5.87	132.76	121.54
1	g	142	ASP	C-N-CA	5.87	132.76	121.54
3	H	59	ARG	NH1-CZ-NH2	5.87	126.93	119.30
1	D	43	LYS	N-CA-C	-5.87	105.88	113.16
3	M	92	SER	CA-C-N	5.87	128.07	120.44
3	M	92	SER	C-N-CA	5.87	128.07	120.44
1	d	146	LYS	CA-C-O	5.87	127.64	120.60
2	m	66	LEU	CA-C-N	5.87	128.14	120.28
2	m	66	LEU	C-N-CA	5.87	128.14	120.28
1	D	108	THR	CA-C-N	5.87	128.75	120.42
1	D	108	THR	C-N-CA	5.87	128.75	120.42
2	5	36	PHE	CA-CB-CG	5.87	119.67	113.80
3	L	205	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	b	141	VAL	N-CA-C	-5.86	99.19	107.75
1	b	170	ALA	CA-C-N	5.86	128.49	120.46
1	b	170	ALA	C-N-CA	5.86	128.49	120.46
1	c	162	THR	CA-C-N	5.86	131.89	121.75
1	c	162	THR	C-N-CA	5.86	131.89	121.75
3	M	282	LYS	CA-C-N	5.86	130.46	123.19
3	M	282	LYS	C-N-CA	5.86	130.46	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	GLN	CA-C-N	5.86	128.74	120.42
1	B	97	GLN	C-N-CA	5.86	128.74	120.42
1	c	42	CYS	CA-C-O	-5.86	114.69	121.49
3	H	56	GLU	CB-CG-CD	-5.86	102.64	112.60
3	M	25	GLU	N-CA-C	5.86	117.67	111.28
1	a	137	LEU	N-CA-CB	5.86	119.91	110.65
2	1	190	LYS	CA-C-O	-5.86	114.49	121.11
2	2	113	GLY	N-CA-C	-5.86	102.23	110.96
2	5	139	ALA	O-C-N	-5.86	116.08	123.17
3	K	83	THR	CA-C-O	5.86	126.76	120.55
3	L	342	ILE	N-CA-C	-5.86	104.64	110.62
1	B	235	ARG	NE-CZ-NH1	-5.86	115.64	121.50
2	l	51	ARG	NE-CZ-NH2	5.86	124.47	119.20
2	7	111	LEU	CB-CA-C	-5.86	101.77	110.62
2	l	208	LEU	N-CA-C	-5.86	106.30	113.50
2	n	137	ILE	O-C-N	-5.86	115.25	122.57
3	H	194	ALA	CA-C-N	5.86	128.06	120.56
3	H	194	ALA	C-N-CA	5.86	128.06	120.56
3	L	243	LEU	CA-C-N	5.86	128.60	120.29
3	L	243	LEU	C-N-CA	5.86	128.60	120.29
2	2	88	ARG	CA-C-O	-5.85	114.34	120.55
1	G	6	MET	CG-SD-CE	-5.85	88.02	100.90
2	n	21	ASP	N-CA-C	-5.85	107.38	114.75
1	B	105	GLU	N-CA-C	-5.85	100.04	109.58
3	L	96	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	33	ARG	CA-C-N	5.85	125.90	120.34
1	B	33	ARG	C-N-CA	5.85	125.90	120.34
1	b	144	VAL	N-CA-C	-5.85	96.25	108.88
1	c	87	VAL	O-C-N	5.85	127.55	121.87
1	c	109	VAL	CA-C-N	5.85	128.12	120.28
1	c	109	VAL	C-N-CA	5.85	128.12	120.28
3	H	61	PRO	N-CA-CB	5.85	108.75	103.08
3	K	237	ILE	N-CA-C	-5.85	99.70	108.12
1	B	215	LYS	N-CA-C	-5.85	101.86	110.52
2	h	194	ASP	CA-C-O	5.85	125.91	118.54
2	2	125	ILE	N-CA-CB	5.85	119.24	111.64
2	4	81	ARG	N-CA-C	-5.85	106.19	113.38
3	M	151	GLU	CB-CG-CD	-5.85	102.66	112.60
3	J	248	ALA	CB-CA-C	-5.85	99.15	109.62
1	A	154	GLY	N-CA-C	-5.84	106.42	116.01
1	B	84	ASP	N-CA-C	-5.84	105.04	111.82
1	e	31	VAL	CA-C-N	5.84	128.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	31	VAL	C-N-CA	5.84	128.11	120.28
1	f	36	THR	N-CA-CB	5.84	118.63	110.04
2	j	106	TYR	CA-CB-CG	-5.84	103.38	113.90
2	5	57	ALA	N-CA-C	-5.84	99.48	109.24
1	c	49	ILE	N-CA-C	-5.84	99.76	108.46
2	5	156	THR	CA-C-O	-5.84	114.86	120.64
3	H	229	LEU	O-C-N	5.84	129.05	122.22
3	L	255	THR	N-CA-C	-5.84	99.09	108.55
1	C	233	VAL	CA-C-N	5.84	128.35	120.65
1	C	233	VAL	C-N-CA	5.84	128.35	120.65
1	c	49	ILE	CB-CA-C	5.84	119.49	110.50
1	D	64	ILE	CA-C-O	-5.84	113.48	120.78
1	B	162	THR	CA-C-O	-5.83	115.19	121.38
1	d	219	ARG	N-CA-CB	5.83	120.78	111.91
1	e	16	SER	CA-C-N	5.83	125.21	118.85
1	e	16	SER	C-N-CA	5.83	125.21	118.85
3	K	22	LYS	CA-CB-CG	5.83	125.77	114.10
2	3	189	VAL	CA-CB-CG1	5.83	120.32	110.40
1	D	48	LEU	O-C-N	-5.83	116.51	123.27
2	5	166	GLU	CA-C-N	5.83	128.57	120.29
2	5	166	GLU	C-N-CA	5.83	128.57	120.29
2	6	91	ALA	CA-C-N	5.83	128.09	120.28
2	6	91	ALA	C-N-CA	5.83	128.09	120.28
3	L	163	LYS	O-C-N	-5.83	114.61	121.32
2	m	154	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	a	151	ASP	CA-C-O	-5.83	115.05	120.94
1	a	181	ASP	N-CA-C	-5.83	103.31	110.65
1	G	178	GLU	CA-C-N	5.83	128.99	120.71
1	G	178	GLU	C-N-CA	5.83	128.99	120.71
2	i	158	GLU	N-CA-C	-5.83	105.48	112.59
2	6	88	ARG	CA-C-N	5.83	128.01	120.44
2	6	88	ARG	C-N-CA	5.83	128.01	120.44
1	C	169	ASN	CB-CA-C	-5.83	101.70	110.90
2	4	35	ASN	N-CA-CB	5.83	120.33	110.49
3	I	307	ILE	CA-C-O	5.83	126.94	120.59
3	M	360	MET	CG-SD-CE	-5.83	88.08	100.90
3	K	28	ARG	NE-CZ-NH2	-5.82	113.96	119.20
3	K	93	GLN	CB-CG-CD	-5.82	102.70	112.60
3	J	154	ARG	CG-CD-NE	-5.82	99.19	112.00
2	h	70	ILE	N-CA-C	5.82	116.56	110.62
3	I	242	GLU	N-CA-CB	5.82	120.33	110.49
3	M	353	ALA	N-CA-C	5.82	117.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	174	SER	CA-C-N	5.82	128.08	120.28
2	n	174	SER	C-N-CA	5.82	128.08	120.28
1	c	10	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	c	60	GLU	N-CA-C	-5.82	100.70	109.95
2	5	60	VAL	CA-C-N	5.82	126.56	119.99
2	5	60	VAL	C-N-CA	5.82	126.56	119.99
3	H	385	LYS	CB-CA-C	-5.82	98.84	110.42
3	I	218	GLU	CA-C-O	-5.82	114.38	120.55
2	5	84	LYS	CA-C-O	-5.82	113.98	119.80
2	6	28	GLU	CB-CG-CD	-5.81	102.72	112.60
1	a	162	THR	CA-C-N	5.81	132.14	121.85
1	a	162	THR	C-N-CA	5.81	132.14	121.85
3	M	329	LYS	CA-CB-CG	-5.81	102.48	114.10
2	6	54	MET	O-C-N	5.81	130.45	123.36
3	K	188	LYS	N-CA-C	-5.81	106.84	114.04
2	6	180	SER	N-CA-C	-5.81	105.20	112.93
3	H	29	ARG	NE-CZ-NH1	-5.81	115.69	121.50
3	I	142	ASP	CA-CB-CG	-5.81	106.79	112.60
2	2	36	PHE	CA-C-N	5.81	128.35	120.63
2	2	36	PHE	C-N-CA	5.81	128.35	120.63
2	i	111	LEU	N-CA-C	-5.81	98.95	108.41
2	4	67	ALA	N-CA-CB	5.80	118.77	110.06
3	L	90	ASN	CA-C-O	-5.80	114.25	120.92
3	H	33	GLU	CA-CB-CG	-5.80	102.49	114.10
1	E	34	GLY	CA-C-N	5.80	130.05	120.94
1	E	34	GLY	C-N-CA	5.80	130.05	120.94
3	K	95	ILE	N-CA-C	-5.80	100.05	108.17
1	D	150	THR	N-CA-CB	5.80	120.03	110.69
1	G	71	ASP	N-CA-C	-5.80	100.74	108.34
1	g	124	THR	N-CA-C	-5.80	104.39	112.45
3	J	217	GLY	CA-C-N	5.80	128.53	120.29
3	J	217	GLY	C-N-CA	5.80	128.53	120.29
3	I	224	ARG	N-CA-C	5.80	117.68	111.36
3	K	218	GLU	CA-C-N	5.80	127.58	120.22
3	K	218	GLU	C-N-CA	5.80	127.58	120.22
3	M	41	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	a	144	VAL	CA-C-O	-5.79	112.19	119.95
3	L	153	ILE	N-CA-C	-5.79	104.87	110.72
1	a	196	MET	CA-C-N	5.79	127.38	120.14
1	a	196	MET	C-N-CA	5.79	127.38	120.14
1	d	26	TYR	CA-C-N	5.79	129.12	120.31
1	d	26	TYR	C-N-CA	5.79	129.12	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	56	SER	CA-C-N	5.79	129.09	120.17
1	G	56	SER	C-N-CA	5.79	129.09	120.17
2	7	210	LYS	N-CA-C	-5.79	105.41	112.88
1	c	121	GLN	CA-C-O	-5.79	114.41	120.55
2	5	158	GLU	CA-C-N	5.79	128.40	120.35
2	5	158	GLU	C-N-CA	5.79	128.40	120.35
3	I	163	LYS	N-CA-CB	5.79	120.68	110.37
1	E	186	ASP	CA-C-O	5.79	126.67	120.24
3	I	167	PHE	O-C-N	5.79	128.25	122.12
3	K	391	ASP	CA-CB-CG	5.79	118.39	112.60
2	h	201	PRO	O-C-N	5.79	130.45	122.64
3	K	190	LEU	CA-C-N	5.79	132.59	121.54
3	K	190	LEU	C-N-CA	5.79	132.59	121.54
1	D	190	VAL	N-CA-C	-5.79	104.72	110.62
2	h	209	ALA	CA-C-N	5.79	131.80	122.14
2	h	209	ALA	C-N-CA	5.79	131.80	122.14
2	n	44	LYS	N-CA-C	-5.79	105.85	114.64
3	K	158	GLU	CA-C-O	-5.79	114.29	120.42
2	l	43	LYS	CA-C-N	5.78	129.89	120.23
2	l	43	LYS	C-N-CA	5.78	129.89	120.23
3	H	59	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	E	179	TYR	N-CA-CB	5.78	118.54	109.69
3	H	377	LYS	O-C-N	5.78	128.74	122.15
3	L	230	ALA	N-CA-C	5.78	117.58	111.28
1	b	154	GLY	N-CA-C	-5.78	107.20	115.64
3	J	114	ALA	CA-C-O	-5.78	113.66	120.60
1	d	44	GLU	CA-C-N	-5.78	113.49	121.23
1	d	44	GLU	C-N-CA	-5.78	113.49	121.23
1	f	222	LYS	N-CA-C	-5.78	100.29	109.07
1	G	56	SER	O-C-N	-5.78	116.55	120.83
2	l	168	ALA	O-C-N	-5.78	115.99	122.12
1	e	117	CYS	CB-CA-C	-5.78	101.20	110.79
1	g	172	THR	CA-C-O	-5.78	114.75	120.82
2	i	205	GLU	N-CA-C	5.78	118.35	111.71
2	m	67	ALA	CA-C-N	5.78	128.02	120.28
2	m	67	ALA	C-N-CA	5.78	128.02	120.28
1	B	233	VAL	CA-C-N	5.78	127.95	120.44
1	B	233	VAL	C-N-CA	5.78	127.95	120.44
1	c	154	GLY	N-CA-C	-5.78	107.02	115.63
1	f	191	LEU	CA-C-N	5.78	127.56	120.22
1	f	191	LEU	C-N-CA	5.78	127.56	120.22
2	7	148	TYR	CA-C-N	5.78	126.35	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	148	TYR	C-N-CA	5.78	126.35	119.94
3	J	36	PHE	CA-C-N	5.78	129.59	120.47
3	J	36	PHE	C-N-CA	5.78	129.59	120.47
3	J	335	ASP	CA-C-N	5.78	128.02	120.28
3	J	335	ASP	C-N-CA	5.78	128.02	120.28
1	c	244	LEU	N-CA-C	-5.77	104.40	112.25
2	1	134	GLU	N-CA-C	-5.77	99.99	109.40
3	K	329	LYS	CA-C-N	5.77	128.91	120.71
3	K	329	LYS	C-N-CA	5.77	128.91	120.71
3	J	95	ILE	N-CA-C	-5.77	99.74	108.17
1	f	232	TYR	CA-C-N	5.77	128.37	120.46
1	f	232	TYR	C-N-CA	5.77	128.37	120.46
2	i	176	MET	CA-C-N	5.77	128.01	120.28
2	i	176	MET	C-N-CA	5.77	128.01	120.28
2	6	58	GLY	CA-C-N	5.77	129.03	120.90
2	6	58	GLY	C-N-CA	5.77	129.03	120.90
3	H	212	VAL	N-CA-CB	5.77	120.75	111.23
1	d	53	ARG	O-C-N	-5.77	116.19	123.17
1	d	234	GLU	N-CA-C	5.77	117.56	111.28
2	k	200	SER	CA-C-N	5.77	125.89	119.32
2	k	200	SER	C-N-CA	5.77	125.89	119.32
3	J	261	VAL	N-CA-C	-5.77	105.47	111.58
1	B	67	ILE	N-CA-CB	5.76	120.74	111.23
3	M	41	ARG	NE-CZ-NH2	5.76	124.39	119.20
3	J	267	GLN	OE1-CD-NE2	-5.76	116.83	122.60
1	a	160	LYS	N-CA-C	-5.76	106.23	113.72
1	B	181	ASP	CA-C-N	5.76	132.54	121.54
1	B	181	ASP	C-N-CA	5.76	132.54	121.54
1	C	238	GLU	N-CA-C	5.76	117.56	111.28
1	G	187	ASP	CA-CB-CG	5.76	118.36	112.60
3	K	307	ILE	CA-C-N	5.76	129.74	121.50
3	K	307	ILE	C-N-CA	5.76	129.74	121.50
1	d	234	GLU	CA-C-N	5.76	128.47	120.29
1	d	234	GLU	C-N-CA	5.76	128.47	120.29
3	H	175	PRO	O-C-N	5.76	129.88	122.85
3	M	333	ASP	N-CA-C	-5.76	100.90	109.83
1	E	63	THR	CB-CA-C	5.76	119.15	109.48
2	7	39	SER	CA-C-N	5.76	128.00	120.28
2	7	39	SER	C-N-CA	5.76	128.00	120.28
1	a	222	LYS	N-CA-C	-5.76	99.27	109.06
1	B	194	VAL	CA-C-O	5.75	127.03	121.05
2	l	165	VAL	CA-C-N	5.75	127.92	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	165	VAL	C-N-CA	5.75	127.92	120.44
3	J	276	ASP	CB-CA-C	-5.75	102.42	110.13
1	B	141	VAL	CA-C-O	-5.75	114.15	120.48
2	2	62	ASP	CB-CA-C	-5.75	101.07	110.85
2	5	49	ALA	O-C-N	-5.75	116.10	122.72
3	J	71	ILE	N-CA-C	-5.75	99.25	107.77
3	K	369	LYS	CA-C-N	-5.75	116.06	123.19
3	K	369	LYS	C-N-CA	-5.75	116.06	123.19
1	E	56	SER	CB-CA-C	-5.75	97.85	110.67
1	f	73	HIS	CB-CG-CD2	-5.75	123.72	131.20
2	4	34	GLY	N-CA-C	-5.75	107.04	115.72
2	n	185	GLY	CA-C-O	5.75	130.57	120.57
3	J	211	PHE	N-CA-CB	5.75	118.74	110.06
1	G	52	LYS	CB-CG-CD	5.75	124.52	111.30
3	K	194	ALA	CA-C-N	5.75	128.58	120.42
3	K	194	ALA	C-N-CA	5.75	128.58	120.42
3	L	331	ALA	N-CA-C	-5.75	101.41	109.69
2	2	78	GLU	O-C-N	5.75	128.70	122.15
1	a	129	VAL	CB-CA-C	-5.75	103.03	110.84
1	b	180	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	c	174	PHE	CA-C-O	-5.75	114.33	120.42
2	i	169	VAL	CA-C-N	5.75	127.98	120.28
2	i	169	VAL	C-N-CA	5.75	127.98	120.28
2	k	89	ALA	CB-CA-C	-5.75	101.82	110.90
3	H	314	PHE	CA-C-O	-5.74	114.79	120.82
1	c	136	LEU	N-CA-CB	5.74	120.50	111.20
2	2	44	LYS	N-CA-C	-5.74	106.14	114.12
3	I	226	VAL	N-CA-CB	5.74	118.35	110.54
1	a	99	ASN	CA-C-O	5.74	126.50	120.42
2	k	157	PRO	N-CA-CB	5.74	108.65	103.20
3	H	173	GLU	O-C-N	5.74	126.52	121.18
3	I	54	GLU	CB-CA-C	-5.74	101.09	110.85
3	L	157	VAL	CA-C-O	-5.74	113.60	120.78
1	A	184	SER	O-C-N	-5.74	115.65	122.65
2	1	76	LEU	CA-C-O	5.74	126.84	120.82
2	1	170	ARG	CA-C-O	-5.74	114.47	120.55
2	6	193	GLU	CA-CB-CG	5.74	125.58	114.10
3	K	200	ARG	N-CA-C	-5.74	105.58	112.58
1	F	19	GLY	CA-C-N	5.74	133.56	122.03
1	F	19	GLY	C-N-CA	5.74	133.56	122.03
2	n	43	LYS	CA-C-O	-5.74	114.38	120.92
2	n	73	GLU	CA-C-N	5.74	128.43	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	73	GLU	C-N-CA	5.74	128.43	120.29
3	H	376	THR	CA-CB-CG2	5.74	120.25	110.50
3	J	299	ARG	CB-CA-C	5.74	118.97	109.56
1	A	62	ASP	CA-CB-CG	5.73	118.33	112.60
1	b	246	LYS	N-CA-CB	5.73	120.25	110.50
2	1	28	GLU	N-CA-C	-5.73	100.33	109.96
2	l	87	VAL	CA-C-N	5.73	127.96	120.28
2	l	87	VAL	C-N-CA	5.73	127.96	120.28
1	D	129	VAL	N-CA-C	-5.73	100.78	108.35
2	1	150	VAL	CB-CA-C	5.73	119.22	111.88
2	5	45	ILE	CA-C-O	-5.73	114.39	120.53
3	M	36	PHE	CA-C-N	5.73	128.56	120.42
3	M	36	PHE	C-N-CA	5.73	128.56	120.42
3	I	260	GLU	O-C-N	-5.73	116.17	122.07
3	J	54	GLU	N-CA-C	5.73	117.61	111.36
1	c	178	GLU	O-C-N	-5.73	116.16	123.26
1	f	171	VAL	N-CA-C	-5.73	103.77	111.44
2	5	155	PHE	CA-C-N	5.73	134.42	123.65
2	5	155	PHE	C-N-CA	5.73	134.42	123.65
3	M	369	LYS	N-CA-CB	5.73	120.17	110.49
2	1	61	GLY	CA-C-N	5.73	129.01	120.31
2	1	61	GLY	C-N-CA	5.73	129.01	120.31
2	2	204	VAL	CA-C-N	5.73	128.74	120.38
2	2	204	VAL	C-N-CA	5.73	128.74	120.38
1	b	82	VAL	CA-C-O	-5.72	114.29	120.47
2	k	126	ASP	CA-C-O	-5.72	114.72	120.96
2	m	69	ILE	CA-C-N	5.72	127.77	120.56
2	m	69	ILE	C-N-CA	5.72	127.77	120.56
2	7	167	LEU	CA-C-N	5.72	127.95	120.28
2	7	167	LEU	C-N-CA	5.72	127.95	120.28
3	I	364	ARG	O-C-N	5.72	129.31	122.27
1	A	125	GLN	CA-C-O	-5.72	114.43	120.55
1	F	239	ARG	CA-C-O	5.72	125.97	119.27
3	L	374	ASP	CB-CA-C	-5.72	101.29	110.79
3	M	142	ASP	CA-CB-CG	-5.72	106.88	112.60
3	I	12	LYS	N-CA-C	5.72	117.19	111.07
1	d	91	ARG	CG-CD-NE	-5.72	99.42	112.00
2	1	210	LYS	N-CA-C	-5.72	105.02	112.23
2	k	72	ILE	CA-C-O	5.72	126.90	120.95
1	d	29	GLU	CA-C-O	5.72	126.41	119.38
1	D	59	LEU	N-CA-CB	5.72	119.73	110.41
1	E	187	ASP	CA-C-N	5.72	127.94	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	ASP	C-N-CA	5.72	127.94	120.28
2	2	87	VAL	CA-C-N	5.72	127.94	120.28
2	2	87	VAL	C-N-CA	5.72	127.94	120.28
1	c	32	LYS	CA-C-N	5.71	128.41	120.29
1	c	32	LYS	C-N-CA	5.71	128.41	120.29
2	5	203	GLU	CA-C-N	5.71	128.54	120.42
2	5	203	GLU	C-N-CA	5.71	128.54	120.42
2	6	47	GLN	OE1-CD-NE2	5.71	128.31	122.60
2	6	168	ALA	CA-C-N	5.71	128.29	120.46
2	6	168	ALA	C-N-CA	5.71	128.29	120.46
2	1	155	PHE	N-CA-C	-5.71	100.51	109.25
3	L	250	ARG	CA-C-O	-5.71	114.76	121.16
2	2	69	ILE	N-CA-CB	5.71	117.23	110.55
2	l	182	SER	N-CA-C	-5.71	105.03	112.23
3	H	268	LEU	CA-C-O	-5.71	114.82	120.70
1	A	11	ALA	N-CA-C	-5.71	100.27	108.60
1	c	24	VAL	CA-C-O	5.71	126.64	120.47
2	5	168	ALA	CA-C-O	-5.71	114.50	120.55
1	C	90	ASP	CA-C-N	5.71	127.86	120.44
1	C	90	ASP	C-N-CA	5.71	127.86	120.44
2	l	211	PHE	CA-CB-CG	-5.71	108.09	113.80
3	H	397	PHE	CA-CB-CG	-5.71	108.09	113.80
2	1	36	PHE	O-C-N	5.71	129.72	123.22
3	K	48	VAL	CA-C-N	5.71	128.39	120.29
3	K	48	VAL	C-N-CA	5.71	128.39	120.29
1	a	104	ASP	CA-CB-CG	-5.70	106.90	112.60
3	L	242	GLU	N-CA-CB	5.70	120.12	110.49
1	a	105	GLU	CA-C-O	-5.70	113.88	120.03
1	G	84	ASP	CA-CB-CG	5.70	118.30	112.60
2	7	207	ILE	O-C-N	5.70	129.63	121.82
3	I	343	THR	N-CA-C	-5.70	106.22	112.72
3	K	353	ALA	CB-CA-C	-5.70	99.73	110.67
3	L	236	SER	N-CA-C	-5.70	100.04	108.99
3	J	380	GLU	N-CA-C	5.70	117.49	111.28
2	6	14	THR	N-CA-C	-5.70	100.50	109.50
1	C	187	ASP	CA-CB-CG	-5.70	106.90	112.60
2	k	48	ILE	N-CA-CB	-5.70	103.28	110.57
3	L	241	ASP	O-C-N	-5.70	116.83	123.27
3	J	202	THR	N-CA-CB	5.70	120.11	110.49
1	C	209	ILE	CA-C-O	-5.69	114.67	121.28
1	c	48	LEU	O-C-N	-5.69	116.65	123.31
1	A	113	ALA	N-CA-C	-5.69	105.22	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CA-C-O	-5.69	113.23	119.95
1	D	83	ALA	N-CA-C	5.69	117.48	111.28
2	6	104	PHE	CA-C-N	5.69	126.96	119.84
2	6	104	PHE	C-N-CA	5.69	126.96	119.84
2	7	102	ARG	NE-CZ-NH2	5.69	124.32	119.20
3	H	347	SER	CA-C-O	5.69	128.48	121.99
1	G	200	ILE	N-CA-C	-5.69	107.44	112.90
2	6	201	PRO	N-CA-CB	5.69	109.22	103.25
3	I	56	GLU	CA-C-O	5.69	126.45	119.05
3	I	149	GLN	CB-CA-C	5.69	121.88	109.99
1	B	118	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	120	LYS	CA-C-N	5.69	127.83	120.44
1	C	120	LYS	C-N-CA	5.69	127.83	120.44
1	F	108	THR	N-CA-CB	-5.69	101.24	109.83
2	4	107	LEU	CA-C-N	-5.69	114.34	121.96
2	4	107	LEU	C-N-CA	-5.69	114.34	121.96
3	M	182	GLY	O-C-N	5.69	127.46	121.77
1	c	16	SER	O-C-N	-5.68	114.78	121.32
1	d	230	LYS	CB-CA-C	-5.68	101.19	112.05
3	I	198	GLN	N-CA-C	-5.68	106.69	113.97
3	J	16	LEU	O-C-N	5.68	128.63	122.15
1	d	86	ARG	N-CA-C	5.68	117.47	111.28
3	I	281	VAL	N-CA-C	-5.68	99.45	107.75
3	J	70	ASP	CA-C-O	5.68	127.40	121.38
1	D	198	LEU	CA-C-N	5.68	127.89	120.28
1	D	198	LEU	C-N-CA	5.68	127.89	120.28
1	F	64	ILE	O-C-N	5.68	127.20	122.09
2	5	63	ALA	N-CA-C	5.68	117.55	111.36
3	I	146	LEU	CA-C-N	5.68	131.93	121.70
3	I	146	LEU	C-N-CA	5.68	131.93	121.70
3	I	330	LEU	N-CA-CB	5.68	120.21	111.46
3	J	228	GLN	N-CA-C	-5.68	105.17	111.36
2	3	61	GLY	CA-C-O	-5.68	114.64	120.66
2	3	65	PHE	CA-C-N	5.68	127.89	120.28
2	3	65	PHE	C-N-CA	5.68	127.89	120.28
3	M	85	PRO	N-CA-C	5.68	120.14	111.11
1	A	218	ASP	CA-CB-CG	-5.68	106.92	112.60
2	3	179	ASP	CA-CB-CG	-5.68	106.92	112.60
3	L	263	ARG	NH1-CZ-NH2	5.68	126.68	119.30
1	D	120	LYS	CA-C-O	-5.68	114.40	120.42
2	1	45	ILE	CA-CB-CG1	5.68	120.05	110.40
2	i	183	GLY	CA-C-N	5.68	132.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	183	GLY	C-N-CA	5.68	132.38	121.54
3	J	286	ALA	N-CA-C	-5.68	99.79	108.76
1	a	107	ILE	CA-C-N	-5.67	112.03	120.94
1	a	107	ILE	C-N-CA	-5.67	112.03	120.94
1	B	229	LEU	CA-C-N	5.67	129.37	120.97
1	B	229	LEU	C-N-CA	5.67	129.37	120.97
1	b	186	ASP	CA-C-N	5.67	127.88	120.28
1	b	186	ASP	C-N-CA	5.67	127.88	120.28
1	F	213	TYR	CA-CB-CG	5.67	124.11	113.90
2	h	97	LEU	CA-C-O	5.67	126.44	120.42
2	3	79	ILE	CA-C-O	-5.67	114.34	120.47
2	5	108	VAL	CA-C-O	-5.67	116.19	120.96
2	l	86	THR	CA-C-O	-5.67	114.94	121.47
3	H	244	ASP	N-CA-CB	5.67	120.08	110.49
3	K	211	PHE	N-CA-CB	5.67	120.78	111.08
3	K	369	LYS	N-CA-CB	5.67	120.36	111.56
3	L	271	GLU	CA-C-N	5.67	127.82	120.44
3	L	271	GLU	C-N-CA	5.67	127.82	120.44
1	D	194	VAL	CB-CA-C	-5.67	104.39	112.22
2	7	108	VAL	O-C-N	5.67	129.67	123.09
1	a	10	ARG	CA-C-N	5.67	131.15	122.93
1	a	10	ARG	C-N-CA	5.67	131.15	122.93
1	E	73	HIS	ND1-CE1-NE2	5.67	114.07	108.40
1	E	232	TYR	CB-CG-CD2	-5.67	112.29	120.80
3	H	22	LYS	O-C-N	5.67	128.62	122.15
3	I	73	GLU	CB-CA-C	-5.67	100.97	110.56
3	L	395	VAL	CA-C-N	5.67	132.37	121.54
3	L	395	VAL	C-N-CA	5.67	132.37	121.54
1	D	132	PHE	CB-CA-C	-5.67	102.18	110.06
1	E	216	VAL	O-C-N	5.67	127.47	121.91
1	g	82	VAL	O-C-N	5.67	128.21	121.80
2	l	135	LYS	N-CA-C	-5.67	103.93	111.24
2	m	153	ASP	N-CA-CB	5.67	118.23	110.01
3	K	72	LEU	N-CA-CB	5.67	120.38	111.20
2	i	87	VAL	CA-C-N	5.67	127.87	120.28
2	i	87	VAL	C-N-CA	5.67	127.87	120.28
2	k	62	ASP	CA-CB-CG	-5.67	106.93	112.60
2	5	149	GLY	O-C-N	5.67	127.74	122.13
3	H	118	VAL	N-CA-CB	5.67	119.79	111.52
3	H	160	PRO	O-C-N	5.67	128.30	122.18
3	M	224	ARG	CA-C-O	5.67	126.43	120.42
2	m	31	ALA	N-CA-C	-5.67	99.05	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	116	VAL	CA-C-O	5.67	125.52	120.70
3	M	281	VAL	N-CA-C	-5.67	99.59	107.80
1	C	59	LEU	CB-CA-C	-5.66	101.06	109.90
2	j	104	PHE	N-CA-C	-5.66	101.59	110.14
2	l	70	ILE	CA-C-N	5.66	127.80	120.44
2	l	70	ILE	C-N-CA	5.66	127.80	120.44
2	7	23	VAL	CA-C-O	5.66	126.33	120.39
2	7	195	GLU	O-C-N	5.66	128.93	123.04
2	n	202	GLU	CA-C-N	5.66	127.80	120.44
2	n	202	GLU	C-N-CA	5.66	127.80	120.44
1	B	83	ALA	O-C-N	5.66	127.92	122.03
3	J	166	LEU	CA-C-N	5.66	128.91	120.31
3	J	166	LEU	C-N-CA	5.66	128.91	120.31
3	J	309	VAL	N-CA-CB	5.66	119.13	111.21
1	A	137	LEU	N-CA-CB	5.66	119.65	110.43
2	7	143	GLY	CA-C-N	5.66	127.86	120.28
2	7	143	GLY	C-N-CA	5.66	127.86	120.28
2	3	202	GLU	O-C-N	5.66	127.97	122.09
2	3	209	ALA	CA-C-O	5.66	126.33	119.31
2	n	143	GLY	CA-C-N	5.66	127.86	120.28
2	n	143	GLY	C-N-CA	5.66	127.86	120.28
2	i	103	TYR	CB-CG-CD2	5.66	129.28	120.80
1	a	174	PHE	CA-CB-CG	-5.65	108.15	113.80
2	6	104	PHE	N-CA-C	-5.65	100.82	108.11
3	I	195	VAL	CA-C-N	5.65	127.85	120.28
3	I	195	VAL	C-N-CA	5.65	127.85	120.28
1	B	100	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	b	214	VAL	CG1-CB-CG2	-5.65	98.37	110.80
3	H	130	PHE	CA-C-N	5.65	131.87	121.70
3	H	130	PHE	C-N-CA	5.65	131.87	121.70
3	K	205	ARG	CB-CG-CD	5.65	124.30	111.30
3	J	241	ASP	CA-CB-CG	-5.65	106.95	112.60
3	K	107	ALA	N-CA-CB	5.65	119.42	110.55
1	f	225	SER	CA-C-O	-5.65	114.32	120.87
3	K	95	ILE	O-C-N	5.65	129.11	123.18
1	d	66	LYS	N-CA-C	-5.64	108.18	114.62
1	E	47	ILE	CA-C-O	5.64	126.46	120.48
1	F	64	ILE	N-CA-C	-5.64	106.98	112.29
1	F	102	THR	O-C-N	-5.64	115.28	122.34
1	g	219	ARG	N-CA-CB	5.64	120.03	110.49
2	4	30	ARG	N-CA-C	-5.64	100.16	108.79
3	J	263	ARG	N-CA-C	-5.64	105.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	110	LYS	CB-CA-C	-5.64	101.42	110.79
2	h	198	GLN	O-C-N	5.64	130.57	123.12
2	5	19	CYS	CB-CA-C	5.64	120.60	109.66
1	B	46	VAL	N-CA-C	-5.64	100.91	108.35
2	h	187	ASP	CA-CB-CG	5.64	118.24	112.60
2	m	154	ARG	NE-CZ-NH1	-5.64	115.86	121.50
3	J	281	VAL	CA-C-N	5.64	131.85	121.70
3	J	281	VAL	C-N-CA	5.64	131.85	121.70
3	L	299	ARG	CB-CA-C	5.64	117.57	109.11
1	a	169	ASN	CA-C-O	-5.64	114.54	120.63
1	f	66	LYS	N-CA-C	-5.64	98.79	110.80
2	i	81	ARG	NE-CZ-NH2	-5.64	114.13	119.20
2	n	18	VAL	O-C-N	5.64	129.37	122.83
3	M	364	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	a	122	GLN	N-CA-C	-5.63	105.14	111.28
3	I	187	GLY	O-C-N	5.63	130.03	122.70
3	L	279	GLY	N-CA-C	-5.63	99.83	113.18
2	m	153	ASP	CA-C-O	-5.63	114.91	120.82
1	G	138	ILE	O-C-N	-5.63	117.23	123.20
1	G	242	GLU	O-C-N	5.63	128.09	122.12
2	1	157	PRO	N-CA-CB	5.63	108.55	103.20
1	B	151	ASP	CA-CB-CG	-5.63	106.97	112.60
3	J	319	GLN	N-CA-C	5.63	118.35	111.82
1	g	103	TYR	N-CA-C	-5.63	106.30	114.12
2	3	171	ALA	CA-C-N	5.63	128.41	120.42
2	3	171	ALA	C-N-CA	5.63	128.41	120.42
3	M	148	VAL	CA-C-O	5.63	126.81	120.85
2	1	138	VAL	CA-CB-CG1	5.62	119.96	110.40
2	3	165	VAL	N-CA-C	-5.62	105.04	110.72
1	D	117	CYS	N-CA-CB	5.62	118.48	110.16
1	E	240	ILE	CA-C-N	5.62	127.81	120.28
1	E	240	ILE	C-N-CA	5.62	127.81	120.28
1	e	157	LEU	CA-C-N	5.62	130.92	122.99
1	e	157	LEU	C-N-CA	5.62	130.92	122.99
2	h	33	MET	N-CA-CB	5.62	121.31	111.13
2	l	206	GLN	CA-C-N	5.62	129.86	120.64
2	l	206	GLN	C-N-CA	5.62	129.86	120.64
3	M	153	ILE	O-C-N	5.62	127.33	121.87
1	B	92	ALA	N-CA-CB	5.62	118.16	110.01
2	3	108	VAL	CA-C-O	-5.62	113.75	120.78
3	I	317	ARG	CA-C-N	5.62	128.16	120.46
3	I	317	ARG	C-N-CA	5.62	128.16	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	182	GLY	CA-C-N	5.62	126.17	120.38
3	J	182	GLY	C-N-CA	5.62	126.17	120.38
2	2	202	GLU	CA-C-N	5.62	127.81	120.28
2	2	202	GLU	C-N-CA	5.62	127.81	120.28
3	M	171	GLY	CA-C-N	5.62	131.69	122.64
3	M	171	GLY	C-N-CA	5.62	131.69	122.64
1	d	78	THR	CA-C-O	5.61	128.03	121.46
2	6	134	GLU	CA-C-N	5.61	128.07	120.38
2	6	134	GLU	C-N-CA	5.61	128.07	120.38
3	H	90	ASN	CB-CA-C	-5.61	100.49	109.75
1	E	147	LEU	N-CA-C	-5.61	98.38	108.48
2	l	173	TYR	N-CA-C	-5.61	104.79	111.69
3	M	56	GLU	N-CA-C	5.61	118.33	111.82
1	b	31	VAL	CA-CB-CG2	5.61	119.94	110.40
1	c	195	ALA	CA-C-O	-5.61	114.47	120.42
3	H	264	THR	CA-C-O	5.61	126.37	120.42
1	f	174	PHE	CA-C-O	5.61	126.50	120.55
2	m	99	ASN	CA-C-N	5.61	128.25	120.29
2	m	99	ASN	C-N-CA	5.61	128.25	120.29
3	L	286	ALA	CA-C-N	5.61	131.06	121.87
3	L	286	ALA	C-N-CA	5.61	131.06	121.87
1	b	84	ASP	CA-C-N	5.61	127.79	120.28
1	b	84	ASP	C-N-CA	5.61	127.79	120.28
1	c	119	PHE	CA-CB-CG	-5.61	108.19	113.80
1	e	73	HIS	ND1-CE1-NE2	5.61	114.01	108.40
2	l	39	SER	CA-C-O	5.61	127.06	120.89
2	6	44	LYS	N-CA-C	-5.61	104.69	112.03
2	m	102	ARG	NE-CZ-NH2	5.61	124.25	119.20
3	H	338	GLU	CA-C-N	5.61	127.73	120.44
3	H	338	GLU	C-N-CA	5.61	127.73	120.44
3	I	224	ARG	O-C-N	5.61	128.54	122.15
3	L	299	ARG	NE-CZ-NH1	-5.61	115.89	121.50
2	2	109	GLN	CA-C-O	5.60	126.30	120.30
3	H	252	ASN	N-CA-C	-5.60	106.33	114.12
1	b	57	LYS	N-CA-C	-5.60	106.28	113.23
1	d	243	LEU	N-CA-C	5.60	117.39	111.28
3	L	50	ARG	N-CA-CB	5.60	118.36	110.12
3	L	232	GLU	O-C-N	-5.60	116.18	122.12
3	L	377	LYS	N-CA-CB	5.60	118.45	110.16
2	i	82	GLU	O-C-N	-5.60	115.08	122.47
2	i	135	LYS	N-CA-CB	-5.60	102.38	110.56
3	H	84	GLY	CA-C-O	-5.60	113.51	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LEU	N-CA-C	5.60	117.38	111.28
1	b	188	ALA	CA-C-N	5.60	128.05	120.44
1	b	188	ALA	C-N-CA	5.60	128.05	120.44
2	m	28	GLU	CA-CB-CG	-5.60	102.90	114.10
1	E	181	ASP	CA-CB-CG	-5.60	107.00	112.60
2	l	133	GLU	CB-CA-C	-5.60	102.10	110.16
3	K	371	THR	N-CA-C	-5.60	100.92	109.65
3	L	324	HIS	ND1-CE1-NE2	5.60	114.00	108.40
2	1	206	GLN	CA-C-N	5.59	129.48	120.30
2	1	206	GLN	C-N-CA	5.59	129.48	120.30
3	I	94	TYR	N-CA-C	-5.59	105.10	111.14
3	J	310	PRO	N-CA-C	-5.59	100.94	112.47
1	E	188	ALA	CA-C-O	5.59	126.48	120.55
1	e	33	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	1	91	ALA	CA-C-O	-5.59	114.49	120.42
2	j	37	ILE	N-CA-C	-5.59	99.18	107.51
2	5	143	GLY	CA-C-O	5.59	126.15	119.10
2	n	23	VAL	N-CA-C	-5.59	99.75	108.81
3	H	250	ARG	CA-C-O	-5.59	115.35	121.89
2	h	50	ASP	CA-CB-CG	-5.59	107.01	112.60
1	G	113	ALA	N-CA-CB	5.59	118.33	110.12
1	b	144	VAL	N-CA-CB	5.59	119.03	111.21
2	1	160	GLY	N-CA-C	-5.59	103.61	112.66
2	h	161	VAL	N-CA-C	-5.59	104.84	113.16
2	3	165	VAL	O-C-N	5.59	127.58	121.83
2	6	28	GLU	N-CA-C	-5.59	100.57	109.96
2	7	68	ARG	CA-C-N	5.59	127.60	120.56
2	7	68	ARG	C-N-CA	5.59	127.60	120.56
3	K	273	ASP	CA-CB-CG	5.59	118.19	112.60
1	g	31	VAL	CB-CA-C	-5.58	104.51	112.22
1	e	83	ALA	CA-C-N	5.58	128.22	120.29
1	e	83	ALA	C-N-CA	5.58	128.22	120.29
1	e	208	ASN	N-CA-C	-5.58	104.00	111.87
2	3	76	LEU	CA-C-O	-5.58	114.92	120.90
2	j	104	PHE	CA-C-N	5.58	126.82	119.84
2	j	104	PHE	C-N-CA	5.58	126.82	119.84
3	J	226	VAL	N-CA-CB	5.58	121.50	110.95
1	E	235	ARG	CA-C-N	5.58	128.22	120.29
1	E	235	ARG	C-N-CA	5.58	128.22	120.29
2	7	149	GLY	N-CA-C	-5.58	106.03	112.50
3	L	207	VAL	CA-CB-CG1	5.58	119.89	110.40
3	J	119	LEU	CA-C-N	5.58	125.58	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	119	LEU	C-N-CA	5.58	125.58	119.89
1	b	103	TYR	CB-CA-C	-5.58	100.01	109.38
2	5	211	PHE	N-CA-C	-5.58	106.06	112.92
2	m	184	ASP	CB-CG-OD1	-5.58	105.57	118.40
3	K	296	ALA	O-C-N	5.58	129.59	122.39
1	D	52	LYS	N-CA-C	-5.58	104.01	112.99
2	j	132	ILE	O-C-N	-5.58	117.24	123.26
3	J	140	TYR	CG-CD2-CE2	5.58	129.57	121.20
2	7	65	PHE	N-CA-CB	5.58	118.05	109.91
3	K	287	THR	O-C-N	-5.58	117.23	123.48
1	F	25	GLU	CA-C-O	5.57	126.33	120.42
1	g	85	ALA	CA-C-N	5.57	127.69	120.44
1	g	85	ALA	C-N-CA	5.57	127.69	120.44
2	3	193	GLU	O-C-N	-5.57	115.18	122.59
3	I	74	ASP	CA-C-N	5.57	131.19	120.66
3	I	74	ASP	C-N-CA	5.57	131.19	120.66
3	I	377	LYS	N-CA-C	5.57	117.36	111.28
2	1	12	THR	CB-CA-C	5.57	121.36	109.10
1	d	94	ILE	CA-C-N	5.57	127.75	120.28
1	d	94	ILE	C-N-CA	5.57	127.75	120.28
2	h	92	THR	CA-CB-OG1	-5.57	101.24	109.60
2	3	134	GLU	O-C-N	5.57	129.62	122.93
2	5	71	LYS	N-CA-C	5.57	117.03	111.07
2	7	86	THR	CA-C-O	-5.57	115.15	121.72
3	K	168	ALA	N-CA-C	5.57	118.28	111.82
3	J	93	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	a	138	ILE	CA-C-N	5.57	130.62	122.77
1	a	138	ILE	C-N-CA	5.57	130.62	122.77
1	E	12	ILE	N-CA-CB	-5.57	103.61	112.07
3	I	184	PRO	N-CA-CB	5.57	108.52	103.34
3	M	283	VAL	CA-C-N	5.57	131.72	121.70
3	M	283	VAL	C-N-CA	5.57	131.72	121.70
1	f	120	LYS	N-CA-C	5.57	117.15	111.14
2	1	132	ILE	O-C-N	-5.57	117.01	122.97
2	7	157	PRO	CA-C-N	5.57	131.23	122.49
2	7	157	PRO	C-N-CA	5.57	131.23	122.49
3	I	303	PHE	CA-C-O	-5.57	114.83	121.56
3	L	104	ALA	CA-C-O	-5.57	114.57	120.92
1	F	130	ARG	N-CA-C	-5.56	103.11	110.40
2	k	39	SER	CA-C-N	5.56	131.73	122.66
2	k	39	SER	C-N-CA	5.56	131.73	122.66
1	B	65	GLU	CB-CG-CD	-5.56	103.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	161	VAL	CA-C-O	5.56	126.52	120.57
1	b	97	GLN	N-CA-CB	5.56	119.62	110.39
1	f	25	GLU	CA-C-N	5.56	127.73	120.28
1	f	25	GLU	C-N-CA	5.56	127.73	120.28
3	I	262	GLN	CB-CG-CD	-5.56	103.15	112.60
3	K	176	LYS	N-CA-C	-5.56	104.74	113.02
3	J	213	GLN	OE1-CD-NE2	5.56	128.16	122.60
1	A	8	TYR	CB-CA-C	5.56	120.66	110.10
1	d	91	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	G	180	ARG	N-CA-C	-5.56	100.91	109.52
1	g	46	VAL	CA-C-O	-5.56	115.47	121.19
2	k	33	MET	N-CA-C	-5.56	102.11	110.06
1	d	191	LEU	N-CA-CB	5.55	118.39	110.06
1	E	8	TYR	N-CA-C	-5.55	104.15	112.54
1	e	15	PHE	N-CA-C	-5.55	102.06	110.28
2	j	92	THR	CA-C-O	5.55	126.44	120.55
2	7	104	PHE	N-CA-C	-5.55	100.52	109.40
3	J	232	GLU	N-CA-CB	-5.55	101.75	110.30
1	A	172	THR	CA-C-N	5.55	127.65	120.44
1	A	172	THR	C-N-CA	5.55	127.65	120.44
1	B	15	PHE	N-CA-C	5.55	118.85	110.64
1	d	169	ASN	N-CA-C	5.55	117.13	111.14
2	l	86	THR	CA-CB-OG1	5.55	117.92	109.60
3	L	311	LEU	N-CA-C	-5.55	102.66	109.65
1	c	239	ARG	CA-C-N	5.55	128.06	120.46
1	c	239	ARG	C-N-CA	5.55	128.06	120.46
1	E	36	THR	CA-C-O	-5.55	115.52	121.56
2	k	37	ILE	N-CA-C	-5.55	100.34	108.99
1	f	34	GLY	N-CA-C	-5.54	104.67	112.60
2	i	121	SER	CA-C-O	-5.54	114.79	120.89
2	n	106	TYR	CA-CB-CG	-5.54	103.92	113.90
3	L	258	ASP	O-C-N	-5.54	116.59	122.30
1	A	232	TYR	CA-C-N	5.54	129.22	120.47
1	A	232	TYR	C-N-CA	5.54	129.22	120.47
1	G	71	ASP	CA-CB-CG	-5.54	107.06	112.60
2	3	211	PHE	CB-CG-CD1	-5.54	111.28	120.70
2	j	42	ALA	N-CA-C	-5.54	102.08	110.28
3	I	205	ARG	N-CA-C	-5.54	99.49	108.52
3	K	255	THR	N-CA-C	-5.54	100.29	108.99
3	M	386	THR	CB-CA-C	5.54	121.45	110.42
1	B	68	TYR	CA-CB-CG	-5.54	103.93	113.90
3	I	236	SER	O-C-N	-5.54	117.75	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	380	GLU	CA-C-O	-5.54	114.68	120.55
1	C	36	THR	N-CA-C	5.54	118.10	110.35
1	F	150	THR	N-CA-CB	5.54	119.66	110.63
2	j	147	ALA	CA-C-N	5.54	127.70	120.28
2	j	147	ALA	C-N-CA	5.54	127.70	120.28
3	I	43	ARG	CA-C-O	5.54	126.63	120.82
1	a	169	ASN	N-CA-C	5.54	118.03	111.33
1	E	229	LEU	N-CA-C	-5.54	106.66	113.41
2	k	29	LYS	CA-C-O	-5.54	115.16	121.58
3	H	78	VAL	N-CA-CB	5.54	117.97	111.66
3	H	253	SER	N-CA-C	-5.54	106.57	113.38
2	7	158	GLU	N-CA-C	-5.53	105.22	112.41
3	I	280	ASP	N-CA-C	-5.53	99.01	110.80
2	3	35	ASN	N-CA-C	-5.53	104.78	112.30
3	J	353	ALA	N-CA-C	5.53	117.31	111.28
1	b	200	ILE	CA-CB-CG1	5.53	119.80	110.40
2	1	204	VAL	CA-C-N	5.53	128.00	120.54
2	1	204	VAL	C-N-CA	5.53	128.00	120.54
2	3	184	ASP	N-CA-CB	5.53	118.05	109.48
3	L	16	LEU	CA-C-N	5.53	127.69	120.28
3	L	16	LEU	C-N-CA	5.53	127.69	120.28
1	c	210	GLU	N-CA-C	-5.53	99.89	108.90
2	3	80	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	n	79	ILE	CA-C-O	-5.53	114.91	121.05
3	I	260	GLU	CA-C-N	5.53	129.36	120.30
3	I	260	GLU	C-N-CA	5.53	129.36	120.30
3	K	290	ILE	N-CA-C	-5.53	106.92	112.17
3	L	266	MET	CG-SD-CE	-5.53	88.74	100.90
1	A	227	GLU	CA-C-N	5.53	127.69	120.28
1	A	227	GLU	C-N-CA	5.53	127.69	120.28
2	7	158	GLU	CA-C-N	5.53	131.34	122.50
2	7	158	GLU	C-N-CA	5.53	131.34	122.50
2	7	208	LEU	N-CA-CB	5.53	119.14	110.46
3	K	20	TYR	O-C-N	-5.53	115.85	122.15
3	J	355	CYS	CA-C-O	-5.53	115.02	120.82
1	c	191	LEU	CA-C-N	5.52	132.24	121.41
1	c	191	LEU	C-N-CA	5.52	132.24	121.41
3	L	317	ARG	NH1-CZ-NH2	5.52	126.48	119.30
2	h	191	ILE	N-CA-C	-5.52	97.85	109.34
2	5	36	PHE	CA-C-N	5.52	130.53	122.69
2	5	36	PHE	C-N-CA	5.52	130.53	122.69
2	7	20	LYS	CA-C-O	5.52	125.81	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	ASP	CA-C-N	5.52	129.09	120.75
1	G	62	ASP	C-N-CA	5.52	129.09	120.75
2	n	192	THR	N-CA-C	-5.52	106.59	113.38
1	E	226	PRO	CA-C-N	5.52	127.68	120.28
1	E	226	PRO	C-N-CA	5.52	127.68	120.28
2	i	49	ALA	O-C-N	-5.52	117.08	122.99
2	7	184	ASP	O-C-N	-5.52	116.65	123.44
3	L	348	GLY	CA-C-N	5.52	128.13	120.29
3	L	348	GLY	C-N-CA	5.52	128.13	120.29
3	L	387	THR	CB-CA-C	-5.52	102.41	109.92
3	M	77	VAL	N-CA-CB	5.52	120.49	111.44
3	M	302	ARG	NE-CZ-NH1	5.52	127.02	121.50
3	J	375	PHE	CB-CG-CD2	5.52	130.08	120.70
1	A	122	GLN	N-CA-CB	5.52	118.72	110.22
1	C	210	GLU	N-CA-C	-5.52	100.41	109.40
1	E	81	LEU	CA-C-O	-5.52	114.47	120.81
1	F	20	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	h	194	ASP	O-C-N	-5.52	114.50	121.67
3	K	103	GLY	N-CA-C	-5.52	107.63	115.30
1	e	100	ARG	N-CA-C	-5.51	105.37	111.71
3	J	211	PHE	CA-C-N	5.51	131.89	121.97
3	J	211	PHE	C-N-CA	5.51	131.89	121.97
2	1	125	ILE	N-CA-CB	5.51	119.57	111.52
2	3	29	LYS	N-CA-CB	5.51	119.94	110.68
2	4	147	ALA	CA-C-N	5.51	128.12	120.29
2	4	147	ALA	C-N-CA	5.51	128.12	120.29
3	H	145	GLY	N-CA-C	-5.51	108.13	114.69
3	K	70	ASP	N-CA-C	-5.51	100.55	108.60
1	a	141	VAL	CA-C-O	-5.51	114.42	120.43
1	c	143	GLU	N-CA-C	-5.51	108.34	114.62
2	i	62	ASP	CA-CB-CG	-5.51	107.09	112.60
1	a	200	ILE	CA-C-N	5.51	129.99	122.34
1	a	200	ILE	C-N-CA	5.51	129.99	122.34
1	F	239	ARG	N-CA-C	5.51	120.06	113.23
1	G	223	GLU	N-CA-C	-5.51	100.27	109.24
2	j	28	GLU	CB-CG-CD	-5.51	103.24	112.60
1	E	105	GLU	CA-C-N	5.50	125.82	119.93
1	E	105	GLU	C-N-CA	5.50	125.82	119.93
3	L	350	ASP	CA-C-N	5.50	128.00	120.46
3	L	350	ASP	C-N-CA	5.50	128.00	120.46
2	1	43	LYS	N-CA-CB	5.50	118.06	109.97
2	5	89	ALA	N-CA-C	-5.50	105.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	166	GLU	CB-CA-C	-5.50	101.49	110.85
2	n	106	TYR	CA-C-O	-5.50	114.83	120.99
3	M	317	ARG	CA-C-N	5.50	128.00	120.46
3	M	317	ARG	C-N-CA	5.50	128.00	120.46
2	k	137	ILE	CA-CB-CG1	5.50	119.75	110.40
3	M	101	LYS	N-CA-C	-5.50	99.97	108.55
2	3	104	PHE	O-C-N	-5.50	116.25	121.20
2	6	37	ILE	N-CA-C	-5.50	99.15	107.73
3	H	157	VAL	CB-CA-C	-5.50	102.27	111.29
3	M	342	ILE	N-CA-C	-5.50	105.00	111.00
1	B	60	GLU	CA-C-N	5.50	128.10	120.29
1	B	60	GLU	C-N-CA	5.50	128.10	120.29
2	j	128	ILE	N-CA-C	-5.50	106.05	111.77
2	l	160	GLY	CA-C-N	5.50	128.22	120.42
2	l	160	GLY	C-N-CA	5.50	128.22	120.42
2	m	146	THR	CA-C-N	5.50	127.64	120.28
2	m	146	THR	C-N-CA	5.50	127.64	120.28
3	I	305	ARG	CA-C-O	5.50	126.17	120.40
3	M	166	LEU	O-C-N	5.50	129.03	122.27
1	f	20	ARG	NE-CZ-NH2	-5.50	114.25	119.20
2	1	188	VAL	N-CA-C	-5.50	100.57	108.48
3	K	351	ILE	O-C-N	-5.50	116.54	121.87
1	E	14	VAL	CA-CB-CG1	-5.49	101.06	110.40
2	n	34	GLY	O-C-N	5.49	128.88	122.45
2	n	60	VAL	N-CA-CB	-5.49	101.39	110.56
3	M	231	LYS	O-C-N	5.49	129.03	122.27
3	J	167	PHE	CA-C-O	-5.49	113.65	119.97
2	3	20	LYS	CA-C-O	5.49	125.99	119.56
1	b	239	ARG	CB-CG-CD	5.49	123.93	111.30
1	C	210	GLU	CA-C-N	-5.49	114.79	122.75
1	C	210	GLU	C-N-CA	-5.49	114.79	122.75
3	L	234	ALA	N-CA-C	5.49	116.61	109.64
1	d	33	ARG	N-CA-C	-5.49	106.42	113.23
1	G	197	GLY	CA-C-N	5.49	128.65	120.31
1	G	197	GLY	C-N-CA	5.49	128.65	120.31
1	c	123	TYR	CA-C-N	5.49	129.96	120.58
1	c	123	TYR	C-N-CA	5.49	129.96	120.58
1	D	235	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	1	20	LYS	N-CA-C	5.49	117.26	111.28
3	I	46	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	c	179	TYR	N-CA-CB	5.49	119.76	110.49
1	D	12	ILE	CA-C-O	-5.49	113.93	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ASN	CA-CB-CG	-5.49	107.11	112.60
2	l	186	ILE	N-CA-C	-5.49	100.16	108.17
1	A	242	GLU	CB-CG-CD	-5.48	103.28	112.60
2	k	35	ASN	CA-CB-CG	-5.48	107.12	112.60
3	I	252	ASN	CA-C-O	-5.48	115.18	122.03
1	D	221	PHE	CA-C-O	5.48	126.43	120.95
2	4	205	GLU	N-CA-CB	5.48	118.18	110.12
2	k	88	ARG	CA-CB-CG	5.48	125.06	114.10
2	m	71	LYS	CA-C-N	5.48	127.97	120.46
2	m	71	LYS	C-N-CA	5.48	127.97	120.46
3	I	28	ARG	O-C-N	5.48	127.93	122.12
1	c	194	VAL	N-CA-C	-5.48	105.19	110.72
2	l	65	PHE	CA-CB-CG	-5.48	108.32	113.80
2	h	39	SER	N-CA-CB	5.48	120.01	110.81
2	l	196	PHE	CB-CG-CD2	-5.48	111.39	120.70
3	H	250	ARG	CA-C-N	5.48	131.54	121.85
3	H	250	ARG	C-N-CA	5.48	131.54	121.85
2	l	112	ILE	N-CA-C	-5.48	100.44	108.11
1	d	236	ALA	CA-C-O	-5.47	114.75	120.55
2	h	104	PHE	CA-C-O	-5.47	114.64	120.28
2	7	180	SER	O-C-N	5.47	128.76	122.25
1	c	62	ASP	CA-CB-CG	5.47	118.07	112.60
1	d	31	VAL	CA-CB-CG2	5.47	119.70	110.40
1	E	203	GLU	CB-CG-CD	-5.47	103.30	112.60
2	2	159	ILE	N-CA-CB	5.47	117.04	110.31
2	k	38	ALA	N-CA-C	-5.47	101.04	109.52
3	K	397	PHE	O-C-N	5.47	130.58	122.81
3	K	298	LEU	N-CA-C	-5.47	106.44	113.23
1	e	143	GLU	N-CA-C	-5.47	99.15	110.80
1	e	186	ASP	CA-CB-CG	-5.47	107.13	112.60
2	m	32	THR	CA-CB-OG1	5.47	117.81	109.60
3	H	239	PHE	CA-CB-CG	-5.47	108.33	113.80
2	m	211	PHE	CA-CB-CG	-5.47	108.33	113.80
3	K	109	ASN	CA-CB-CG	5.47	118.07	112.60
1	C	33	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	D	229	LEU	CA-C-N	5.47	129.06	120.97
1	D	229	LEU	C-N-CA	5.47	129.06	120.97
2	l	134	GLU	N-CA-CB	5.47	120.34	110.83
3	I	258	ASP	CA-C-O	-5.47	115.08	120.82
3	K	364	ARG	N-CA-C	-5.47	106.11	112.89
3	L	62	PRO	O-C-N	5.47	130.02	122.64
3	L	317	ARG	CA-C-N	5.47	128.18	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	317	ARG	C-N-CA	5.47	128.18	120.42
1	A	223	GLU	CA-C-O	5.46	127.26	120.54
1	D	141	VAL	CB-CA-C	-5.46	103.89	110.99
1	D	237	ASN	N-CA-C	5.46	118.00	111.71
2	j	34	GLY	CA-C-N	5.46	127.60	120.28
2	j	34	GLY	C-N-CA	5.46	127.60	120.28
3	H	367	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	B	130	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	b	88	LEU	CB-CA-C	-5.46	101.56	110.85
1	A	17	PRO	N-CA-CB	-5.46	98.27	103.51
1	C	118	ASP	CA-C-N	5.46	127.60	120.28
1	C	118	ASP	C-N-CA	5.46	127.60	120.28
1	c	77	ALA	CA-C-O	-5.46	115.24	121.58
1	f	175	PHE	CA-C-N	5.46	128.05	120.29
1	f	175	PHE	C-N-CA	5.46	128.05	120.29
1	G	42	CYS	N-CA-C	-5.46	101.42	109.18
2	2	22	GLY	CA-C-N	5.46	130.10	122.23
2	2	22	GLY	C-N-CA	5.46	130.10	122.23
3	H	72	LEU	N-CA-CB	5.46	119.08	110.56
3	L	332	GLU	N-CA-C	-5.46	105.84	112.88
1	C	169	ASN	CA-C-O	-5.46	115.08	120.70
2	7	129	GLY	N-CA-C	-5.46	102.63	110.60
3	K	101	LYS	N-CA-C	-5.46	100.68	109.58
1	d	135	SER	N-CA-C	-5.46	101.06	109.52
1	d	33	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	G	192	GLY	N-CA-C	-5.45	107.90	114.66
2	1	43	LYS	CA-C-N	5.45	128.57	120.17
2	1	43	LYS	C-N-CA	5.45	128.57	120.17
3	H	137	GLU	N-CA-CB	5.45	119.90	111.39
1	e	232	TYR	CA-C-N	5.45	127.93	120.46
1	e	232	TYR	C-N-CA	5.45	127.93	120.46
2	n	18	VAL	N-CA-CB	5.45	118.08	110.56
3	K	61	PRO	CB-CA-C	-5.45	104.27	110.92
1	D	12	ILE	N-CA-C	-5.45	105.38	113.39
1	D	199	SER	CB-CA-C	-5.45	101.75	110.79
2	5	58	GLY	O-C-N	-5.45	115.62	122.70
3	L	159	LEU	CA-C-N	5.45	125.79	119.47
3	L	159	LEU	C-N-CA	5.45	125.79	119.47
2	1	23	VAL	N-CA-C	-5.45	101.16	108.35
2	1	161	VAL	CA-C-N	5.45	128.02	120.29
2	1	161	VAL	C-N-CA	5.45	128.02	120.29
2	7	67	ALA	CA-C-N	5.45	127.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	67	ALA	C-N-CA	5.45	127.58	120.28
3	L	116	VAL	O-C-N	5.45	129.17	123.02
3	L	149	GLN	CA-C-N	5.45	127.92	120.46
3	L	149	GLN	C-N-CA	5.45	127.92	120.46
1	a	98	ILE	N-CA-CB	5.44	117.54	110.57
1	B	92	ALA	CA-C-N	5.44	127.52	120.44
1	B	92	ALA	C-N-CA	5.44	127.52	120.44
2	5	53	ALA	N-CA-CB	-5.44	102.88	111.05
3	M	173	GLU	CA-C-N	5.44	123.58	119.66
3	M	173	GLU	C-N-CA	5.44	123.58	119.66
1	B	224	VAL	N-CA-CB	5.44	117.72	110.26
1	b	218	ASP	CA-CB-CG	5.44	118.04	112.60
1	G	132	PHE	N-CA-C	-5.44	102.42	110.48
1	G	168	ARG	CA-C-N	5.44	129.88	120.58
1	G	168	ARG	C-N-CA	5.44	129.88	120.58
1	g	150	THR	N-CA-C	-5.44	100.83	109.59
2	4	86	THR	N-CA-C	-5.44	102.41	110.46
2	4	178	ARG	N-CA-C	-5.44	106.69	113.38
2	5	146	THR	N-CA-CB	5.44	118.22	110.16
3	I	124	ASP	N-CA-C	-5.44	97.78	109.81
1	f	211	VAL	N-CA-C	-5.44	100.35	108.46
2	h	154	ARG	NE-CZ-NH1	-5.44	116.06	121.50
3	H	319	GLN	CA-C-O	5.44	126.23	119.97
1	a	205	VAL	CA-C-N	5.44	125.05	119.56
1	a	205	VAL	C-N-CA	5.44	125.05	119.56
1	g	174	PHE	O-C-N	-5.44	116.36	122.12
2	i	88	ARG	CA-C-O	-5.44	114.79	120.55
3	I	54	GLU	N-CA-CB	5.44	118.21	110.16
3	I	222	LEU	N-CA-CB	5.44	118.04	109.94
1	C	81	LEU	N-CA-CB	5.44	118.00	110.17
1	D	56	SER	CB-CA-C	5.44	121.24	110.42
1	c	14	VAL	CA-C-N	5.43	128.81	120.82
1	c	14	VAL	C-N-CA	5.43	128.81	120.82
2	3	152	GLU	CB-CG-CD	-5.43	103.36	112.60
2	3	202	GLU	CA-C-O	-5.43	115.08	120.90
3	H	387	THR	CA-C-O	-5.43	114.37	119.80
3	L	249	ARG	NE-CZ-NH1	5.43	126.94	121.50
3	J	34	LYS	CA-C-N	5.43	127.83	120.44
3	J	34	LYS	C-N-CA	5.43	127.83	120.44
3	J	195	VAL	CB-CA-C	-5.43	104.72	112.22
1	c	53	ARG	NE-CZ-NH1	-5.43	116.07	121.50
2	i	176	MET	O-C-N	-5.43	115.87	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	241	ARG	CA-C-N	5.43	129.86	120.58
1	a	241	ARG	C-N-CA	5.43	129.86	120.58
1	c	168	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	E	132	PHE	CB-CG-CD1	5.43	129.93	120.70
3	H	389	ILE	CA-C-N	5.43	125.42	120.21
3	H	389	ILE	C-N-CA	5.43	125.42	120.21
3	J	140	TYR	N-CA-CB	5.43	118.05	110.56
1	c	130	ARG	CA-C-O	-5.43	115.27	120.97
2	7	159	ILE	N-CA-C	-5.43	100.62	108.87
3	I	213	GLN	O-C-N	5.43	129.23	123.42
1	C	115	LYS	CA-C-O	5.43	126.19	119.79
3	K	85	PRO	CA-C-O	-5.43	114.66	122.31
3	L	333	ASP	CA-C-O	5.43	125.34	119.15
3	J	200	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	C	170	ALA	CB-CA-C	-5.42	101.63	110.85
1	D	233	VAL	N-CA-C	-5.42	105.09	110.62
1	g	79	SER	N-CA-C	-5.42	99.76	108.55
2	4	129	GLY	CA-C-N	5.42	129.45	121.96
2	4	129	GLY	C-N-CA	5.42	129.45	121.96
3	H	218	GLU	CA-C-N	5.42	127.11	120.22
3	H	218	GLU	C-N-CA	5.42	127.11	120.22
1	c	118	ASP	CA-C-N	5.42	127.49	120.44
1	c	118	ASP	C-N-CA	5.42	127.49	120.44
2	j	192	THR	CA-C-N	5.42	131.90	121.54
2	j	192	THR	C-N-CA	5.42	131.90	121.54
2	4	211	PHE	O-C-N	5.42	126.71	120.58
3	J	156	ALA	CB-CA-C	-5.42	101.63	110.85
1	e	226	PRO	N-CA-CB	5.42	109.37	103.30
1	G	151	ASP	N-CA-C	-5.42	103.80	110.31
2	m	186	ILE	CB-CA-C	5.42	119.41	111.33
3	I	35	LYS	CA-C-N	5.42	128.55	120.31
3	I	35	LYS	C-N-CA	5.42	128.55	120.31
3	K	61	PRO	CA-C-O	-5.42	112.70	120.56
3	K	252	ASN	CA-C-N	5.42	131.46	121.70
3	K	252	ASN	C-N-CA	5.42	131.46	121.70
3	M	173	GLU	CA-C-O	-5.42	114.65	119.75
1	A	103	TYR	CA-C-O	5.42	125.37	118.54
1	d	151	ASP	CB-CA-C	-5.42	100.98	109.22
2	3	193	GLU	N-CA-CB	5.42	119.65	110.49
2	l	196	PHE	CA-CB-CG	-5.42	108.38	113.80
2	n	104	PHE	CA-C-N	5.42	126.27	119.98
2	n	104	PHE	C-N-CA	5.42	126.27	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	234	ALA	O-C-N	-5.42	115.72	121.30
1	B	85	ALA	CA-C-N	5.42	127.54	120.28
1	B	85	ALA	C-N-CA	5.42	127.54	120.28
1	b	99	ASN	CA-CB-CG	-5.42	107.18	112.60
3	H	324	HIS	CA-C-N	5.42	128.54	120.31
3	H	324	HIS	C-N-CA	5.42	128.54	120.31
3	I	232	GLU	N-CA-CB	5.42	118.33	110.26
3	K	20	TYR	N-CA-C	-5.42	105.46	111.36
3	L	326	ARG	CA-C-O	5.42	126.29	120.55
1	g	130	ARG	CB-CG-CD	5.42	123.75	111.30
1	B	53	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	b	106	PRO	CA-C-O	-5.41	114.81	121.31
1	b	239	ARG	NE-CZ-NH1	-5.41	116.09	121.50
2	3	167	LEU	O-C-N	5.41	128.32	122.15
2	5	59	SER	CA-C-N	5.41	129.21	120.55
2	5	59	SER	C-N-CA	5.41	129.21	120.55
2	5	88	ARG	O-C-N	5.41	127.86	122.12
3	M	309	VAL	CA-C-O	5.41	124.64	119.98
1	D	191	LEU	CA-C-O	5.41	126.16	120.42
1	c	38	ILE	CA-C-N	5.41	125.33	121.65
1	c	38	ILE	C-N-CA	5.41	125.33	121.65
2	k	33	MET	CA-C-N	5.41	128.15	119.98
2	k	33	MET	C-N-CA	5.41	128.15	119.98
3	H	99	GLU	O-C-N	5.41	128.83	122.34
3	K	9	LEU	CA-C-N	5.41	128.53	120.31
3	K	9	LEU	C-N-CA	5.41	128.53	120.31
3	K	158	GLU	CA-C-N	5.41	126.85	120.09
3	K	158	GLU	C-N-CA	5.41	126.85	120.09
1	b	32	LYS	CA-C-N	5.41	127.97	120.29
1	b	32	LYS	C-N-CA	5.41	127.97	120.29
1	c	227	GLU	N-CA-C	5.41	117.26	111.36
1	G	171	VAL	CA-C-N	5.41	127.47	120.44
1	G	171	VAL	C-N-CA	5.41	127.47	120.44
1	g	159	TYR	CA-C-N	5.41	127.47	120.44
1	g	159	TYR	C-N-CA	5.41	127.47	120.44
3	H	147	ASP	CA-CB-CG	-5.41	107.19	112.60
3	I	294	ASP	CA-C-N	5.41	125.42	119.90
3	I	294	ASP	C-N-CA	5.41	125.42	119.90
2	2	23	VAL	N-CA-C	-5.41	100.69	108.42
3	K	19	ASP	CB-CA-C	-5.41	101.66	110.85
3	L	148	VAL	N-CA-C	5.41	115.61	110.53
2	h	165	VAL	N-CA-CB	5.40	117.49	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	138	VAL	N-CA-C	-5.40	100.70	108.48
1	c	68	TYR	CB-CA-C	-5.40	100.37	109.50
2	1	101	TYR	CB-CA-C	-5.40	103.82	111.76
2	2	72	ILE	CA-C-O	-5.40	115.12	120.85
2	6	88	ARG	CD-NE-CZ	-5.40	116.83	124.40
2	m	62	ASP	O-C-N	5.40	128.31	122.15
3	I	192	ALA	CA-C-N	5.40	128.52	120.31
3	I	192	ALA	C-N-CA	5.40	128.52	120.31
3	L	60	SER	CB-CA-C	-5.40	100.83	109.69
1	B	117	CYS	N-CA-C	5.40	117.17	111.28
1	b	90	ASP	CA-CB-CG	5.40	118.00	112.60
3	I	338	GLU	N-CA-C	-5.40	105.47	111.36
1	A	71	ASP	N-CA-C	-5.40	99.30	110.80
1	f	36	THR	CA-CB-OG1	5.40	117.70	109.60
1	d	242	GLU	N-CA-C	5.40	116.84	111.07
2	3	28	GLU	N-CA-C	-5.40	99.49	108.34
3	M	202	THR	CB-CA-C	5.40	118.68	109.72
2	1	169	VAL	CA-C-N	5.40	127.51	120.28
2	1	169	VAL	C-N-CA	5.40	127.51	120.28
2	2	192	THR	CA-C-N	5.40	130.22	122.40
2	2	192	THR	C-N-CA	5.40	130.22	122.40
2	n	202	GLU	CB-CG-CD	-5.40	103.43	112.60
1	A	100	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	244	LEU	N-CA-CB	5.39	118.76	110.61
1	D	142	ASP	CA-CB-CG	5.39	117.99	112.60
1	F	16	SER	CA-C-N	5.39	126.58	119.84
1	F	16	SER	C-N-CA	5.39	126.58	119.84
2	2	99	ASN	CA-C-O	5.39	126.27	120.55
2	6	45	ILE	N-CA-C	-5.39	101.23	108.35
2	1	43	LYS	N-CA-C	-5.39	102.30	110.28
2	6	206	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	C	40	ILE	N-CA-C	-5.39	100.30	108.17
1	e	49	ILE	N-CA-C	-5.39	100.72	108.48
1	B	142	ASP	CB-CA-C	5.39	119.24	110.24
2	3	165	VAL	CA-C-O	-5.39	115.14	120.85
3	M	13	LEU	N-CA-C	5.39	117.23	111.36
3	M	311	LEU	CA-C-N	5.39	125.40	119.90
3	M	311	LEU	C-N-CA	5.39	125.40	119.90
1	b	135	SER	N-CA-C	-5.39	100.99	109.50
2	1	104	PHE	N-CA-CB	5.39	116.80	110.71
2	7	71	LYS	CA-C-N	5.39	128.07	120.42
2	7	71	LYS	C-N-CA	5.39	128.07	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	121	GLN	OE1-CD-NE2	5.39	127.99	122.60
1	b	10	ARG	CB-CG-CD	5.39	123.69	111.30
1	G	63	THR	CA-C-O	-5.39	115.84	121.55
2	j	75	ASN	CA-C-N	5.39	128.50	120.31
2	j	75	ASN	C-N-CA	5.39	128.50	120.31
3	H	223	VAL	N-CA-C	5.39	115.59	110.42
3	H	319	GLN	O-C-N	-5.39	115.64	122.27
3	J	372	MET	CA-C-N	5.38	127.94	120.29
3	J	372	MET	C-N-CA	5.38	127.94	120.29
2	i	29	LYS	CG-CD-CE	5.38	123.68	111.30
2	4	190	LYS	N-CA-C	-5.38	100.13	108.90
3	L	381	LYS	CA-C-N	5.38	127.34	120.56
3	L	381	LYS	C-N-CA	5.38	127.34	120.56
3	H	170	VAL	N-CA-C	-5.38	107.18	111.81
3	K	174	PRO	N-CA-CB	5.38	108.30	103.08
1	F	208	ASN	O-C-N	5.38	128.55	122.20
1	f	56	SER	N-CA-C	-5.38	100.54	108.99
2	j	163	GLU	CA-C-N	5.38	129.83	120.68
2	j	163	GLU	C-N-CA	5.38	129.83	120.68
2	7	210	LYS	CA-C-N	5.38	130.66	122.37
2	7	210	LYS	C-N-CA	5.38	130.66	122.37
3	H	327	LYS	O-C-N	5.38	127.90	122.09
3	K	288	ASN	CA-CB-CG	5.38	117.98	112.60
1	D	45	GLY	N-CA-C	-5.38	103.17	110.43
1	e	198	LEU	N-CA-CB	5.38	118.21	110.20
1	F	48	LEU	N-CA-C	-5.38	99.17	108.69
1	f	59	LEU	N-CA-C	-5.38	101.21	109.76
2	5	68	ARG	NE-CZ-NH2	-5.38	114.36	119.20
2	l	210	LYS	CA-CB-CG	-5.38	103.34	114.10
2	7	33	MET	N-CA-C	-5.38	104.30	111.24
3	K	20	TYR	CA-C-N	5.38	128.03	120.28
3	K	20	TYR	C-N-CA	5.38	128.03	120.28
3	K	46	ARG	O-C-N	5.38	127.82	122.12
3	L	368	ALA	CA-C-O	5.38	126.30	120.55
3	J	47	GLU	CA-C-N	5.38	127.34	120.56
3	J	47	GLU	C-N-CA	5.38	127.34	120.56
1	E	96	ALA	N-CA-C	-5.38	105.46	112.23
3	L	348	GLY	O-C-N	5.38	127.94	122.24
3	J	29	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	E	202	SER	CA-C-O	5.38	127.47	121.40
3	M	156	ALA	CA-C-O	-5.38	114.27	120.24
1	a	169	ASN	O-C-N	5.37	127.82	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	181	ASP	N-CA-CB	5.37	116.53	110.35
1	B	172	THR	CA-C-N	5.37	127.74	120.38
1	B	172	THR	C-N-CA	5.37	127.74	120.38
2	1	103	TYR	N-CA-C	-5.37	106.57	113.23
3	I	190	LEU	N-CA-C	-5.37	105.50	111.36
3	H	47	GLU	O-C-N	-5.37	115.67	122.27
1	C	241	ARG	CA-C-N	5.37	127.91	120.29
1	C	241	ARG	C-N-CA	5.37	127.91	120.29
1	D	88	LEU	CA-C-N	5.37	129.10	120.30
1	D	88	LEU	C-N-CA	5.37	129.10	120.30
2	j	95	SER	CB-CA-C	-5.37	101.88	110.79
2	n	66	LEU	N-CA-CB	5.37	118.57	110.30
3	L	264	THR	CA-C-N	5.37	127.42	120.44
3	L	264	THR	C-N-CA	5.37	127.42	120.44
1	e	180	ARG	N-CA-C	-5.37	100.97	108.96
1	e	210	GLU	N-CA-C	-5.37	99.94	109.06
1	g	220	THR	N-CA-C	-5.37	96.90	107.69
2	l	72	ILE	CB-CA-C	5.37	119.38	112.14
2	n	66	LEU	CA-C-N	5.37	127.47	120.28
2	n	66	LEU	C-N-CA	5.37	127.47	120.28
3	K	43	ARG	CA-C-O	-5.37	115.19	120.82
1	A	136	LEU	N-CA-CB	5.36	119.43	110.85
1	B	74	ILE	O-C-N	-5.36	117.60	123.18
1	D	213	TYR	CA-C-N	5.36	130.23	123.10
1	D	213	TYR	C-N-CA	5.36	130.23	123.10
1	f	236	ALA	N-CA-C	5.36	117.20	111.36
1	B	115	LYS	CA-C-N	5.36	128.03	120.42
1	B	115	LYS	C-N-CA	5.36	128.03	120.42
2	3	205	GLU	CA-C-O	5.36	126.16	120.10
2	2	144	SER	N-CA-CB	5.36	118.00	110.12
2	k	164	ALA	CA-C-N	5.36	127.80	120.46
2	k	164	ALA	C-N-CA	5.36	127.80	120.46
1	B	141	VAL	O-C-N	5.36	128.72	122.99
1	e	11	ALA	O-C-N	5.36	128.65	123.29
3	J	222	LEU	CA-C-N	5.36	129.12	120.55
3	J	222	LEU	C-N-CA	5.36	129.12	120.55
1	F	26	TYR	CB-CG-CD1	-5.35	112.77	120.80
1	G	205	VAL	CA-C-N	5.35	125.07	119.82
1	G	205	VAL	C-N-CA	5.35	125.07	119.82
2	i	96	ASN	CA-C-N	5.35	127.89	120.29
2	i	96	ASN	C-N-CA	5.35	127.89	120.29
3	H	320	ILE	CA-C-N	5.35	127.45	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	320	ILE	C-N-CA	5.35	127.45	120.28
1	d	220	THR	O-C-N	-5.35	117.05	123.31
1	g	211	VAL	CA-C-O	5.35	126.65	120.76
2	j	158	GLU	N-CA-C	-5.35	106.53	113.16
3	J	231	LYS	N-CA-CB	5.35	118.08	110.16
2	j	205	GLU	CB-CA-C	-5.35	101.91	110.79
2	5	95	SER	N-CA-C	5.35	117.11	111.28
2	m	127	PRO	N-CA-CB	5.35	108.83	103.48
1	A	213	TYR	N-CA-CB	5.35	119.85	111.56
1	a	72	GLU	CB-CG-CD	-5.35	103.51	112.60
1	F	46	VAL	N-CA-C	-5.35	100.14	108.86
2	4	211	PHE	CB-CG-CD1	-5.35	111.61	120.70
2	k	83	ARG	CD-NE-CZ	-5.35	116.91	124.40
2	5	176	MET	N-CA-C	-5.35	104.54	111.71
3	H	45	GLU	CA-C-N	5.35	127.45	120.28
3	H	45	GLU	C-N-CA	5.35	127.45	120.28
3	K	241	ASP	N-CA-CB	5.35	119.15	110.43
3	M	317	ARG	N-CA-C	-5.35	105.35	111.07
1	f	197	GLY	CA-C-N	5.35	127.88	120.29
1	f	197	GLY	C-N-CA	5.35	127.88	120.29
3	M	171	GLY	CA-C-O	5.35	125.65	119.13
1	A	239	ARG	N-CA-C	-5.34	105.50	112.23
1	F	159	TYR	CA-C-O	-5.34	115.13	121.60
3	L	312	PRO	CA-C-N	5.34	130.59	121.29
3	L	312	PRO	C-N-CA	5.34	130.59	121.29
3	M	224	ARG	NE-CZ-NH2	-5.34	114.39	119.20
3	J	305	ARG	N-CA-CB	5.34	119.13	110.42
1	B	214	VAL	CA-C-O	5.34	125.67	120.27
1	B	63	THR	O-C-N	5.34	130.11	123.01
1	B	226	PRO	CA-C-N	5.34	127.88	120.29
1	B	226	PRO	C-N-CA	5.34	127.88	120.29
1	e	23	GLN	CA-C-N	5.34	128.00	120.42
1	e	23	GLN	C-N-CA	5.34	128.00	120.42
1	f	232	TYR	N-CA-C	5.34	117.18	111.36
2	1	71	LYS	O-C-N	5.34	127.64	122.09
2	2	135	LYS	N-CA-C	-5.34	106.44	113.17
2	j	36	PHE	CA-C-N	5.34	129.93	122.93
2	j	36	PHE	C-N-CA	5.34	129.93	122.93
3	M	184	PRO	CA-C-O	-5.34	115.32	121.36
1	F	41	LYS	CA-C-N	5.34	132.51	123.01
1	F	41	LYS	C-N-CA	5.34	132.51	123.01
2	4	176	MET	CA-C-O	5.34	125.95	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	224	ARG	N-CA-CB	-5.34	102.27	110.12
3	I	57	ARG	CA-C-N	5.34	127.70	120.44
3	I	57	ARG	C-N-CA	5.34	127.70	120.44
2	2	142	SER	CA-C-O	5.34	125.73	119.06
2	j	70	ILE	CB-CA-C	5.34	119.58	112.22
2	4	98	LEU	N-CA-CB	5.33	117.96	110.12
3	I	139	SER	N-CA-C	-5.33	101.61	109.18
3	L	202	THR	CB-CA-C	5.33	117.47	110.06
3	M	356	THR	N-CA-C	-5.33	105.55	111.36
1	c	188	ALA	CA-C-N	5.33	127.37	120.44
1	c	188	ALA	C-N-CA	5.33	127.37	120.44
2	6	81	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	M	127	VAL	CA-C-N	5.33	127.42	120.28
3	M	127	VAL	C-N-CA	5.33	127.42	120.28
2	n	179	ASP	CA-CB-CG	-5.33	107.27	112.60
1	e	241	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	h	151	LEU	O-C-N	5.33	127.77	122.12
2	3	69	ILE	CB-CA-C	-5.33	105.15	111.97
2	l	155	PHE	CA-CB-CG	5.33	119.13	113.80
2	6	132	ILE	N-CA-C	-5.33	101.02	108.80
2	7	171	ALA	CA-C-N	5.33	127.99	120.42
2	7	171	ALA	C-N-CA	5.33	127.99	120.42
2	n	40	LYS	N-CA-C	-5.33	105.55	111.36
3	K	198	GLN	O-C-N	-5.33	115.30	122.23
3	M	194	ALA	CA-C-N	5.33	127.98	120.42
3	M	194	ALA	C-N-CA	5.33	127.98	120.42
1	D	93	ARG	N-CA-C	-5.33	105.37	111.07
1	E	44	GLU	N-CA-C	-5.33	106.46	113.17
1	b	141	VAL	CB-CA-C	-5.32	103.21	110.77
1	F	154	GLY	N-CA-C	-5.32	107.68	115.72
2	i	66	LEU	N-CA-C	5.32	117.08	111.28
3	J	119	LEU	CB-CA-C	-5.32	102.76	109.31
1	D	153	SER	CA-C-O	5.32	126.15	120.24
1	d	143	GLU	CA-C-N	5.32	131.97	122.13
1	d	143	GLU	C-N-CA	5.32	131.97	122.13
1	E	35	ALA	CA-C-N	5.32	129.30	120.94
1	E	35	ALA	C-N-CA	5.32	129.30	120.94
2	h	196	PHE	CA-C-O	5.32	127.92	120.52
2	5	136	ASP	CA-CB-CG	5.32	117.92	112.60
3	J	278	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	162	THR	CA-CB-OG1	5.32	117.58	109.60
1	G	99	ASN	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	240	ILE	N-CA-C	-5.32	100.22	107.99
3	L	297	ILE	O-C-N	5.32	127.03	121.87
1	F	216	VAL	CA-C-O	5.32	123.76	119.29
2	1	109	GLN	N-CA-C	-5.32	99.85	108.52
2	3	109	GLN	N-CA-C	-5.32	100.23	108.90
3	I	131	GLU	CA-C-N	5.32	131.27	121.70
3	I	131	GLU	C-N-CA	5.32	131.27	121.70
1	C	213	TYR	N-CA-C	5.32	116.93	108.79
1	c	169	ASN	CB-CA-C	-5.32	101.81	110.85
1	e	240	ILE	CA-CB-CG2	5.32	119.54	110.50
2	4	202	GLU	N-CA-CB	5.32	117.86	109.94
3	I	253	SER	CB-CA-C	-5.32	100.00	110.10
3	I	321	PHE	CA-C-N	5.32	127.72	120.54
3	I	321	PHE	C-N-CA	5.32	127.72	120.54
3	M	322	LYS	CB-CG-CD	5.32	123.53	111.30
1	A	67	ILE	N-CA-C	-5.32	98.29	109.34
1	c	86	ARG	CD-NE-CZ	-5.32	116.96	124.40
1	c	181	ASP	CA-CB-CG	-5.32	107.28	112.60
1	c	215	LYS	CB-CA-C	-5.32	98.86	109.33
2	4	35	ASN	CA-CB-CG	-5.32	107.28	112.60
2	m	24	VAL	N-CA-C	-5.32	100.83	108.48
2	7	193	GLU	N-CA-CB	5.32	119.47	110.49
3	H	272	LEU	CA-C-N	5.32	130.44	121.14
3	H	272	LEU	C-N-CA	5.32	130.44	121.14
3	L	130	PHE	N-CA-C	-5.32	105.65	111.82
3	I	237	ILE	CA-C-N	5.31	130.17	123.10
3	I	237	ILE	C-N-CA	5.31	130.17	123.10
3	K	240	ILE	N-CA-C	-5.31	99.99	107.75
3	L	174	PRO	N-CA-C	5.31	116.27	110.58
1	E	28	ARG	N-CA-CB	5.31	118.30	110.33
1	F	216	VAL	CA-CB-CG2	-5.31	101.37	110.40
2	1	118	GLU	N-CA-C	-5.31	105.16	111.69
2	j	137	ILE	CA-C-N	5.31	131.53	121.97
2	j	137	ILE	C-N-CA	5.31	131.53	121.97
2	l	152	GLU	CB-CG-CD	-5.31	103.57	112.60
2	6	84	LYS	N-CA-C	5.31	116.39	109.64
2	n	178	ARG	NE-CZ-NH1	-5.31	116.19	121.50
3	L	278	ARG	CA-C-N	5.31	131.82	121.41
3	L	278	ARG	C-N-CA	5.31	131.82	121.41
3	M	392	LEU	N-CA-C	-5.31	99.44	108.26
1	a	225	SER	N-CA-C	-5.31	103.24	110.36
1	b	132	PHE	CA-CB-CG	-5.31	108.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	104	PHE	CA-C-O	-5.31	114.49	119.91
3	I	383	LEU	CA-C-O	-5.31	114.92	120.55
1	B	154	GLY	CA-C-N	5.31	130.63	122.93
1	B	154	GLY	C-N-CA	5.31	130.63	122.93
3	J	384	LYS	CA-C-N	5.31	127.34	120.44
3	J	384	LYS	C-N-CA	5.31	127.34	120.44
1	B	17	PRO	CA-C-N	5.31	131.93	122.06
1	B	17	PRO	C-N-CA	5.31	131.93	122.06
2	n	117	SER	CA-C-O	-5.31	114.92	120.55
3	J	83	THR	CA-C-N	5.31	130.20	121.87
3	J	83	THR	C-N-CA	5.31	130.20	121.87
3	J	355	CYS	O-C-N	5.31	127.54	122.07
1	B	183	LEU	CA-C-N	5.31	131.66	122.64
1	B	183	LEU	C-N-CA	5.31	131.66	122.64
2	h	125	ILE	N-CA-CB	5.31	117.36	110.99
3	H	340	ALA	N-CA-C	-5.31	105.50	111.28
1	d	53	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	G	206	PRO	CB-CA-C	-5.30	103.87	111.62
3	J	367	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	a	62	ASP	CA-CB-CG	5.30	117.90	112.60
1	E	73	HIS	CA-CB-CG	-5.30	108.50	113.80
2	3	68	ARG	NE-CZ-NH2	-5.30	114.43	119.20
2	4	161	VAL	CA-C-N	5.30	127.82	120.29
2	4	161	VAL	C-N-CA	5.30	127.82	120.29
3	K	173	GLU	O-C-N	-5.30	114.91	121.64
1	C	106	PRO	CA-C-N	5.30	131.51	121.97
1	C	106	PRO	C-N-CA	5.30	131.51	121.97
3	K	321	PHE	CA-C-N	5.30	127.70	120.54
3	K	321	PHE	C-N-CA	5.30	127.70	120.54
3	L	123	LYS	O-C-N	5.30	126.78	121.85
1	F	35	ALA	CA-C-N	5.30	129.26	120.94
1	F	35	ALA	C-N-CA	5.30	129.26	120.94
2	h	162	ASP	CA-CB-CG	-5.30	107.30	112.60
2	m	75	ASN	N-CA-C	5.30	116.74	111.07
2	m	117	SER	N-CA-CB	5.30	117.91	110.12
3	K	152	GLU	O-C-N	5.30	127.74	122.12
3	M	268	LEU	N-CA-CB	5.30	118.00	110.16
1	g	144	VAL	N-CA-C	-5.30	101.31	107.61
2	l	73	GLU	N-CA-C	5.30	117.05	111.28
2	l	90	ILE	CA-C-N	5.30	127.81	120.29
2	l	90	ILE	C-N-CA	5.30	127.81	120.29
2	m	101	TYR	CA-C-O	-5.30	113.07	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	206	VAL	N-CA-CB	5.30	119.26	111.52
1	G	200	ILE	CA-C-O	-5.30	113.79	119.35
2	3	165	VAL	CA-CB-CG1	-5.30	101.40	110.40
2	6	79	ILE	N-CA-C	5.30	115.51	110.53
3	I	352	LYS	CA-C-O	5.30	126.16	120.55
3	J	118	VAL	N-CA-CB	5.30	120.80	110.95
1	B	83	ALA	CA-C-O	-5.29	115.44	121.00
2	m	193	GLU	CA-C-N	-5.29	111.43	121.54
2	m	193	GLU	C-N-CA	-5.29	111.43	121.54
3	L	384	LYS	CA-CB-CG	5.29	124.69	114.10
1	F	112	LEU	CA-C-N	5.29	127.37	120.28
1	F	112	LEU	C-N-CA	5.29	127.37	120.28
2	i	124	SER	N-CA-C	-5.29	100.77	109.40
2	k	83	ARG	NE-CZ-NH1	-5.29	116.21	121.50
2	l	78	GLU	CB-CG-CD	-5.29	103.60	112.60
3	J	236	SER	N-CA-CB	5.29	119.76	111.56
1	A	172	THR	CA-CB-CG2	5.29	119.50	110.50
2	m	27	THR	N-CA-C	-5.29	101.25	109.14
2	7	101	TYR	CB-CG-CD1	-5.29	112.86	120.80
3	I	112	THR	CA-C-N	5.29	130.46	122.68
3	I	112	THR	C-N-CA	5.29	130.46	122.68
1	b	240	ILE	CA-C-N	5.29	127.37	120.28
1	b	240	ILE	C-N-CA	5.29	127.37	120.28
1	c	92	ALA	N-CA-CB	5.29	117.68	110.01
3	J	228	GLN	CA-C-N	5.29	127.80	120.29
3	J	228	GLN	C-N-CA	5.29	127.80	120.29
1	d	160	LYS	O-C-N	5.29	128.68	122.34
1	e	144	VAL	CA-C-N	5.29	125.20	119.76
1	e	144	VAL	C-N-CA	5.29	125.20	119.76
1	F	68	TYR	O-C-N	5.29	129.50	123.31
2	7	212	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	a	56	SER	CA-C-N	5.29	128.34	120.31
1	a	56	SER	C-N-CA	5.29	128.34	120.31
1	d	23	GLN	OE1-CD-NE2	5.29	127.89	122.60
3	I	300	PRO	CA-C-N	5.29	130.20	120.79
3	I	300	PRO	C-N-CA	5.29	130.20	120.79
3	K	40	GLU	N-CA-CB	5.29	118.47	110.28
1	b	239	ARG	N-CA-C	5.28	117.95	111.82
1	d	215	LYS	N-CA-C	-5.28	101.92	110.32
1	e	40	ILE	CA-CB-CG1	5.28	119.38	110.40
2	3	71	LYS	CA-C-N	5.28	127.70	120.46
2	3	71	LYS	C-N-CA	5.28	127.70	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	291	ASP	CB-CA-C	-5.28	101.79	110.72
1	b	123	TYR	N-CA-CB	5.28	118.52	110.44
3	J	317	ARG	CB-CA-C	-5.28	101.87	110.85
1	f	69	LYS	CA-C-N	5.28	128.58	122.35
1	f	69	LYS	C-N-CA	5.28	128.58	122.35
1	C	87	VAL	N-CA-C	5.28	116.05	110.72
1	f	73	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	f	93	ARG	N-CA-C	-5.28	105.61	111.36
3	M	201	ALA	CA-C-N	5.28	128.21	120.71
3	M	201	ALA	C-N-CA	5.28	128.21	120.71
1	A	105	GLU	O-C-N	-5.28	116.70	121.66
1	d	226	PRO	CA-C-N	5.28	127.88	120.28
1	d	226	PRO	C-N-CA	5.28	127.88	120.28
2	2	42	ALA	O-C-N	5.28	128.87	122.85
2	7	22	GLY	CA-C-O	5.28	127.54	121.47
2	7	85	PRO	N-CD-CG	5.28	111.12	103.20
3	H	9	LEU	CA-C-O	5.28	129.77	120.80
3	I	23	LEU	CA-C-N	5.28	127.35	120.28
3	I	23	LEU	C-N-CA	5.28	127.35	120.28
3	K	218	GLU	CA-C-O	5.28	126.01	120.42
3	K	320	ILE	CA-C-O	-5.28	115.25	120.85
1	A	115	LYS	O-C-N	-5.28	115.18	122.46
1	G	90	ASP	N-CA-C	-5.28	105.44	111.14
2	j	71	LYS	CA-C-N	5.28	127.69	120.46
2	j	71	LYS	C-N-CA	5.28	127.69	120.46
2	n	161	VAL	N-CA-C	-5.28	104.37	111.44
3	M	312	PRO	N-CA-CB	5.27	107.89	103.25
1	D	149	GLU	CB-CA-C	-5.27	101.70	110.14
2	j	163	GLU	N-CA-CB	5.27	118.24	110.33
3	J	364	ARG	CA-C-O	5.27	126.01	120.42
3	I	254	ASP	CA-C-O	5.27	126.93	120.55
1	B	194	VAL	N-CA-CB	5.27	117.06	110.47
1	D	171	VAL	CA-C-O	-5.27	114.56	120.25
2	i	88	ARG	CA-C-N	5.27	127.29	120.44
2	i	88	ARG	C-N-CA	5.27	127.29	120.44
2	4	51	ARG	O-C-N	5.27	129.32	122.15
2	l	70	ILE	CB-CA-C	-5.27	105.22	111.97
2	7	119	GLY	O-C-N	5.27	129.55	122.70
3	H	109	ASN	N-CA-CB	5.27	117.60	110.38
3	L	116	VAL	CA-C-O	-5.27	116.41	121.63
2	7	90	ILE	CA-C-O	5.27	126.43	120.85
2	7	211	PHE	N-CA-C	-5.27	105.51	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	364	ARG	NE-CZ-NH1	-5.27	116.23	121.50
3	M	63	LEU	N-CA-C	-5.27	100.81	109.40
3	K	388	PRO	N-CA-C	-5.27	101.97	110.55
1	B	48	LEU	N-CA-C	-5.26	99.86	108.76
1	f	125	GLN	N-CA-CB	5.26	117.95	110.16
2	4	94	THR	N-CA-C	5.26	117.02	111.28
2	5	58	GLY	CA-C-O	5.26	129.73	120.57
3	I	269	LEU	CA-C-N	5.26	127.60	120.44
3	I	269	LEU	C-N-CA	5.26	127.60	120.44
3	L	99	GLU	CB-CG-CD	-5.26	103.65	112.60
3	J	393	LYS	CA-C-N	5.26	131.73	121.41
3	J	393	LYS	C-N-CA	5.26	131.73	121.41
1	c	184	SER	CA-C-N	5.26	127.33	120.28
1	c	184	SER	C-N-CA	5.26	127.33	120.28
1	d	126	TYR	N-CA-CB	5.26	118.29	110.29
2	h	156	THR	O-C-N	-5.26	118.34	121.71
2	j	85	PRO	N-CA-CB	5.26	108.22	103.33
2	6	165	VAL	CA-CB-CG1	-5.26	101.45	110.40
3	H	321	PHE	CA-C-N	5.26	127.86	120.28
3	H	321	PHE	C-N-CA	5.26	127.86	120.28
3	J	130	PHE	N-CA-C	-5.26	98.67	107.99
1	A	25	GLU	CA-C-N	5.26	128.30	120.31
1	A	25	GLU	C-N-CA	5.26	128.30	120.31
1	a	103	TYR	N-CA-C	-5.26	107.88	114.56
1	a	130	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	C	137	LEU	N-CA-C	-5.26	99.95	108.52
1	c	79	SER	N-CA-C	-5.26	100.73	108.99
2	3	112	ILE	CA-C-O	-5.26	114.87	120.39
2	n	86	THR	N-CA-C	-5.26	101.30	109.72
1	b	108	THR	CA-C-O	-5.26	115.27	121.16
1	d	239	ARG	NE-CZ-NH1	-5.26	116.24	121.50
2	2	25	MET	N-CA-C	-5.26	101.30	109.24
2	j	167	LEU	CA-C-N	5.26	127.76	120.29
2	j	167	LEU	C-N-CA	5.26	127.76	120.29
3	H	258	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	60	GLU	CB-CA-C	5.26	118.94	109.64
1	b	58	LEU	N-CA-C	-5.26	106.71	113.23
1	b	145	PRO	O-C-N	5.26	128.99	123.10
1	E	36	THR	N-CA-C	5.26	117.91	110.50
2	4	85	PRO	N-CA-CB	5.26	108.33	103.39
2	7	150	VAL	O-C-N	5.26	127.37	121.90
3	K	152	GLU	CB-CG-CD	-5.26	103.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	27	THR	N-CA-C	-5.25	101.37	109.52
2	6	133	GLU	N-CA-C	-5.25	101.55	109.85
3	M	26	LEU	N-CA-CB	5.25	117.63	110.01
1	e	26	TYR	CB-CG-CD1	5.25	128.68	120.80
1	e	103	TYR	N-CA-C	-5.25	107.89	114.56
3	H	372	MET	CA-C-N	5.25	127.27	120.44
3	H	372	MET	C-N-CA	5.25	127.27	120.44
1	d	81	LEU	N-CA-CB	5.25	117.72	109.69
1	E	206	PRO	N-CA-C	-5.25	109.22	114.68
1	F	143	GLU	N-CA-C	-5.25	107.53	114.04
2	1	22	GLY	CA-C-N	5.25	130.49	122.25
2	1	22	GLY	C-N-CA	5.25	130.49	122.25
2	j	175	ALA	CA-C-N	5.25	127.32	120.28
2	j	175	ALA	C-N-CA	5.25	127.32	120.28
2	l	189	VAL	N-CA-C	-5.25	100.30	108.86
3	I	140	TYR	CB-CG-CD2	-5.25	112.92	120.80
3	L	286	ALA	N-CA-CB	5.25	120.64	111.13
3	M	220	ALA	CA-C-N	5.25	128.70	120.82
3	M	220	ALA	C-N-CA	5.25	128.70	120.82
1	A	201	GLU	N-CA-C	5.25	118.83	111.74
3	K	93	GLN	N-CA-C	-5.25	105.16	112.30
1	d	137	LEU	N-CA-C	-5.25	99.86	108.41
1	e	230	LYS	CA-C-N	5.25	124.57	118.85
1	e	230	LYS	C-N-CA	5.25	124.57	118.85
3	M	249	ARG	N-CA-C	-5.25	99.89	108.76
1	A	16	SER	O-C-N	-5.25	113.67	121.12
1	F	37	ALA	N-CA-C	-5.25	99.78	108.75
2	j	144	SER	N-CA-C	5.25	118.47	111.75
2	k	80	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	m	85	PRO	O-C-N	5.25	129.72	122.64
1	b	15	PHE	N-CA-C	-5.24	101.32	109.24
1	c	90	ASP	CA-C-N	5.24	127.26	120.44
1	c	90	ASP	C-N-CA	5.24	127.26	120.44
2	4	88	ARG	CD-NE-CZ	-5.24	117.06	124.40
3	J	387	THR	N-CA-CB	5.24	119.70	110.37
2	k	192	THR	CA-C-N	5.24	130.00	122.35
2	k	192	THR	C-N-CA	5.24	130.00	122.35
1	F	92	ALA	N-CA-CB	5.24	118.40	110.28
2	k	92	THR	CA-CB-OG1	-5.24	101.74	109.60
2	k	170	ARG	CA-C-N	5.24	127.73	120.29
2	k	170	ARG	C-N-CA	5.24	127.73	120.29
2	5	192	THR	N-CA-C	-5.24	106.57	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	35	ASN	N-CA-C	-5.24	104.33	111.56
2	m	86	THR	CA-C-N	5.24	128.75	120.47
2	m	86	THR	C-N-CA	5.24	128.75	120.47
3	I	289	ARG	N-CA-CB	5.24	119.41	110.71
3	J	21	TYR	N-CA-CB	5.24	117.91	110.16
1	C	15	PHE	CA-C-O	-5.24	115.43	121.19
1	f	147	LEU	N-CA-C	-5.24	100.16	109.06
2	h	202	GLU	N-CA-C	5.24	116.67	111.07
3	M	150	ILE	CA-CB-CG2	5.24	119.40	110.50
1	E	211	VAL	O-C-N	5.24	128.91	123.26
1	G	10	ARG	O-C-N	5.24	128.12	122.15
2	m	104	PHE	CA-C-N	5.24	125.53	119.93
2	m	104	PHE	C-N-CA	5.24	125.53	119.93
3	I	44	TYR	CB-CA-C	-5.24	101.95	110.85
3	I	110	GLN	O-C-N	5.24	127.67	122.12
1	C	225	SER	N-CA-CB	5.23	117.93	110.03
1	E	28	ARG	N-CA-C	-5.23	106.04	112.90
1	g	128	GLY	N-CA-C	-5.23	106.67	115.62
3	L	363	ILE	O-C-N	5.23	127.34	121.90
1	B	46	VAL	CA-C-N	5.23	130.26	122.99
1	B	46	VAL	C-N-CA	5.23	130.26	122.99
2	i	202	GLU	N-CA-C	5.23	117.39	111.11
2	k	71	LYS	CA-C-N	5.23	127.63	120.46
2	k	71	LYS	C-N-CA	5.23	127.63	120.46
2	l	162	ASP	CA-C-N	5.23	129.53	120.58
2	l	162	ASP	C-N-CA	5.23	129.53	120.58
3	I	369	LYS	N-CA-C	-5.23	101.35	109.72
3	L	394	GLY	CA-C-O	-5.23	115.13	122.51
1	C	63	THR	CA-C-O	5.23	125.39	119.27
2	j	45	ILE	CA-CB-CG1	5.23	119.29	110.40
2	m	140	THR	N-CA-C	-5.23	100.50	109.24
2	7	82	GLU	CB-CG-CD	-5.23	103.71	112.60
1	a	104	ASP	N-CA-CB	5.23	119.86	111.91
1	G	29	GLU	CA-C-N	5.23	127.81	120.28
1	G	29	GLU	C-N-CA	5.23	127.81	120.28
2	5	139	ALA	N-CA-C	-5.23	101.35	109.24
2	m	167	LEU	CA-C-N	5.23	127.71	120.29
2	m	167	LEU	C-N-CA	5.23	127.71	120.29
3	K	303	PHE	CA-C-N	5.23	131.52	121.54
3	K	303	PHE	C-N-CA	5.23	131.52	121.54
2	l	102	ARG	NE-CZ-NH2	5.23	123.90	119.20
2	k	97	LEU	N-CA-C	-5.23	105.48	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	316	GLY	O-C-N	5.23	127.21	122.19
3	I	321	PHE	CB-CA-C	-5.23	102.11	110.79
3	L	385	LYS	O-C-N	5.23	129.13	122.39
3	J	61	PRO	O-C-N	5.23	123.61	121.15
1	b	150	THR	N-CA-C	-5.22	101.64	109.95
2	k	198	GLN	OE1-CD-NE2	5.22	127.82	122.60
3	H	367	ARG	CG-CD-NE	-5.22	100.51	112.00
3	L	130	PHE	N-CA-CB	5.22	118.38	110.28
1	f	196	MET	CA-C-N	5.22	125.78	119.98
1	f	196	MET	C-N-CA	5.22	125.78	119.98
2	2	154	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	A	73	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	a	186	ASP	N-CA-CB	5.22	117.89	110.16
1	c	132	PHE	CB-CA-C	5.22	119.07	109.46
2	k	21	ASP	N-CA-C	-5.22	105.20	112.30
3	I	363	ILE	O-C-N	5.22	127.21	121.83
1	b	47	ILE	N-CA-CB	5.22	118.61	111.41
1	C	91	ARG	N-CA-CB	5.22	117.58	110.01
1	c	65	GLU	N-CA-CB	5.22	117.94	110.06
1	D	146	LYS	CA-C-O	-5.22	114.34	120.60
2	3	68	ARG	CA-C-N	5.22	127.14	120.56
2	3	68	ARG	C-N-CA	5.22	127.14	120.56
3	K	23	LEU	CA-C-N	5.22	127.27	120.28
3	K	23	LEU	C-N-CA	5.22	127.27	120.28
3	J	302	ARG	CB-CA-C	-5.22	101.05	110.23
2	1	91	ALA	N-CA-CB	5.22	117.88	110.16
2	2	204	VAL	CA-CB-CG2	-5.22	101.53	110.40
2	3	153	ASP	N-CA-C	-5.22	105.51	111.14
2	3	169	VAL	CA-CB-CG1	5.22	119.27	110.40
3	K	47	GLU	CA-C-N	5.22	127.13	120.56
3	K	47	GLU	C-N-CA	5.22	127.13	120.56
3	K	278	ARG	CD-NE-CZ	-5.22	117.10	124.40
3	J	14	LYS	CA-C-N	5.22	127.27	120.28
3	J	14	LYS	C-N-CA	5.22	127.27	120.28
1	b	180	ARG	CB-CA-C	-5.21	99.10	109.79
1	c	217	ASP	N-CA-CB	5.21	118.36	110.28
1	e	233	VAL	CA-C-O	-5.21	115.53	120.95
2	2	73	GLU	N-CA-C	5.21	117.87	111.82
2	5	63	ALA	CA-C-N	5.21	127.69	120.29
2	5	63	ALA	C-N-CA	5.21	127.69	120.29
3	L	28	ARG	N-CA-C	-5.21	105.49	111.07
1	F	123	TYR	CA-CB-CG	-5.21	104.52	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	174	SER	CB-CA-C	-5.21	102.14	110.79
3	K	225	GLU	CA-C-O	-5.21	115.35	120.82
3	H	63	LEU	N-CA-C	-5.21	100.41	108.90
3	J	70	ASP	O-C-N	-5.21	117.79	123.26
1	G	61	ALA	CA-C-O	5.21	125.58	119.28
1	g	155	ALA	N-CA-CB	5.21	118.76	110.16
2	n	201	PRO	CA-C-N	5.21	127.57	120.54
2	n	201	PRO	C-N-CA	5.21	127.57	120.54
3	L	55	VAL	CA-C-O	-5.21	115.65	121.17
1	f	16	SER	N-CA-C	-5.21	102.47	110.07
1	g	211	VAL	N-CA-C	-5.21	100.74	108.45
2	h	60	VAL	CA-C-N	5.21	125.61	119.94
2	h	60	VAL	C-N-CA	5.21	125.61	119.94
2	k	103	TYR	N-CA-C	-5.21	106.32	113.30
2	7	184	ASP	CA-CB-CG	-5.21	107.39	112.60
3	J	301	GLY	O-C-N	5.21	129.47	122.70
2	h	132	ILE	N-CA-C	-5.21	99.00	107.28
2	k	81	ARG	CA-C-N	5.21	129.95	122.40
2	k	81	ARG	C-N-CA	5.21	129.95	122.40
2	5	38	ALA	N-CA-CB	5.21	117.56	110.01
2	m	201	PRO	N-CA-C	5.21	123.19	112.47
3	M	336	PHE	CA-C-O	-5.21	112.99	119.18
3	J	74	ASP	CA-CB-CG	5.21	117.81	112.60
1	d	83	ALA	CA-C-O	-5.20	115.34	120.70
2	3	92	THR	CA-C-N	5.20	127.25	120.28
2	3	92	THR	C-N-CA	5.20	127.25	120.28
2	m	72	ILE	N-CA-C	5.20	115.93	110.62
1	f	205	VAL	N-CA-C	-5.20	97.64	108.88
2	3	151	LEU	N-CA-C	5.20	116.95	111.28
1	c	140	GLY	N-CA-C	-5.20	102.59	111.27
1	G	232	TYR	N-CA-CB	5.20	117.77	110.12
3	H	67	VAL	N-CA-C	-5.20	100.58	108.17
1	d	172	THR	N-CA-C	-5.20	105.69	111.36
1	G	97	GLN	N-CA-C	-5.20	105.79	111.82
2	i	82	GLU	CA-C-O	5.20	127.43	120.98
2	l	148	TYR	CA-C-O	5.20	126.06	120.55
3	L	391	ASP	N-CA-CB	5.20	119.28	110.49
2	i	174	SER	CA-C-N	5.20	127.24	120.28
2	i	174	SER	C-N-CA	5.20	127.24	120.28
2	3	129	GLY	CA-C-N	5.20	131.60	121.41
2	3	129	GLY	C-N-CA	5.20	131.60	121.41
2	7	65	PHE	CB-CA-C	-5.20	102.96	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	119	LEU	CA-C-N	5.20	125.20	119.90
3	L	119	LEU	C-N-CA	5.20	125.20	119.90
1	e	14	VAL	O-C-N	-5.19	116.08	122.57
1	e	182	ASP	N-CA-C	-5.19	106.72	113.16
2	2	118	GLU	CB-CA-C	-5.19	101.02	110.63
3	I	382	VAL	N-CA-C	5.19	115.41	110.42
1	B	144	VAL	N-CA-C	-5.19	104.93	109.19
1	c	141	VAL	O-C-N	-5.19	117.46	123.07
2	l	194	ASP	CA-CB-CG	5.19	117.79	112.60
2	6	181	ALA	N-CA-C	5.19	117.36	111.02
2	i	189	VAL	N-CA-C	-5.19	100.90	108.17
2	1	180	SER	N-CA-C	-5.19	106.35	113.30
2	l	60	VAL	N-CA-CB	5.19	116.62	110.55
3	H	135	LYS	CA-C-N	5.19	126.33	119.84
3	H	135	LYS	C-N-CA	5.19	126.33	119.84
1	e	67	ILE	CA-C-N	5.19	130.45	122.93
1	e	67	ILE	C-N-CA	5.19	130.45	122.93
2	4	101	TYR	N-CA-CB	5.19	118.02	110.65
2	l	170	ARG	N-CA-CB	5.19	117.75	110.12
3	M	72	LEU	CA-C-N	5.19	131.10	122.54
3	M	72	LEU	C-N-CA	5.19	131.10	122.54
2	h	167	LEU	CA-C-N	5.19	127.65	120.29
2	h	167	LEU	C-N-CA	5.19	127.65	120.29
1	a	192	GLY	N-CA-C	-5.18	106.42	113.37
1	b	86	ARG	CA-C-N	5.18	127.56	120.46
1	b	86	ARG	C-N-CA	5.18	127.56	120.46
1	c	86	ARG	N-CA-C	5.18	116.93	111.28
1	e	99	ASN	CA-C-N	5.18	127.75	120.28
1	e	99	ASN	C-N-CA	5.18	127.75	120.28
2	2	82	GLU	CA-C-O	-5.18	112.80	119.59
2	7	157	PRO	CB-CA-C	5.18	115.62	109.92
2	n	204	VAL	N-CA-CB	-5.18	102.80	110.58
3	H	30	LEU	CA-C-N	5.18	127.18	120.44
3	H	30	LEU	C-N-CA	5.18	127.18	120.44
3	M	88	VAL	N-CA-CB	5.18	118.43	111.90
3	M	201	ALA	N-CA-CB	-5.18	103.27	111.05
3	J	225	GLU	CA-C-N	5.18	129.21	120.29
3	J	225	GLU	C-N-CA	5.18	129.21	120.29
1	E	144	VAL	CB-CA-C	-5.18	104.29	109.89
1	e	195	ALA	N-CA-C	5.18	116.93	111.28
2	i	166	GLU	CA-C-N	5.18	127.22	120.28
2	i	166	GLU	C-N-CA	5.18	127.22	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	37	ILE	O-C-N	-5.18	117.16	123.02
3	M	275	PHE	N-CA-C	-5.18	99.76	110.80
1	g	67	ILE	CA-CB-CG1	-5.18	101.59	110.40
2	3	156	THR	N-CA-C	-5.18	100.06	108.82
3	K	345	GLY	N-CA-C	-5.18	106.58	115.08
2	j	95	SER	CA-C-N	5.18	127.22	120.28
2	j	95	SER	C-N-CA	5.18	127.22	120.28
2	5	156	THR	N-CA-C	-5.18	100.08	109.09
3	I	141	GLU	N-CA-CB	5.18	118.15	110.49
3	L	288	ASN	OD1-CG-ND2	-5.18	117.42	122.60
3	J	241	ASP	CA-C-O	-5.18	114.93	120.42
1	f	55	GLY	CA-C-N	5.18	131.01	121.85
1	f	55	GLY	C-N-CA	5.18	131.01	121.85
3	K	179	LEU	O-C-N	-5.18	116.72	122.93
3	L	315	GLU	CA-C-O	5.18	125.91	120.42
1	a	108	THR	N-CA-CB	5.18	117.62	110.17
1	e	45	GLY	N-CA-C	-5.18	103.03	110.38
1	f	194	VAL	CA-C-O	-5.18	115.57	120.95
2	2	187	ASP	N-CA-C	5.18	118.66	109.96
1	d	98	ILE	N-CA-CB	5.17	117.58	110.54
1	e	184	SER	N-CA-C	-5.17	102.80	110.46
2	2	68	ARG	CB-CA-C	-5.17	102.05	110.85
2	2	208	LEU	N-CA-C	-5.17	106.56	112.92
3	H	78	VAL	CA-C-O	-5.17	114.99	121.04
3	J	360	MET	CA-C-N	5.17	127.21	120.28
3	J	360	MET	C-N-CA	5.17	127.21	120.28
2	i	191	ILE	CA-C-N	5.17	131.74	122.38
2	i	191	ILE	C-N-CA	5.17	131.74	122.38
2	5	182	SER	CA-C-O	5.17	126.05	119.95
2	7	166	GLU	CA-C-N	5.17	129.43	120.58
2	7	166	GLU	C-N-CA	5.17	129.43	120.58
3	J	319	GLN	CA-C-N	5.17	127.55	120.46
3	J	319	GLN	C-N-CA	5.17	127.55	120.46
1	b	94	ILE	CA-C-N	5.17	127.21	120.28
1	b	94	ILE	C-N-CA	5.17	127.21	120.28
1	e	173	GLU	CA-C-O	-5.17	114.94	120.42
1	F	42	CYS	N-CA-C	-5.17	101.84	109.18
2	i	132	ILE	O-C-N	5.17	128.61	123.18
1	E	136	LEU	N-CA-C	-5.17	101.33	109.50
1	G	149	GLU	N-CA-C	-5.17	100.97	109.40
2	3	89	ALA	CB-CA-C	-5.17	102.11	110.79
3	J	156	ALA	N-CA-CB	5.17	117.81	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASP	CB-CA-C	-5.17	102.73	110.90
1	f	242	GLU	CB-CA-C	-5.17	102.21	110.79
2	3	49	ALA	N-CA-CB	5.17	118.67	110.87
1	B	207	GLU	N-CA-CB	-5.17	102.72	110.73
1	e	132	PHE	N-CA-CB	5.17	117.63	109.83
1	g	12	ILE	CA-CB-CG2	5.17	119.28	110.50
3	H	179	LEU	CB-CA-C	5.17	118.66	109.72
3	I	278	ARG	N-CA-C	-5.17	101.22	109.07
3	I	377	LYS	CA-C-N	5.17	127.62	120.29
3	I	377	LYS	C-N-CA	5.17	127.62	120.29
3	M	158	GLU	CB-CA-C	-5.17	102.74	110.90
1	a	93	ARG	N-CA-CB	5.17	117.71	110.12
1	E	12	ILE	CA-C-O	5.17	124.67	119.20
2	i	177	LYS	N-CA-C	5.17	116.91	111.28
2	l	143	GLY	CA-C-N	5.17	128.86	120.60
2	l	143	GLY	C-N-CA	5.17	128.86	120.60
2	7	98	LEU	O-C-N	-5.17	116.64	122.12
1	f	222	LYS	N-CA-CB	5.16	120.28	111.66
2	1	197	TYR	CA-CB-CG	-5.16	104.60	113.90
2	k	44	LYS	N-CA-C	-5.16	105.33	113.02
3	I	342	ILE	O-C-N	5.16	127.15	121.83
3	K	302	ARG	N-CA-C	-5.16	107.65	114.31
3	K	150	ILE	O-C-N	-5.16	116.51	121.83
3	J	311	LEU	CA-C-N	5.16	125.44	119.92
3	J	311	LEU	C-N-CA	5.16	125.44	119.92
1	a	63	THR	CA-CB-OG1	5.16	117.34	109.60
1	b	159	TYR	O-C-N	5.16	129.94	123.23
2	i	203	GLU	CA-C-N	5.16	127.75	120.42
2	i	203	GLU	C-N-CA	5.16	127.75	120.42
2	l	200	SER	CA-C-N	5.16	126.29	119.84
2	l	200	SER	C-N-CA	5.16	126.29	119.84
2	n	115	ILE	N-CA-CB	5.16	118.53	111.41
3	L	249	ARG	NE-CZ-NH2	-5.16	114.56	119.20
3	M	27	TYR	CA-C-N	5.16	127.46	120.44
3	M	27	TYR	C-N-CA	5.16	127.46	120.44
3	M	375	PHE	N-CA-CB	5.16	117.49	110.01
1	d	34	GLY	O-C-N	5.16	126.73	122.71
1	e	73	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	g	24	VAL	O-C-N	5.16	126.87	121.87
2	3	211	PHE	O-C-N	5.16	128.29	122.20
2	j	174	SER	CA-CB-OG	-5.16	100.78	111.10
2	4	111	LEU	CA-C-O	5.16	125.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	267	GLN	CA-C-O	-5.16	113.70	119.79
3	K	211	PHE	N-CA-C	-5.16	101.47	109.72
1	c	172	THR	O-C-N	5.16	128.03	122.15
1	g	67	ILE	CA-C-O	-5.16	115.03	120.39
2	h	18	VAL	CA-C-O	-5.16	115.06	120.57
2	2	210	LYS	N-CA-C	-5.16	106.50	112.89
2	n	51	ARG	NE-CZ-NH2	5.16	123.84	119.20
3	I	44	TYR	CA-C-N	5.16	127.19	120.28
3	I	44	TYR	C-N-CA	5.16	127.19	120.28
3	K	263	ARG	CA-C-O	5.16	125.90	119.97
3	J	112	THR	CA-C-N	5.16	130.72	122.93
3	J	112	THR	C-N-CA	5.16	130.72	122.93
3	J	290	ILE	CA-C-N	-5.16	115.51	123.14
3	J	290	ILE	C-N-CA	-5.16	115.51	123.14
1	a	94	ILE	N-CA-C	-5.15	105.38	111.00
2	4	75	ASN	CA-CB-CG	5.15	117.75	112.60
2	4	94	THR	N-CA-CB	5.15	117.70	110.12
2	4	167	LEU	CA-C-N	5.15	127.19	120.28
2	4	167	LEU	C-N-CA	5.15	127.19	120.28
2	j	171	ALA	N-CA-CB	-5.15	102.53	110.16
2	k	106	TYR	N-CA-CB	5.15	118.69	110.65
3	J	10	LEU	CA-C-N	5.15	127.19	120.28
3	J	10	LEU	C-N-CA	5.15	127.19	120.28
3	J	364	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	a	230	LYS	CA-C-O	-5.15	113.89	118.63
2	3	20	LYS	O-C-N	-5.15	116.16	122.34
2	l	81	ARG	NE-CZ-NH1	-5.15	116.35	121.50
3	M	387	THR	N-CA-C	-5.15	97.33	108.81
1	a	129	VAL	N-CA-CB	5.15	117.17	110.99
3	I	230	ALA	CA-C-N	5.15	127.69	120.28
3	I	230	ALA	C-N-CA	5.15	127.69	120.28
3	M	46	ARG	CB-CA-C	-5.15	102.24	110.79
3	H	395	VAL	CB-CA-C	-5.15	104.82	111.20
3	I	388	PRO	CA-C-N	5.15	131.65	122.13
3	I	388	PRO	C-N-CA	5.15	131.65	122.13
3	L	76	ARG	CD-NE-CZ	-5.15	117.19	124.40
3	M	320	ILE	CA-C-O	5.15	126.31	120.85
2	1	81	ARG	CA-C-O	5.15	124.48	118.97
2	h	94	THR	CA-C-N	5.15	127.17	120.28
2	h	94	THR	C-N-CA	5.15	127.17	120.28
2	2	182	SER	N-CA-C	-5.15	101.94	109.81
3	M	351	ILE	CA-C-O	5.15	126.31	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	101	LEU	O-C-N	5.14	127.65	122.09
2	n	83	ARG	NE-CZ-NH1	-5.14	116.36	121.50
3	L	385	LYS	CA-C-O	-5.14	113.20	119.43
1	a	100	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	6	156	THR	CA-C-O	-5.14	115.55	120.64
3	L	260	GLU	N-CA-C	-5.14	107.39	113.97
3	J	82	SER	N-CA-C	-5.14	106.59	112.92
1	a	117	CYS	O-C-N	5.14	127.57	122.12
2	2	151	LEU	CA-C-N	5.14	129.31	120.72
2	2	151	LEU	C-N-CA	5.14	129.31	120.72
2	k	148	TYR	O-C-N	-5.14	116.67	122.12
3	M	386	THR	N-CA-C	-5.14	99.85	110.80
1	C	115	LYS	CA-CB-CG	-5.14	103.82	114.10
1	D	225	SER	N-CA-CB	5.14	116.87	109.78
1	f	69	LYS	N-CA-CB	-5.14	101.49	109.87
2	h	162	ASP	N-CA-C	-5.14	107.01	113.28
2	5	39	SER	CA-C-N	5.14	127.48	120.54
2	5	39	SER	C-N-CA	5.14	127.48	120.54
3	L	171	GLY	N-CA-C	-5.14	101.00	113.18
3	L	213	GLN	CA-C-N	5.14	129.42	120.68
3	L	213	GLN	C-N-CA	5.14	129.42	120.68
3	L	397	PHE	N-CA-C	-5.14	107.04	113.72
2	k	130	GLY	CA-C-N	-5.14	112.90	121.94
2	k	130	GLY	C-N-CA	-5.14	112.90	121.94
2	5	164	ALA	N-CA-CB	5.14	118.21	110.30
1	d	202	SER	O-C-N	-5.14	117.92	123.42
1	E	232	TYR	N-CA-CB	5.14	117.67	110.12
2	1	59	SER	CB-CA-C	5.14	118.25	109.72
3	K	336	PHE	CB-CG-CD2	-5.14	111.97	120.70
1	A	68	TYR	CB-CA-C	-5.13	100.85	109.48
1	F	18	ASP	CA-C-O	-5.13	112.94	119.31
1	F	106	PRO	CB-CA-C	5.13	118.04	111.21
3	K	296	ALA	CB-CA-C	-5.13	101.23	110.37
3	K	308	GLU	CA-C-O	-5.13	114.84	120.69
3	M	133	GLU	N-CA-C	-5.13	106.77	112.57
1	C	219	ARG	NE-CZ-NH1	5.13	126.63	121.50
2	h	59	SER	CA-C-N	5.13	127.71	120.42
2	h	59	SER	C-N-CA	5.13	127.71	120.42
2	2	60	VAL	N-CA-C	5.13	115.35	110.42
2	2	154	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	5	23	VAL	N-CA-C	-5.13	101.24	108.27
1	F	25	GLU	O-C-N	-5.13	116.30	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	99	ASN	CA-CB-CG	5.13	117.73	112.60
2	l	44	LYS	N-CA-C	-5.13	105.03	113.50
2	j	91	ALA	CB-CA-C	-5.13	102.27	110.79
3	I	358	ALA	CA-C-N	5.13	125.64	120.00
3	I	358	ALA	C-N-CA	5.13	125.64	120.00
3	L	388	PRO	O-C-N	5.13	129.57	122.64
3	J	322	LYS	N-CA-CB	5.13	117.66	110.12
1	b	196	MET	CA-C-N	5.13	125.63	119.94
1	b	196	MET	C-N-CA	5.13	125.63	119.94
1	g	228	GLU	CA-C-N	5.13	127.15	120.28
1	g	228	GLU	C-N-CA	5.13	127.15	120.28
1	g	82	VAL	CA-C-O	-5.13	114.93	120.47
2	6	75	ASN	CA-C-N	5.13	127.15	120.28
2	6	75	ASN	C-N-CA	5.13	127.15	120.28
1	C	67	ILE	N-CA-C	-5.13	98.68	109.34
1	d	212	GLY	N-CA-C	-5.13	103.55	112.06
2	3	102	ARG	N-CA-C	-5.13	106.80	113.16
2	n	62	ASP	O-C-N	-5.13	116.31	122.15
3	I	299	ARG	N-CA-CB	5.13	117.21	110.29
3	I	315	GLU	CA-C-N	5.13	125.64	120.00
3	I	315	GLU	C-N-CA	5.13	125.64	120.00
3	J	359	GLY	O-C-N	-5.13	116.69	122.28
1	c	179	TYR	N-CA-C	-5.12	99.88	110.80
1	d	89	ILE	CB-CA-C	5.12	120.56	112.26
1	f	164	ILE	O-C-N	-5.12	117.35	123.04
2	l	109	GLN	N-CA-C	-5.12	100.55	108.90
2	m	144	SER	CA-C-O	-5.12	115.44	120.82
1	F	8	TYR	CB-CG-CD2	5.12	128.48	120.80
1	F	134	VAL	N-CA-C	-5.12	100.50	108.95
2	l	104	PHE	O-C-N	-5.12	116.41	121.17
2	h	187	ASP	N-CA-C	-5.12	101.81	109.95
2	l	87	VAL	CB-CA-C	5.12	119.06	112.14
2	n	155	PHE	N-CA-CB	5.12	118.61	110.16
3	I	30	LEU	CA-C-N	5.12	127.41	120.44
3	I	30	LEU	C-N-CA	5.12	127.41	120.44
3	J	147	ASP	CB-CA-C	-5.12	100.37	110.10
1	e	84	ASP	CA-CB-CG	-5.12	107.48	112.60
1	f	120	LYS	CA-C-N	5.12	127.65	120.28
1	f	120	LYS	C-N-CA	5.12	127.65	120.28
1	G	163	ALA	N-CA-C	-5.12	101.33	108.96
2	l	30	ARG	N-CA-C	-5.12	100.11	108.76
2	i	192	THR	CA-CB-OG1	5.12	117.28	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	92	THR	CA-C-N	5.12	127.56	120.29
2	j	92	THR	C-N-CA	5.12	127.56	120.29
2	m	143	GLY	CA-C-N	5.12	127.09	120.44
2	m	143	GLY	C-N-CA	5.12	127.09	120.44
3	I	243	LEU	N-CA-C	-5.12	104.65	111.87
1	c	214	VAL	N-CA-C	-5.12	100.75	108.12
2	l	74	ALA	O-C-N	-5.12	116.32	122.15
3	K	195	VAL	N-CA-C	5.12	115.89	110.72
3	M	118	VAL	CA-CB-CG1	5.12	119.10	110.40
1	c	228	GLU	O-C-N	-5.12	116.32	122.15
1	g	98	ILE	O-C-N	5.12	127.10	121.83
2	m	190	LYS	CA-C-N	5.12	128.22	122.59
2	m	190	LYS	C-N-CA	5.12	128.22	122.59
2	7	25	MET	N-CA-C	-5.12	101.52	109.24
3	K	321	PHE	CA-C-O	-5.12	115.13	120.55
3	M	55	VAL	N-CA-C	-5.12	105.51	110.42
1	A	100	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	245	LYS	N-CA-CB	5.11	118.64	110.46
1	g	170	ALA	CA-C-N	5.11	127.47	120.46
1	g	170	ALA	C-N-CA	5.11	127.47	120.46
2	2	58	GLY	O-C-N	-5.11	117.86	124.15
2	m	204	VAL	CA-C-N	5.11	127.64	120.28
2	m	204	VAL	C-N-CA	5.11	127.64	120.28
1	D	141	VAL	N-CA-C	5.11	115.41	107.28
2	3	48	ILE	N-CA-C	-5.11	106.81	111.67
3	K	21	TYR	CB-CG-CD1	5.11	128.47	120.80
3	L	46	ARG	CA-C-O	5.11	125.85	119.97
1	B	156	LEU	CA-C-O	-5.11	114.86	120.43
2	i	28	GLU	CA-C-O	5.11	126.80	120.92
3	I	27	TYR	CB-CG-CD2	5.11	128.47	120.80
3	K	114	ALA	N-CA-CB	5.11	119.13	110.49
1	d	46	VAL	CB-CA-C	5.11	118.35	110.28
1	G	101	LEU	N-CA-C	5.11	116.93	111.36
3	I	121	THR	N-CA-C	-5.11	99.65	108.69
3	J	158	GLU	CA-C-N	5.11	127.11	120.26
3	J	158	GLU	C-N-CA	5.11	127.11	120.26
2	i	108	VAL	O-C-N	-5.11	118.53	122.97
2	j	27	THR	CA-CB-CG2	5.11	119.18	110.50
2	5	193	GLU	N-CA-CB	5.11	120.23	112.47
2	6	161	VAL	CA-CB-CG2	5.11	119.08	110.40
2	m	22	GLY	O-C-N	-5.11	117.92	124.00
2	7	116	ASP	N-CA-C	-5.11	101.69	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	320	ILE	CA-C-N	5.11	127.08	120.44
3	M	320	ILE	C-N-CA	5.11	127.08	120.44
1	a	100	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
2	h	80	ARG	N-CA-C	5.11	116.65	111.14
2	3	180	SER	CA-C-O	5.11	126.01	120.55
2	6	37	ILE	CA-C-N	5.11	127.54	120.29
2	6	37	ILE	C-N-CA	5.11	127.54	120.29
3	L	40	GLU	CA-C-N	5.11	127.54	120.29
3	L	40	GLU	C-N-CA	5.11	127.54	120.29
3	L	273	ASP	N-CA-C	-5.11	101.53	109.14
3	M	61	PRO	N-CA-C	5.11	116.93	110.70
3	M	245	ALA	N-CA-C	-5.11	106.18	114.09
3	L	41	ARG	NE-CZ-NH1	-5.10	116.40	121.50
3	J	18	GLU	N-CA-C	5.10	116.84	111.28
1	B	130	ARG	CA-C-N	5.10	126.22	119.84
1	B	130	ARG	C-N-CA	5.10	126.22	119.84
2	h	97	LEU	CA-C-N	5.10	128.06	120.31
2	h	97	LEU	C-N-CA	5.10	128.06	120.31
2	l	34	GLY	O-C-N	5.10	128.96	122.58
2	m	85	PRO	N-CA-C	5.10	122.98	112.47
3	K	127	VAL	CA-CB-CG1	-5.10	101.72	110.40
3	K	259	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	e	190	VAL	N-CA-CB	5.10	117.48	110.54
2	j	109	GLN	OE1-CD-NE2	-5.10	117.50	122.60
2	l	110	LEU	CA-C-O	5.10	126.92	121.16
2	6	153	ASP	CA-C-O	-5.10	115.14	120.55
2	n	68	ARG	CA-C-N	5.10	126.99	120.56
2	n	68	ARG	C-N-CA	5.10	126.99	120.56
3	M	371	THR	CA-CB-OG1	5.10	117.25	109.60
1	C	27	ALA	CA-C-O	5.10	125.63	119.11
1	F	87	VAL	CA-C-N	5.10	127.53	120.29
1	F	87	VAL	C-N-CA	5.10	127.53	120.29
1	f	102	THR	CA-C-O	5.10	125.31	119.35
2	1	210	LYS	O-C-N	5.10	129.16	122.33
2	k	97	LEU	N-CA-CB	5.10	117.40	110.01
2	l	212	ARG	O-C-N	-5.10	115.81	122.59
3	I	51	LEU	CA-C-N	5.10	127.11	120.28
3	I	51	LEU	C-N-CA	5.10	127.11	120.28
3	J	76	ARG	CA-C-O	-5.10	115.48	121.44
1	A	90	ASP	N-CA-CB	5.09	117.46	110.07
1	B	109	VAL	CA-C-N	5.09	127.11	120.28
1	B	109	VAL	C-N-CA	5.09	127.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	VAL	CA-C-O	5.09	126.57	121.17
1	D	186	ASP	N-CA-C	5.09	116.91	111.36
1	e	152	PRO	N-CD-CG	5.09	110.84	103.20
1	F	73	HIS	CG-CD2-NE2	5.09	112.29	107.20
2	6	118	GLU	CA-C-N	5.09	131.39	121.41
2	6	118	GLU	C-N-CA	5.09	131.39	121.41
2	6	131	ALA	CA-C-N	5.09	130.26	122.92
2	6	131	ALA	C-N-CA	5.09	130.26	122.92
3	H	113	LEU	O-C-N	-5.09	115.82	122.59
2	1	145	LEU	N-CA-CB	5.09	117.39	110.01
2	h	49	ALA	CA-C-O	5.09	126.76	121.36
2	h	146	THR	N-CA-C	5.09	116.64	111.14
2	j	47	GLN	OE1-CD-NE2	-5.09	117.51	122.60
3	L	31	GLU	CA-C-N	5.09	127.52	120.29
3	L	31	GLU	C-N-CA	5.09	127.52	120.29
3	L	350	ASP	CB-CA-C	-5.09	102.34	110.79
1	G	29	GLU	CB-CG-CD	-5.09	103.95	112.60
1	g	103	TYR	CB-CA-C	-5.09	100.83	109.38
1	g	185	PHE	CA-CB-CG	-5.09	108.71	113.80
3	K	199	THR	N-CA-CB	5.09	117.45	110.07
3	M	48	VAL	N-CA-C	5.09	117.45	111.09
1	A	16	SER	N-CA-CB	5.09	116.17	109.55
1	D	172	THR	N-CA-C	-5.09	105.63	111.07
1	e	116	ILE	CA-CB-CG1	5.09	119.05	110.40
2	3	83	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	c	94	ILE	CB-CA-C	-5.09	105.20	112.22
2	2	163	GLU	N-CA-C	-5.09	107.12	113.38
2	4	132	ILE	CA-CB-CG2	-5.09	101.85	110.50
2	n	86	THR	N-CA-CB	5.09	119.78	111.08
3	J	17	GLU	O-C-N	5.09	127.31	122.07
2	6	66	LEU	CA-C-N	5.08	128.04	120.31
2	6	66	LEU	C-N-CA	5.08	128.04	120.31
1	g	196	MET	CG-SD-CE	-5.08	89.72	100.90
2	i	133	GLU	N-CA-CB	5.08	117.92	110.35
1	e	224	VAL	CA-CB-CG1	-5.08	101.76	110.40
1	F	50	ALA	CA-C-N	5.08	128.69	121.42
1	F	50	ALA	C-N-CA	5.08	128.69	121.42
1	g	194	VAL	CA-CB-CG2	-5.08	101.76	110.40
2	l	122	ILE	CA-C-O	-5.08	114.98	120.67
2	l	140	THR	N-CA-CB	5.08	117.50	109.83
3	I	267	GLN	CA-C-N	5.08	127.05	120.44
3	I	267	GLN	C-N-CA	5.08	127.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	144	VAL	CA-C-N	5.08	124.99	119.76
1	c	144	VAL	C-N-CA	5.08	124.99	119.76
2	i	114	GLY	CA-C-N	5.08	130.17	122.91
2	i	114	GLY	C-N-CA	5.08	130.17	122.91
2	5	43	LYS	CA-C-O	-5.08	114.84	120.38
2	6	59	SER	CA-C-N	5.08	127.42	120.46
2	6	59	SER	C-N-CA	5.08	127.42	120.46
3	I	134	GLU	CB-CG-CD	-5.08	103.97	112.60
1	a	150	THR	CA-C-N	-5.08	116.65	123.96
1	a	150	THR	C-N-CA	-5.08	116.65	123.96
1	G	200	ILE	O-C-N	5.08	126.78	122.16
2	2	17	LEU	N-CA-C	-5.08	101.02	108.99
2	k	86	THR	N-CA-CB	5.08	119.77	111.08
2	l	161	VAL	CA-C-N	5.08	127.50	120.29
2	l	161	VAL	C-N-CA	5.08	127.50	120.29
3	I	121	THR	N-CA-CB	5.08	119.34	110.81
3	K	308	GLU	N-CA-C	-5.08	101.69	109.76
3	J	324	HIS	CA-C-N	5.08	127.08	120.28
3	J	324	HIS	C-N-CA	5.08	127.08	120.28
1	F	30	ALA	O-C-N	5.08	127.94	122.15
1	B	68	TYR	CA-C-N	5.08	127.98	120.82
1	B	68	TYR	C-N-CA	5.08	127.98	120.82
1	b	119	PHE	CA-C-N	5.08	127.50	120.29
1	b	119	PHE	C-N-CA	5.08	127.50	120.29
1	b	220	THR	CA-C-N	5.08	131.24	121.54
1	b	220	THR	C-N-CA	5.08	131.24	121.54
2	3	205	GLU	O-C-N	-5.08	116.28	122.22
2	5	114	GLY	N-CA-C	-5.08	103.85	110.45
3	K	198	GLN	OE1-CD-NE2	5.08	127.68	122.60
3	K	286	ALA	N-CA-CB	5.08	119.14	110.71
3	M	146	LEU	N-CA-C	-5.08	103.99	111.81
1	D	227	GLU	N-CA-C	5.07	116.62	111.14
2	h	157	PRO	N-CA-C	-5.07	107.42	114.27
2	5	203	GLU	O-C-N	-5.07	116.37	122.15
3	I	311	LEU	CA-C-O	-5.07	114.77	120.25
3	M	130	PHE	N-CA-C	-5.07	105.82	112.41
3	J	385	LYS	N-CA-C	5.07	116.50	111.07
1	b	245	LYS	CA-C-N	5.07	130.83	121.70
1	b	245	LYS	C-N-CA	5.07	130.83	121.70
1	F	152	PRO	CA-C-N	5.07	128.02	120.31
1	F	152	PRO	C-N-CA	5.07	128.02	120.31
2	l	78	GLU	N-CA-CB	5.07	117.66	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	392	LEU	N-CA-C	5.07	121.60	110.80
1	F	172	THR	CA-C-N	5.07	127.49	120.29
1	F	172	THR	C-N-CA	5.07	127.49	120.29
1	G	64	ILE	O-C-N	-5.07	117.68	123.10
1	G	183	LEU	N-CA-CB	5.07	117.51	110.26
2	1	167	LEU	CA-C-N	5.07	127.07	120.28
2	1	167	LEU	C-N-CA	5.07	127.07	120.28
2	3	96	ASN	O-C-N	5.07	127.49	122.12
1	a	63	THR	CA-C-O	5.07	124.62	119.05
1	c	138	ILE	N-CA-C	-5.07	101.08	108.17
1	a	180	ARG	N-CA-C	-5.07	101.59	109.24
1	e	73	HIS	CE1-NE2-CD2	-5.07	103.94	109.00
2	h	43	LYS	CA-C-N	5.07	129.83	122.08
2	h	43	LYS	C-N-CA	5.07	129.83	122.08
2	5	148	TYR	O-C-N	-5.07	116.85	122.07
2	6	30	ARG	CD-NE-CZ	-5.07	117.31	124.40
3	J	181	TYR	N-CA-CB	5.07	120.12	111.66
3	H	52	ARG	CD-NE-CZ	-5.06	117.31	124.40
2	2	69	ILE	CB-CA-C	-5.06	105.49	111.97
2	n	196	PHE	CA-CB-CG	-5.06	108.74	113.80
3	I	131	GLU	CA-C-O	-5.06	115.86	121.33
3	M	13	LEU	CA-C-N	5.06	127.06	120.28
3	M	13	LEU	C-N-CA	5.06	127.06	120.28
3	J	148	VAL	CB-CA-C	-5.06	105.31	112.14
2	4	191	ILE	N-CA-C	-5.06	99.23	107.28
3	H	241	ASP	N-CA-CB	5.06	118.43	110.23
3	I	180	LEU	N-CA-CB	5.06	118.52	110.57
1	B	237	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	g	113	ALA	O-C-N	-5.06	116.05	122.27
2	k	87	VAL	CA-C-N	5.06	127.06	120.28
2	k	87	VAL	C-N-CA	5.06	127.06	120.28
3	H	210	GLU	N-CA-C	-5.06	105.77	111.28
3	I	148	VAL	CA-C-N	5.06	129.99	121.14
3	I	148	VAL	C-N-CA	5.06	129.99	121.14
3	K	378	ALA	CA-C-N	5.06	127.61	120.42
3	K	378	ALA	C-N-CA	5.06	127.61	120.42
3	M	353	ALA	O-C-N	5.06	127.48	122.12
1	F	196	MET	N-CA-C	5.06	116.87	111.36
2	h	123	TYR	CA-CB-CG	-5.06	104.80	113.90
2	j	155	PHE	CA-CB-CG	-5.06	108.74	113.80
2	5	117	SER	N-CA-C	5.06	118.55	112.38
3	I	364	ARG	N-CA-C	5.06	117.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	69	SER	N-CA-C	-5.06	104.76	112.04
2	n	67	ALA	CB-CA-C	-5.06	102.40	110.79
3	J	315	GLU	N-CA-C	5.06	116.87	111.36
1	C	20	ARG	N-CA-C	-5.05	100.03	110.80
1	f	165	GLY	N-CA-C	-5.05	104.86	112.84
2	5	211	PHE	CB-CA-C	-5.05	102.02	110.56
2	6	87	VAL	CB-CA-C	-5.05	105.32	112.14
2	m	196	PHE	CA-CB-CG	-5.05	108.75	113.80
2	n	102	ARG	NE-CZ-NH1	-5.05	116.45	121.50
3	I	265	MET	CA-C-N	5.05	127.05	120.28
3	I	265	MET	C-N-CA	5.05	127.05	120.28
1	d	73	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	E	240	ILE	O-C-N	5.05	126.77	121.87
2	2	27	THR	CA-CB-OG1	5.05	117.18	109.60
3	M	152	GLU	CA-C-N	5.05	127.38	120.46
3	M	152	GLU	C-N-CA	5.05	127.38	120.46
1	C	158	GLU	CA-CB-CG	5.05	124.20	114.10
1	c	59	LEU	N-CA-CB	5.05	118.10	110.42
1	d	233	VAL	CA-CB-CG2	-5.05	101.81	110.40
1	e	111	GLU	CA-C-N	5.05	127.01	120.44
1	e	111	GLU	C-N-CA	5.05	127.01	120.44
1	F	36	THR	N-CA-C	5.05	117.62	110.50
2	j	165	VAL	CA-C-O	5.05	126.20	120.95
3	L	107	ALA	N-CA-C	-5.05	101.69	109.52
1	a	77	ALA	N-CA-C	-5.05	102.42	109.69
1	a	185	PHE	CA-C-N	5.05	127.46	120.29
1	a	185	PHE	C-N-CA	5.05	127.46	120.29
1	E	203	GLU	CA-C-O	-5.05	116.01	121.87
2	5	132	ILE	N-CA-CB	5.05	118.03	111.67
3	J	44	TYR	CA-C-O	-5.05	115.07	120.42
1	a	25	GLU	O-C-N	-5.05	116.87	122.07
1	f	174	PHE	CA-C-N	5.05	129.97	121.14
1	f	174	PHE	C-N-CA	5.05	129.97	121.14
2	n	128	ILE	N-CA-C	-5.05	105.62	110.72
3	L	13	LEU	CA-C-N	5.05	127.46	120.29
3	L	13	LEU	C-N-CA	5.05	127.46	120.29
1	c	116	ILE	CA-CB-CG1	5.05	118.98	110.40
2	k	73	GLU	CA-C-O	-5.05	115.07	120.42
3	J	167	PHE	CA-C-N	5.05	127.45	120.29
3	J	167	PHE	C-N-CA	5.05	127.45	120.29
1	b	90	ASP	N-CA-C	-5.04	105.86	111.36
1	D	49	ILE	CA-C-O	5.04	126.57	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	137	ILE	N-CA-C	-5.04	100.64	108.86
3	H	70	ASP	CA-C-N	-5.04	114.97	122.23
3	H	70	ASP	C-N-CA	-5.04	114.97	122.23
3	I	27	TYR	CB-CG-CD1	-5.04	113.23	120.80
3	J	324	HIS	CA-CB-CG	-5.04	108.76	113.80
1	D	226	PRO	N-CA-CB	-5.04	97.94	103.39
1	f	35	ALA	CA-C-N	5.04	128.36	120.75
1	f	35	ALA	C-N-CA	5.04	128.36	120.75
2	2	12	THR	CA-C-O	5.04	129.37	120.80
2	4	31	ALA	N-CA-C	-5.04	101.08	108.79
3	H	273	ASP	CA-C-N	5.04	126.44	120.14
3	H	273	ASP	C-N-CA	5.04	126.44	120.14
3	I	86	LYS	N-CA-C	-5.04	101.49	109.96
3	K	174	PRO	CB-CA-C	-5.04	104.77	110.92
1	a	126	TYR	N-CA-CB	5.04	117.57	110.36
1	B	216	VAL	CA-C-N	5.04	127.34	120.54
1	B	216	VAL	C-N-CA	5.04	127.34	120.54
1	c	201	GLU	CB-CG-CD	-5.04	104.03	112.60
2	i	151	LEU	N-CA-CB	-5.04	102.70	110.01
2	l	96	ASN	CB-CA-C	-5.04	102.29	110.85
3	K	309	VAL	N-CA-C	-5.04	98.00	108.88
3	M	377	LYS	O-C-N	-5.04	116.41	122.15
3	H	86	LYS	N-CA-CB	5.04	118.84	110.63
3	L	120	PRO	N-CA-CB	5.04	107.68	103.25
3	J	137	GLU	N-CA-C	5.04	116.77	111.28
2	2	51	ARG	CB-CG-CD	5.04	122.88	111.30
3	J	397	PHE	N-CA-C	-5.04	101.03	109.24
1	C	228	GLU	N-CA-C	-5.03	107.19	113.38
1	F	190	VAL	CA-C-O	5.03	126.19	120.85
3	K	324	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
3	J	67	VAL	CA-C-N	5.03	128.12	120.77
3	J	67	VAL	C-N-CA	5.03	128.12	120.77
1	b	145	PRO	N-CA-CB	5.03	107.79	103.36
1	F	174	PHE	O-C-N	-5.03	116.89	122.07
3	H	169	GLU	CA-C-O	-5.03	115.09	120.42
3	K	387	THR	O-C-N	5.03	126.21	121.38
3	M	109	ASN	CA-CB-CG	-5.03	107.57	112.60
2	3	24	VAL	N-CA-C	-5.03	100.66	108.86
1	a	150	THR	N-CA-C	-5.03	101.96	109.95
1	e	223	GLU	N-CA-C	-5.03	100.84	109.24
1	G	190	VAL	CA-CB-CG1	5.03	118.94	110.40
2	j	35	ASN	N-CA-CB	5.03	117.51	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	174	PRO	CA-C-O	-5.03	113.27	120.56
1	C	205	VAL	O-C-N	-5.02	115.37	121.10
2	h	154	ARG	CD-NE-CZ	-5.02	117.37	124.40
2	j	172	ILE	CB-CA-C	5.02	119.15	112.22
3	H	71	ILE	CB-CA-C	5.02	120.22	111.18
2	l	66	LEU	CA-C-N	5.02	127.51	120.28
2	l	66	LEU	C-N-CA	5.02	127.51	120.28
2	m	188	VAL	CA-C-O	5.02	126.30	120.67
1	c	99	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	d	196	MET	N-CA-C	5.02	116.83	111.36
2	l	132	ILE	CB-CA-C	-5.02	104.28	111.31
1	B	223	GLU	N-CA-C	-5.02	101.53	109.96
2	l	71	LYS	N-CA-CB	5.02	117.29	110.01
3	H	248	ALA	N-CA-CB	5.02	119.69	111.31
3	M	301	GLY	N-CA-C	-5.02	108.39	115.32
1	a	141	VAL	CG1-CB-CG2	-5.02	99.76	110.80
1	d	200	ILE	CA-C-N	5.02	130.51	122.93
1	d	200	ILE	C-N-CA	5.02	130.51	122.93
1	E	120	LYS	CA-C-N	5.02	127.51	120.28
1	E	120	LYS	C-N-CA	5.02	127.51	120.28
1	e	11	ALA	CA-C-O	-5.02	115.91	121.28
2	h	152	GLU	CA-C-N	5.02	126.96	120.44
2	h	152	GLU	C-N-CA	5.02	126.96	120.44
2	i	79	ILE	O-C-N	-5.02	116.68	121.90
2	n	121	SER	N-CA-CB	5.02	118.97	110.49
3	H	101	LYS	CA-C-N	5.02	125.25	119.83
3	H	101	LYS	C-N-CA	5.02	125.25	119.83
3	H	272	LEU	CB-CA-C	-5.02	102.46	110.79
3	I	305	ARG	O-C-N	-5.02	116.50	123.12
3	K	364	ARG	CD-NE-CZ	-5.02	117.38	124.40
2	j	98	LEU	CA-C-O	-5.02	115.10	120.42
2	k	68	ARG	CD-NE-CZ	-5.02	117.38	124.40
3	M	25	GLU	CA-C-O	-5.02	115.23	120.55
1	B	149	GLU	CB-CA-C	-5.01	100.62	109.70
1	f	200	ILE	N-CA-C	-5.01	107.05	113.22
2	h	83	ARG	CB-CG-CD	5.01	122.83	111.30
2	n	176	MET	CG-SD-CE	-5.01	89.87	100.90
1	f	137	LEU	CB-CA-C	-5.01	102.67	110.74
2	l	64	GLN	CA-C-N	5.01	127.41	120.29
2	l	64	GLN	C-N-CA	5.01	127.41	120.29
1	a	73	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	E	111	GLU	O-C-N	-5.01	115.25	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	145	LEU	CB-CA-C	-5.01	103.01	110.88
2	7	212	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
3	K	69	SER	N-CA-C	-5.01	105.92	112.23
1	a	83	ALA	CA-C-N	5.01	127.41	120.29
1	a	83	ALA	C-N-CA	5.01	127.41	120.29
1	B	160	LYS	N-CA-C	-5.01	106.33	114.09
1	a	235	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	k	98	LEU	CA-C-N	5.01	127.40	120.29
2	k	98	LEU	C-N-CA	5.01	127.40	120.29
2	m	92	THR	CA-C-N	5.01	126.99	120.28
2	m	92	THR	C-N-CA	5.01	126.99	120.28
1	A	178	GLU	O-C-N	5.01	128.74	122.23
1	B	234	GLU	O-C-N	5.01	127.23	122.07
1	C	168	ARG	CA-C-N	5.01	127.25	120.44
1	C	168	ARG	C-N-CA	5.01	127.25	120.44
1	c	32	LYS	N-CA-CB	-5.01	102.72	110.98
2	3	165	VAL	N-CA-CB	5.01	118.09	110.58
2	l	212	ARG	NE-CZ-NH1	5.01	126.51	121.50
2	6	209	ALA	CA-C-O	5.01	125.52	119.31
3	I	352	LYS	CA-C-N	5.01	126.99	120.28
3	I	352	LYS	C-N-CA	5.01	126.99	120.28
1	D	62	ASP	N-CA-C	-5.00	104.98	112.54
1	G	89	ILE	O-C-N	5.00	127.45	121.80
1	B	69	LYS	CB-CA-C	5.00	117.70	109.90
1	E	172	THR	N-CA-C	5.00	116.81	111.36
2	m	156	THR	N-CA-C	-5.00	100.13	108.23
3	I	381	LYS	N-CA-C	5.00	117.12	111.02
3	L	367	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	h	65	PHE	CA-CB-CG	-5.00	108.80	113.80
3	M	142	ASP	CA-C-N	5.00	129.60	121.95
3	M	142	ASP	C-N-CA	5.00	129.60	121.95
3	J	320	ILE	CA-C-O	-5.00	115.75	120.95

There are no chirality outliers.

All (323) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	101	TYR	Sidechain
2	1	106	TYR	Sidechain
2	1	148	TYR	Sidechain
2	1	170	ARG	Sidechain
2	1	173	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	1	68	ARG	Sidechain
2	1	81	ARG	Sidechain
2	2	103	TYR	Sidechain
2	2	139	ALA	Peptide
2	2	170	ARG	Sidechain
2	2	196	PHE	Sidechain
2	2	197	TYR	Sidechain
2	2	211	PHE	Sidechain
2	2	51	ARG	Sidechain
2	2	83	ARG	Sidechain
2	3	51	ARG	Sidechain
2	4	101	TYR	Sidechain
2	4	103	TYR	Sidechain
2	4	106	TYR	Sidechain
2	4	123	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	197	TYR	Sidechain
2	5	132	ILE	Mainchain
2	5	170	ARG	Sidechain
2	5	212	ARG	Sidechain
2	5	68	ARG	Sidechain
2	6	103	TYR	Sidechain
2	6	123	TYR	Sidechain
2	6	148	TYR	Sidechain
2	6	199	TYR	Sidechain
2	6	46	TYR	Sidechain
2	6	68	ARG	Sidechain
2	6	77	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	154	ARG	Sidechain
2	7	170	ARG	Sidechain
2	7	197	TYR	Sidechain
2	7	77	TYR	Sidechain
1	A	100	ARG	Sidechain
1	A	179	TYR	Sidechain
1	A	180	ARG	Sidechain
1	A	213	TYR	Sidechain
1	A	232	TYR	Sidechain
1	A	241	ARG	Sidechain
1	A	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	65	GLU	Peptide
1	B	14	VAL	Peptide
1	B	159	TYR	Sidechain
1	B	220	THR	Peptide
1	B	33	ARG	Sidechain
1	B	68	TYR	Sidechain
1	B	93	ARG	Sidechain
1	C	103	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	185	PHE	Sidechain
1	C	219	ARG	Sidechain
1	C	22	PHE	Sidechain
1	C	220	THR	Peptide
1	C	221	PHE	Sidechain
1	C	235	ARG	Sidechain
1	C	26	TYR	Sidechain
1	C	28	ARG	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	D	126	TYR	Sidechain
1	D	168	ARG	Sidechain
1	D	220	THR	Peptide
1	D	232	TYR	Sidechain
1	D	26	TYR	Sidechain
1	E	123	TYR	Sidechain
1	E	130	ARG	Sidechain
1	E	148	TYR	Sidechain
1	E	159	TYR	Sidechain
1	E	179	TYR	Sidechain
1	E	211	VAL	Peptide
1	E	219	ARG	Sidechain
1	E	220	THR	Peptide
1	E	235	ARG	Sidechain
1	E	25	GLU	Sidechain
1	E	53	ARG	Sidechain
1	E	77	ALA	Peptide
1	F	123	TYR	Sidechain
1	F	126	TYR	Sidechain
1	F	213	TYR	Sidechain
1	F	219	ARG	Sidechain
1	F	220	THR	Peptide
1	F	8	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	G	103	TYR	Sidechain
1	G	123	TYR	Sidechain
1	G	148	TYR	Sidechain
1	G	15	PHE	Sidechain
1	G	213	TYR	Sidechain
1	G	220	THR	Peptide
1	G	235	ARG	Sidechain
1	G	5	GLN	Peptide
1	G	8	TYR	Sidechain
3	H	105	ARG	Sidechain
3	H	167	PHE	Sidechain
3	H	20	TYR	Sidechain
3	H	215	TYR	Peptide
3	H	254	ASP	Peptide
3	H	259	ARG	Sidechain
3	H	27	TYR	Sidechain
3	H	29	ARG	Sidechain
3	H	305	ARG	Sidechain
3	H	364	ARG	Sidechain
3	H	371	THR	Peptide
3	H	375	PHE	Sidechain
3	H	386	THR	Peptide
3	H	387	THR	Peptide
3	H	59	ARG	Sidechain
3	I	140	TYR	Sidechain
3	I	162	LEU	Mainchain
3	I	21	TYR	Sidechain
3	I	215	TYR	Peptide
3	I	217	GLY	Peptide
3	I	218	GLU	Peptide
3	I	236	SER	Peptide
3	I	24	ARG	Sidechain
3	I	240	ILE	Peptide
3	I	254	ASP	Peptide
3	I	263	ARG	Sidechain
3	I	276	ASP	Peptide
3	I	289	ARG	Sidechain
3	I	305	ARG	Sidechain
3	I	311	LEU	Peptide
3	I	36	PHE	Sidechain
3	I	361	PHE	Sidechain
3	I	386	THR	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
3	I	387	THR	Peptide
3	I	46	ARG	Sidechain
3	I	49	ARG	Sidechain
3	I	50	ARG	Sidechain
3	I	59	ARG	Sidechain
3	J	140	TYR	Sidechain
3	J	154	ARG	Sidechain
3	J	181	TYR	Sidechain,Peptide
3	J	254	ASP	Peptide
3	J	259	ARG	Sidechain
3	J	303	PHE	Peptide
3	J	341	ARG	Sidechain
3	J	364	ARG	Sidechain
3	J	367	ARG	Sidechain
3	J	371	THR	Peptide
3	J	385	LYS	Peptide
3	J	386	THR	Peptide
3	J	43	ARG	Sidechain
3	J	94	TYR	Sidechain
3	K	167	PHE	Sidechain
3	K	181	TYR	Sidechain
3	K	186	THR	Peptide
3	K	190	LEU	Peptide
3	K	20	TYR	Sidechain
3	K	200	ARG	Sidechain
3	K	205	ARG	Sidechain
3	K	207	VAL	Peptide
3	K	21	TYR	Sidechain
3	K	27	TYR	Sidechain
3	K	289	ARG	Sidechain
3	K	299	ARG	Sidechain
3	K	303	PHE	Sidechain
3	K	305	ARG	Sidechain
3	K	367	ARG	Sidechain
3	K	386	THR	Peptide
3	K	94	TYR	Sidechain
3	L	118	VAL	Peptide
3	L	128	TYR	Sidechain
3	L	140	TYR	Sidechain
3	L	154	ARG	Sidechain
3	L	181	TYR	Sidechain
3	L	20	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	L	200	ARG	Sidechain
3	L	201	ALA	Peptide
3	L	215	TYR	Sidechain
3	L	249	ARG	Sidechain
3	L	269	LEU	Mainchain,Peptide
3	L	277	PRO	Peptide
3	L	278	ARG	Sidechain
3	L	28	ARG	Sidechain
3	L	302	ARG	Sidechain
3	L	305	ARG	Sidechain
3	L	314	PHE	Sidechain
3	L	317	ARG	Sidechain
3	L	364	ARG	Sidechain
3	L	43	ARG	Sidechain
3	L	49	ARG	Sidechain
3	L	52	ARG	Sidechain
3	L	57	ARG	Sidechain
3	M	118	VAL	Peptide
3	M	20	TYR	Sidechain
3	M	200	ARG	Sidechain
3	M	205	ARG	Sidechain
3	M	215	TYR	Sidechain,Peptide
3	M	250	ARG	Sidechain
3	M	259	ARG	Sidechain
3	M	27	TYR	Sidechain
3	M	289	ARG	Sidechain
3	M	305	ARG	Sidechain
3	M	326	ARG	Sidechain
3	M	385	LYS	Peptide
3	M	386	THR	Mainchain,Peptide
3	M	65	VAL	Peptide
3	M	87	PHE	Sidechain
1	a	10	ARG	Sidechain
1	a	123	TYR	Sidechain
1	a	130	ARG	Sidechain
1	a	132	PHE	Sidechain
1	a	168	ARG	Sidechain
1	a	180	ARG	Sidechain
1	a	213	TYR	Sidechain
1	a	22	PHE	Sidechain
1	a	220	THR	Peptide
1	a	235	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	a	241	ARG	Sidechain
1	a	26	TYR	Sidechain
1	a	68	TYR	Sidechain
1	a	91	ARG	Sidechain
1	a	93	ARG	Sidechain
1	b	10	ARG	Sidechain
1	b	123	TYR	Sidechain
1	b	148	TYR	Sidechain
1	b	179	TYR	Sidechain
1	b	185	PHE	Sidechain
1	b	20	ARG	Sidechain
1	b	220	THR	Peptide
1	b	241	ARG	Sidechain
1	b	26	TYR	Sidechain
1	b	91	ARG	Sidechain
1	c	10	ARG	Sidechain
1	c	100	ARG	Sidechain
1	c	148	TYR	Sidechain
1	c	159	TYR	Sidechain
1	c	168	ARG	Sidechain
1	c	219	ARG	Sidechain
1	c	232	TYR	Sidechain
1	c	28	ARG	Sidechain
1	c	68	TYR	Sidechain
1	c	86	ARG	Sidechain
1	d	159	TYR	Sidechain
1	d	213	TYR	Sidechain
1	d	220	THR	Peptide
1	d	235	ARG	Sidechain
1	d	26	TYR	Sidechain
1	d	68	TYR	Sidechain
1	d	73	HIS	Sidechain
1	d	86	ARG	Sidechain
1	e	132	PHE	Sidechain
1	e	168	ARG	Sidechain
1	e	179	TYR	Sidechain
1	e	220	THR	Peptide
1	e	28	ARG	Sidechain
1	e	68	TYR	Sidechain
1	e	91	ARG	Sidechain
1	f	100	ARG	Sidechain
1	f	103	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	f	126	TYR	Sidechain
1	f	148	TYR	Sidechain
1	f	168	ARG	Sidechain
1	f	179	TYR	Sidechain
1	f	185	PHE	Sidechain
1	f	213	TYR	Sidechain
1	f	220	THR	Mainchain,Peptide
1	f	232	TYR	Sidechain
1	g	123	TYR	Sidechain
1	g	130	ARG	Sidechain
1	g	148	TYR	Sidechain
1	g	20	ARG	Sidechain
1	g	220	THR	Peptide
1	g	239	ARG	Sidechain
1	g	68	TYR	Sidechain
1	g	73	HIS	Sidechain
2	h	123	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	154	ARG	Sidechain
2	h	173	TYR	Sidechain
2	h	178	ARG	Sidechain
2	h	212	ARG	Sidechain
2	h	51	ARG	Sidechain
2	h	68	ARG	Sidechain
2	h	77	TYR	Sidechain
2	i	106	TYR	Sidechain
2	i	139	ALA	Peptide
2	i	154	ARG	Sidechain
2	i	173	TYR	Sidechain
2	i	197	TYR	Sidechain
2	i	51	ARG	Sidechain
2	i	68	ARG	Sidechain
2	i	80	ARG	Sidechain
2	j	103	TYR	Sidechain,Peptide
2	j	123	TYR	Sidechain
2	j	212	ARG	Sidechain
2	j	80	ARG	Sidechain
2	k	106	TYR	Sidechain
2	k	30	ARG	Sidechain
2	k	68	ARG	Sidechain
2	l	139	ALA	Peptide
2	l	46	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	l	51	ARG	Sidechain
2	m	102	ARG	Sidechain
2	m	106	TYR	Sidechain
2	m	197	TYR	Sidechain
2	m	51	ARG	Sidechain
2	m	77	TYR	Sidechain
2	m	81	ARG	Sidechain
2	m	83	ARG	Sidechain
2	n	101	TYR	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	178	ARG	Sidechain
2	n	197	TYR	Sidechain
2	n	30	ARG	Sidechain
2	n	46	TYR	Sidechain
2	n	77	TYR	Sidechain
2	n	81	ARG	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	4	0
1	B	1907	0	1941	7	0
1	C	1907	0	1941	8	0
1	D	1907	0	1941	11	0
1	E	1907	0	1941	14	0
1	F	1907	0	1941	5	0
1	G	1907	0	1941	8	0
1	a	1866	0	1908	8	0
1	b	1866	0	1908	5	0
1	c	1866	0	1908	5	0
1	d	1866	0	1908	6	0
1	e	1866	0	1908	7	0
1	f	1866	0	1908	10	0
1	g	1866	0	1908	7	0
2	1	1553	0	1580	4	0
2	2	1553	0	1580	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	1553	0	1580	2	0
2	4	1553	0	1580	2	0
2	5	1553	0	1580	28	0
2	6	1553	0	1580	4	0
2	7	1553	0	1580	5	0
2	h	1553	0	1580	1	0
2	i	1553	0	1580	5	0
2	j	1553	0	1580	5	0
2	k	1553	0	1580	4	0
2	l	1553	0	1580	24	0
2	m	1553	0	1580	2	0
2	n	1553	0	1580	0	0
3	H	3100	0	3220	12	0
3	I	3100	0	3220	40	0
3	J	3100	0	3220	25	0
3	K	3100	0	3220	24	0
3	L	3100	0	3220	27	0
3	M	3100	0	3220	47	0
4	I	31	0	12	0	0
4	J	31	0	12	1	0
4	K	31	0	12	0	0
4	L	31	0	12	2	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
5	M	1	0	0	0	0
6	M	27	0	12	0	0
All	All	66909	0	68443	329	0

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

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:211:PHE:CE2	2:5:211:PHE:CD2	2.00	1.49
2:1:211:PHE:CZ	2:1:211:PHE:CE2	2.00	1.47
2:1:211:PHE:CE1	2:1:211:PHE:CD1	2.02	1.47
2:1:211:PHE:CE2	2:1:211:PHE:CD2	2.02	1.46
2:5:211:PHE:CE2	2:5:211:PHE:CZ	2.03	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:211:PHE:CE1	2:5:211:PHE:CD1	2.01	1.46
2:1:211:PHE:CZ	2:1:211:PHE:CE1	2.05	1.44
2:5:211:PHE:CD1	2:5:211:PHE:CG	2.03	1.44
2:5:211:PHE:CD2	2:5:211:PHE:CG	2.06	1.42
2:5:211:PHE:CZ	2:5:211:PHE:CE1	2.07	1.41
2:1:211:PHE:CD1	2:1:211:PHE:CG	2.10	1.39
2:1:211:PHE:CD2	2:1:211:PHE:CG	2.14	1.36
3:M:342:ILE:CG2	3:M:379:ILE:CG2	2.10	1.28
3:M:342:ILE:CG2	3:M:379:ILE:HG22	1.65	1.27
3:M:342:ILE:HG22	3:M:379:ILE:CG2	1.72	1.17
2:1:170:ARG:CZ	2:1:170:ARG:NH1	2.10	1.14
3:M:342:ILE:HG21	3:M:379:ILE:HG22	1.29	1.12
2:1:170:ARG:NH1	2:1:211:PHE:CD2	2.20	1.09
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.36	1.09
2:1:170:ARG:CZ	2:1:211:PHE:CE2	2.35	1.08
2:5:170:ARG:NH1	2:5:211:PHE:CZ	2.23	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.23	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.23	1.06
2:1:170:ARG:NH1	2:1:211:PHE:CE2	2.23	1.06
2:1:170:ARG:NH1	2:1:211:PHE:CG	2.22	1.06
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.39	1.06
2:1:170:ARG:NH1	2:1:211:PHE:CD1	2.23	1.06
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.22	1.06
2:1:170:ARG:CZ	2:1:211:PHE:CD1	2.37	1.06
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.38	1.05
2:1:170:ARG:NH1	2:1:211:PHE:CE1	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.24	1.05
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.18	1.05
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.40	1.05
2:1:170:ARG:NH1	2:1:211:PHE:CZ	2.24	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.41	1.04
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.25	1.04
2:1:170:ARG:CZ	2:1:211:PHE:CD2	2.40	1.04
2:1:170:ARG:CZ	2:1:211:PHE:CE1	2.41	1.04
3:M:342:ILE:CG2	3:M:379:ILE:HG21	1.85	1.03
3:M:342:ILE:HG21	3:M:379:ILE:CG2	1.81	1.02
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.42	1.01
2:1:170:ARG:CZ	2:1:211:PHE:CZ	2.44	1.00
2:1:170:ARG:CZ	2:1:211:PHE:CG	2.44	1.00
3:M:342:ILE:HG22	3:M:379:ILE:HG22	1.42	0.86
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.45	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:170:ARG:NE	2:l:211:PHE:CZ	2.47	0.82
2:l:170:ARG:NE	2:l:211:PHE:CE1	2.49	0.81
2:l:170:ARG:NH2	2:l:211:PHE:CD2	2.49	0.80
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.50	0.79
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.50	0.79
3:M:384:LYS:H	3:M:389:ILE:HD11	1.48	0.79
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.50	0.79
3:M:354:ILE:HG21	3:M:379:ILE:HG13	1.63	0.78
3:I:398:VAL:HG22	3:I:398:VAL:OXT	1.83	0.78
1:f:21:LEU:HD22	1:f:21:LEU:H	1.46	0.78
2:l:170:ARG:NH2	2:l:211:PHE:CG	2.52	0.78
3:I:161:LEU:HD22	3:I:237:ILE:HD11	1.65	0.77
3:I:236:SER:HA	3:I:237:ILE:HG12	1.68	0.75
3:I:227:PHE:CE2	3:I:238:ILE:HD13	2.21	0.74
1:A:65:GLU:H	1:A:66:LYS:HA	1.53	0.74
3:I:216:ILE:CG2	3:I:263:ARG:HH22	2.02	0.73
3:M:230:ALA:HB2	3:M:238:ILE:HD11	1.70	0.73
3:K:246:ILE:HG23	3:L:263:ARG:HE	1.52	0.72
3:M:342:ILE:CB	3:M:379:ILE:HG21	2.20	0.71
3:K:261:VAL:HG22	3:L:216:ILE:CG2	2.21	0.71
3:I:398:VAL:OXT	3:I:398:VAL:CG2	2.38	0.70
1:B:56:SER:H	1:B:59:LEU:HD13	1.58	0.69
3:I:167:PHE:CE2	3:I:172:ILE:HD11	2.28	0.69
1:E:38:ILE:HD12	1:E:196:MET:HE3	1.73	0.68
3:I:236:SER:CA	3:I:237:ILE:HG12	2.23	0.68
3:I:146:LEU:H	3:I:147:ASP:HA	1.58	0.68
3:K:153:ILE:HD11	3:K:180:LEU:HD21	1.74	0.68
3:L:256:SER:OG	3:M:216:ILE:HD11	1.94	0.68
3:K:249:ARG:H	3:K:249:ARG:HD3	1.58	0.68
3:M:354:ILE:HG21	3:M:379:ILE:CG1	2.24	0.67
3:L:321:PHE:CE1	3:L:351:ILE:HD12	2.30	0.66
2:1:95:SER:HB3	2:1:130:GLY:H	1.61	0.66
3:L:342:ILE:HG21	3:L:379:ILE:HG21	1.77	0.65
3:I:292:ILE:HD12	3:I:292:ILE:C	2.22	0.65
3:M:342:ILE:HB	3:M:379:ILE:HG21	1.78	0.65
2:i:68:ARG:HH11	2:j:92:THR:HG23	1.62	0.64
3:I:236:SER:HA	3:I:237:ILE:CG1	2.27	0.64
1:b:10:ARG:HH11	1:g:10:ARG:HH12	1.46	0.64
2:6:186:ILE:HG23	2:6:204:VAL:HG11	1.82	0.62
3:K:261:VAL:HG22	3:L:216:ILE:HG21	1.82	0.62
1:E:70:ILE:HG21	1:E:112:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:398:VAL:HG22	3:J:398:VAL:OXT	1.99	0.61
3:K:55:VAL:HG13	3:J:55:VAL:HG22	1.81	0.61
1:b:141:VAL:H	1:b:214:VAL:HG11	1.65	0.61
3:I:243:LEU:HA	3:I:246:ILE:HG22	1.81	0.61
3:K:320:ILE:HG22	3:K:351:ILE:HG21	1.81	0.61
3:L:359:GLY:O	3:L:363:ILE:HG13	2.00	0.60
3:L:320:ILE:HG22	3:L:351:ILE:HG21	1.83	0.60
3:L:206:VAL:HG22	3:L:207:VAL:H	1.65	0.60
3:L:212:VAL:CG1	3:M:216:ILE:HG22	2.32	0.60
3:M:269:LEU:HD11	3:M:297:ILE:HD12	1.82	0.60
3:H:398:VAL:HG22	3:H:398:VAL:OXT	2.02	0.59
3:J:170:VAL:HG12	3:J:172:ILE:HG23	1.85	0.59
2:m:107:LEU:H	2:m:107:LEU:HD22	1.68	0.59
3:I:216:ILE:HG23	3:I:263:ARG:HH22	1.66	0.59
3:I:201:ALA:HB3	3:I:237:ILE:HG13	1.84	0.57
3:H:363:ILE:HG23	3:I:166:LEU:HD23	1.87	0.57
1:D:8:TYR:HA	1:D:14:VAL:HG21	1.85	0.57
3:L:398:VAL:HG22	3:L:398:VAL:OXT	2.05	0.57
3:K:363:ILE:HD12	3:K:363:ILE:C	2.30	0.57
3:I:354:ILE:HD13	3:I:379:ILE:HG12	1.88	0.56
3:M:216:ILE:HG23	3:M:263:ARG:HH12	1.71	0.56
1:G:60:GLU:HG3	1:G:62:ASP:H	1.70	0.56
3:I:236:SER:C	3:I:237:ILE:HG12	2.31	0.56
1:G:132:PHE:HB3	1:G:134:VAL:HG12	1.88	0.56
2:1:13:THR:HB	2:1:143:GLY:H	1.71	0.55
2:i:137:ILE:HD13	2:i:137:ILE:H	1.71	0.55
3:M:283:VAL:HA	3:M:284:ILE:HB	1.89	0.55
1:b:73:HIS:CE1	1:b:106:PRO:HB3	2.42	0.55
3:I:212:VAL:HB	3:J:216:ILE:HD12	1.89	0.55
2:5:27:THR:HG22	2:5:55:THR:HB	1.89	0.54
3:K:299:ARG:HH21	4:J:401:ATP:H5'1	1.72	0.54
3:L:256:SER:CB	3:M:216:ILE:HD11	2.37	0.54
1:D:237:ASN:HA	1:D:240:ILE:HD12	1.90	0.54
3:M:320:ILE:HG22	3:M:351:ILE:CG2	2.38	0.54
2:i:25:MET:HB3	2:i:55:THR:HG21	1.90	0.54
3:I:91:THR:HG22	3:I:92:SER:H	1.74	0.53
2:4:173:TYR:CE1	2:4:208:LEU:HD13	2.43	0.53
1:f:21:LEU:H	1:f:21:LEU:CD2	2.17	0.53
3:H:398:VAL:OXT	3:H:398:VAL:CG2	2.57	0.53
3:M:350:ASP:O	3:M:354:ILE:HG12	2.09	0.52
2:6:65:PHE:HA	2:6:68:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:398:VAL:OXT	3:J:398:VAL:CG2	2.57	0.52
2:7:212:ARG:HG3	2:7:213:LYS:H	1.73	0.52
3:I:161:LEU:CD2	3:I:237:ILE:HD11	2.39	0.52
1:g:53:ARG:HA	1:g:61:ALA:HB1	1.90	0.52
3:J:320:ILE:HG22	3:J:351:ILE:HG21	1.91	0.51
3:H:113:LEU:HD12	3:H:113:LEU:H	1.76	0.51
1:a:215:LYS:HB3	1:a:217:ASP:H	1.74	0.51
1:G:197:GLY:HA3	1:G:240:ILE:HD13	1.93	0.51
1:e:34:GLY:HA3	1:e:80:GLY:H	1.76	0.51
1:E:158:GLU:HB2	1:F:63:THR:HG21	1.94	0.50
3:I:264:THR:HA	3:I:267:GLN:HE21	1.76	0.50
3:H:292:ILE:O	3:H:292:ILE:HG13	2.12	0.50
3:L:212:VAL:HG12	3:M:216:ILE:HG22	1.94	0.50
3:H:363:ILE:HG23	3:I:166:LEU:CD2	2.42	0.50
3:J:312:PRO:HD2	3:J:347:SER:HA	1.94	0.50
2:3:13:THR:HB	2:3:143:GLY:H	1.77	0.49
1:G:82:VAL:HA	1:G:85:ALA:HB3	1.93	0.49
2:4:14:THR:HG22	2:4:27:THR:HA	1.93	0.49
3:I:238:ILE:HD11	3:I:240:ILE:HD11	1.93	0.49
1:a:50:ALA:N	1:a:67:ILE:HD11	2.27	0.49
3:I:246:ILE:O	3:I:246:ILE:HG13	2.12	0.49
3:L:385:LYS:HE2	3:M:307:ILE:HD13	1.93	0.49
3:K:261:VAL:CG2	3:L:216:ILE:HG23	2.43	0.49
3:J:182:GLY:H	3:J:188:LYS:HD3	1.77	0.49
1:E:156:LEU:HD12	1:E:156:LEU:O	2.13	0.48
3:K:398:VAL:OXT	3:K:398:VAL:HG22	2.13	0.48
1:E:56:SER:HB3	1:E:58:LEU:H	1.77	0.48
1:G:97:GLN:HA	1:G:97:GLN:NE2	2.28	0.48
3:M:230:ALA:CB	3:M:238:ILE:HD11	2.42	0.48
3:I:359:GLY:HA3	3:J:172:ILE:HG21	1.94	0.48
3:M:305:ARG:HD2	3:M:307:ILE:HD11	1.95	0.48
3:L:256:SER:HB2	3:M:216:ILE:HD11	1.95	0.48
1:B:49:ILE:HD13	1:B:193:LEU:HD12	1.95	0.48
3:K:260:GLU:HB3	3:L:216:ILE:HD13	1.95	0.48
1:c:21:LEU:HD12	1:c:21:LEU:H	1.79	0.47
1:e:27:ALA:O	1:e:30:ALA:HB3	2.14	0.47
3:M:157:VAL:HG21	3:M:284:ILE:HD11	1.96	0.47
3:J:146:LEU:HB2	3:J:150:ILE:HG13	1.97	0.47
2:6:101:TYR:HB3	2:6:106:TYR:CD1	2.49	0.47
3:K:102:PRO:HB2	3:J:128:TYR:CE1	2.49	0.47
3:L:320:ILE:HD12	4:L:401:ATP:HN62	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:384:LYS:HB3	3:M:389:ILE:CD1	2.44	0.47
3:M:239:PHE:HA	3:M:284:ILE:HG22	1.97	0.47
2:h:165:VAL:HG11	2:h:199:TYR:CE1	2.50	0.47
1:C:73:HIS:CE1	1:C:106:PRO:HB3	2.50	0.47
3:I:318:ILE:HD13	3:I:337:LYS:HG2	1.97	0.47
1:D:53:ARG:HB2	1:D:208:ASN:HD22	1.80	0.47
1:B:64:ILE:HA	1:B:65:GLU:HB3	1.95	0.46
3:M:320:ILE:HG22	3:M:351:ILE:HG21	1.96	0.46
2:5:200:SER:HB3	2:5:201:PRO:HD2	1.97	0.46
1:a:87:VAL:HG21	1:g:121:GLN:HE21	1.81	0.46
3:L:137:GLU:CD	3:L:137:GLU:H	2.23	0.46
3:J:250:ARG:HH22	3:J:265:MET:CE	2.29	0.46
3:H:51:LEU:O	3:H:55:VAL:HG23	2.16	0.46
3:M:321:PHE:CZ	3:M:379:ILE:HD11	2.51	0.46
2:5:18:VAL:HB	2:5:136:ASP:HA	1.98	0.46
3:K:261:VAL:HG22	3:L:216:ILE:HG23	1.98	0.46
3:L:281:VAL:HB	3:L:283:VAL:HG23	1.97	0.46
1:D:141:VAL:HG22	1:D:145:PRO:HA	1.97	0.46
3:H:343:THR:HG22	3:H:383:LEU:HD12	1.96	0.46
3:M:384:LYS:CB	3:M:389:ILE:CD1	2.94	0.46
1:B:12:ILE:HB	1:B:23:GLN:HG2	1.98	0.46
1:E:47:ILE:HD11	1:E:185:PHE:CD2	2.51	0.45
3:M:216:ILE:HD13	3:M:260:GLU:OE1	2.16	0.45
3:I:324:HIS:CE1	3:I:352:LYS:HA	2.51	0.45
2:6:56:THR:HG22	2:6:110:LEU:CD2	2.47	0.45
3:K:234:ALA:HA	3:K:235:PRO:C	2.42	0.45
3:J:212:VAL:HG12	3:J:263:ARG:HH22	1.81	0.45
1:G:73:HIS:CE1	1:G:106:PRO:HB2	2.51	0.45
2:m:49:ALA:HB3	2:m:52:MET:HB2	1.98	0.45
1:a:82:VAL:CG1	1:a:86:ARG:HH21	2.30	0.45
1:C:204:LEU:H	1:C:237:ASN:HD21	1.64	0.45
1:E:121:GLN:HE21	1:F:87:VAL:HG21	1.81	0.45
1:e:126:TYR:HB2	1:e:129:VAL:HG22	1.99	0.45
1:f:78:THR:HG21	1:f:85:ALA:HB1	1.98	0.45
1:f:141:VAL:HG11	1:f:216:VAL:HA	1.98	0.45
1:a:27:ALA:HB1	1:a:152:PRO:HB2	1.98	0.45
1:g:214:VAL:HA	1:g:221:PHE:H	1.81	0.45
1:C:15:PHE:CE2	1:D:27:ALA:HB2	2.52	0.45
1:G:109:VAL:HG13	1:G:138:ILE:HG22	1.99	0.44
3:J:195:VAL:HG22	3:J:199:THR:HG23	1.99	0.44
1:C:69:LYS:HG3	2:3:79:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:HIS:HA	1:D:221:PHE:H	1.83	0.44
2:1:192:THR:HG23	2:1:194:ASP:H	1.82	0.44
3:K:250:ARG:HH22	3:J:249:ARG:HB3	1.82	0.44
1:E:70:ILE:HD11	1:E:89:ILE:HD11	2.00	0.44
1:d:98:ILE:O	1:d:102:THR:HG22	2.18	0.44
3:H:121:THR:HG23	3:I:78:VAL:HG21	1.98	0.44
3:I:227:PHE:CD2	3:I:238:ILE:HD13	2.51	0.44
3:I:174:PRO:HD2	3:I:278:ARG:HG2	1.98	0.44
1:B:129:VAL:HG22	1:B:130:ARG:H	1.83	0.44
1:f:28:ARG:O	1:f:31:VAL:HG22	2.17	0.44
2:1:54:MET:HE3	2:1:56:THR:CG2	2.48	0.44
3:I:246:ILE:O	3:I:246:ILE:HG23	2.17	0.44
1:c:182:ASP:O	1:c:183:LEU:HG	2.17	0.44
3:K:216:ILE:HD12	3:K:260:GLU:HG2	2.00	0.44
3:L:68:VAL:HG12	3:L:102:PRO:HA	2.00	0.44
1:d:94:ILE:CG1	2:k:80:ARG:HH12	2.31	0.43
1:f:143:GLU:HA	1:f:219:ARG:HE	1.83	0.43
1:g:38:ILE:HG12	1:g:196:MET:HE3	1.99	0.43
2:5:27:THR:CG2	2:5:55:THR:HB	2.46	0.43
1:A:34:GLY:HA3	1:A:80:GLY:H	1.83	0.43
1:C:109:VAL:HG13	1:C:138:ILE:HG22	1.99	0.43
3:M:385:LYS:H	3:M:389:ILE:HG12	1.82	0.43
3:I:292:ILE:C	3:I:292:ILE:CD1	2.91	0.43
3:M:216:ILE:CG2	3:M:263:ARG:NH1	2.81	0.43
1:a:31:VAL:HA	1:a:80:GLY:HA2	2.00	0.43
3:M:146:LEU:HD23	3:M:146:LEU:HA	1.93	0.43
1:g:211:VAL:HB	1:g:229:LEU:HD21	2.01	0.43
2:j:15:VAL:HG22	2:j:172:ILE:HD11	1.99	0.43
2:5:24:VAL:HG21	2:5:164:ALA:HB3	2.00	0.43
3:K:200:ARG:HE	3:K:200:ARG:HA	1.83	0.43
4:L:401:ATP:H5'1	3:M:299:ARG:HH12	1.83	0.43
3:J:375:PHE:O	3:J:379:ILE:HG13	2.18	0.43
1:C:15:PHE:CD2	1:D:27:ALA:HB2	2.53	0.43
1:D:141:VAL:H	1:D:214:VAL:HG11	1.84	0.43
2:j:66:LEU:HD23	2:j:66:LEU:HA	1.95	0.43
3:I:216:ILE:HD12	3:I:260:GLU:HG3	2.00	0.43
3:L:71:ILE:HA	3:L:77:VAL:HG13	2.01	0.43
1:e:158:GLU:OE2	1:f:63:THR:HB	2.19	0.43
2:i:32:THR:HA	2:i:38:ALA:H	1.83	0.43
1:A:31:VAL:HG11	1:A:164:ILE:HD11	2.01	0.43
1:d:21:LEU:HD22	1:d:21:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:146:LEU:H	3:J:147:ASP:HA	1.84	0.43
1:D:113:ALA:HB1	1:D:156:LEU:HD13	2.01	0.42
1:E:230:LYS:HB3	1:E:231:PRO:HD3	2.01	0.42
3:J:127:VAL:HA	3:J:130:PHE:CD1	2.54	0.42
1:c:97:GLN:HE22	2:j:75:ASN:HB3	1.83	0.42
2:7:156:THR:HG22	2:7:158:GLU:HB2	2.01	0.42
3:K:239:PHE:CD1	3:K:284:ILE:CG2	3.02	0.42
1:e:184:SER:H	1:e:187:ASP:HB3	1.84	0.42
2:k:97:LEU:HD23	2:k:97:LEU:HA	1.88	0.42
3:K:200:ARG:HA	3:K:200:ARG:NE	2.33	0.42
1:E:16:SER:HB2	1:E:17:PRO:HD2	2.01	0.42
2:7:207:ILE:HG22	2:7:211:PHE:CE1	2.55	0.42
1:B:197:GLY:HA3	1:B:240:ILE:HD13	2.01	0.42
1:D:184:SER:H	1:D:187:ASP:HB2	1.84	0.42
2:7:24:VAL:HG23	2:7:161:VAL:HG12	2.01	0.42
3:L:356:THR:HG23	3:M:173:GLU:O	2.20	0.42
3:M:109:ASN:HB2	3:M:116:VAL:HG11	2.01	0.42
3:M:384:LYS:HB3	3:M:389:ILE:HG12	2.01	0.42
1:E:14:VAL:HG13	1:F:23:GLN:HE22	1.84	0.42
1:f:31:VAL:HA	1:f:80:GLY:HA2	2.02	0.42
1:f:70:ILE:HA	1:f:93:ARG:HG2	2.02	0.42
1:g:79:SER:O	1:g:134:VAL:HG23	2.20	0.41
3:M:250:ARG:HE	3:M:295:PRO:HD2	1.85	0.41
1:b:209:ILE:O	1:b:209:ILE:HD12	2.20	0.41
1:C:204:LEU:H	1:C:237:ASN:ND2	2.18	0.41
3:L:394:GLY:HA3	3:L:397:PHE:H	1.85	0.41
1:A:49:ILE:HG23	1:A:211:VAL:HG22	2.02	0.41
1:F:170:ALA:HB1	1:F:198:LEU:HD21	2.02	0.41
2:2:107:LEU:H	2:2:107:LEU:HG	1.74	0.41
2:k:21:ASP:OD2	2:k:161:VAL:HG22	2.21	0.41
3:H:173:GLU:HA	3:H:174:PRO:HD3	1.93	0.41
3:I:216:ILE:HG23	3:I:263:ARG:NH2	2.33	0.41
3:I:216:ILE:HD12	3:I:260:GLU:CG	2.51	0.41
3:K:275:PHE:CD1	3:J:205:ARG:CZ	3.04	0.41
3:L:178:VAL:HG13	3:L:307:ILE:HG12	2.02	0.41
3:M:384:LYS:N	3:M:389:ILE:HD11	2.27	0.41
3:K:250:ARG:HH22	3:J:249:ARG:CB	2.33	0.41
3:J:178:VAL:HG23	3:J:284:ILE:CD1	2.50	0.41
1:B:14:VAL:HG13	1:C:23:GLN:HE22	1.85	0.41
1:D:121:GLN:HG2	1:D:154:GLY:HA3	2.03	0.41
1:d:94:ILE:HG13	2:k:80:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:GLN:HA	1:G:130:ARG:HE	1.86	0.41
3:J:110:GLN:HA	3:J:113:LEU:HD23	2.03	0.41
3:J:211:PHE:CD2	3:J:246:ILE:HG21	2.56	0.41
3:I:179:LEU:HD23	3:I:179:LEU:HA	1.83	0.41
2:l:29:LYS:HA	2:l:29:LYS:HD3	1.93	0.41
3:I:238:ILE:O	3:I:284:ILE:HG12	2.21	0.41
3:M:181:TYR:CG	3:M:290:ILE:CG2	3.03	0.41
3:J:203:PHE:CE1	3:J:237:ILE:HG21	2.56	0.41
1:a:203:GLU:HA	1:a:240:ILE:HG21	2.01	0.41
1:c:73:HIS:HA	1:c:221:PHE:H	1.86	0.41
1:d:21:LEU:HD22	1:d:21:LEU:N	2.36	0.41
1:e:141:VAL:HG11	1:e:216:VAL:HA	2.02	0.41
2:j:70:ILE:HD11	2:j:94:THR:HG23	2.02	0.41
3:L:398:VAL:OXT	3:L:398:VAL:CG2	2.64	0.41
3:J:130:PHE:CE1	3:J:226:VAL:HG12	2.55	0.41
1:b:198:LEU:HD23	1:b:243:LEU:HB3	2.03	0.41
1:e:102:THR:HG23	1:e:103:TYR:CD2	2.56	0.41
3:I:236:SER:HA	3:I:237:ILE:CB	2.51	0.41
3:I:239:PHE:HA	3:I:284:ILE:HG13	2.03	0.41
1:E:20:ARG:H	1:E:20:ARG:HG3	1.73	0.40
2:2:150:VAL:HG21	2:2:171:ALA:HA	2.03	0.40
2:7:27:THR:HG23	2:7:55:THR:HG22	2.03	0.40
3:K:230:ALA:CB	3:K:238:ILE:HD11	2.51	0.40
3:M:105:ARG:H	3:M:121:THR:HB	1.86	0.40
1:c:21:LEU:HD13	1:c:24:VAL:HG21	2.03	0.40
1:d:49:ILE:HG13	1:d:211:VAL:HG22	2.03	0.40
3:I:216:ILE:HG22	3:I:263:ARG:HH22	1.80	0.40
1:E:20:ARG:HH21	3:M:393:LYS:HB2	1.85	0.40
2:i:101:TYR:HB3	2:i:106:TYR:CD1	2.56	0.40
3:H:186:THR:HG21	3:H:309:VAL:HG12	2.03	0.40
3:H:371:THR:O	3:H:375:PHE:CD1	2.75	0.40
1:f:109:VAL:H	1:f:109:VAL:HG23	1.57	0.40
1:a:130:ARG:HG2	1:a:131:PRO:HD2	2.04	0.40
1:E:49:ILE:HG13	1:E:211:VAL:HG22	2.03	0.40
3:K:293:LEU:HD23	3:K:293:LEU:HA	1.89	0.40
3:M:337:LYS:O	3:M:341:ARG:HG3	2.22	0.40
3:M:384:LYS:CB	3:M:389:ILE:HD13	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%)	231 (96%)	6 (2%)	3 (1%)	9	42
1	B	240/242 (99%)	219 (91%)	18 (8%)	3 (1%)	9	42
1	C	240/242 (99%)	219 (91%)	17 (7%)	4 (2%)	7	36
1	D	240/242 (99%)	222 (92%)	14 (6%)	4 (2%)	7	36
1	E	240/242 (99%)	231 (96%)	7 (3%)	2 (1%)	16	54
1	F	240/242 (99%)	226 (94%)	11 (5%)	3 (1%)	9	42
1	G	240/242 (99%)	229 (95%)	9 (4%)	2 (1%)	16	54
1	a	235/242 (97%)	220 (94%)	10 (4%)	5 (2%)	5	30
1	b	235/242 (97%)	216 (92%)	17 (7%)	2 (1%)	14	51
1	c	235/242 (97%)	222 (94%)	11 (5%)	2 (1%)	14	51
1	d	235/242 (97%)	219 (93%)	12 (5%)	4 (2%)	7	36
1	e	235/242 (97%)	219 (93%)	13 (6%)	3 (1%)	9	42
1	f	235/242 (97%)	225 (96%)	8 (3%)	2 (1%)	14	51
1	g	235/242 (97%)	220 (94%)	9 (4%)	6 (3%)	4	25
2	1	200/202 (99%)	190 (95%)	8 (4%)	2 (1%)	12	48
2	2	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	6	31
2	3	200/202 (99%)	182 (91%)	14 (7%)	4 (2%)	6	31
2	4	200/202 (99%)	187 (94%)	9 (4%)	4 (2%)	6	31
2	5	200/202 (99%)	183 (92%)	10 (5%)	7 (4%)	3	20
2	6	200/202 (99%)	180 (90%)	13 (6%)	7 (4%)	3	20
2	7	200/202 (99%)	181 (90%)	14 (7%)	5 (2%)	4	26
2	h	200/202 (99%)	179 (90%)	15 (8%)	6 (3%)	3	23
2	i	200/202 (99%)	184 (92%)	14 (7%)	2 (1%)	12	48
2	j	200/202 (99%)	181 (90%)	17 (8%)	2 (1%)	12	48
2	k	200/202 (99%)	186 (93%)	11 (6%)	3 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	6	31
2	m	200/202 (99%)	186 (93%)	9 (4%)	5 (2%)	4	26
2	n	200/202 (99%)	178 (89%)	10 (5%)	12 (6%)	1	13
3	H	388/390 (100%)	348 (90%)	31 (8%)	9 (2%)	5	28
3	I	388/390 (100%)	350 (90%)	27 (7%)	11 (3%)	4	24
3	J	388/390 (100%)	345 (89%)	29 (8%)	14 (4%)	2	20
3	K	388/390 (100%)	344 (89%)	29 (8%)	15 (4%)	2	19
3	L	388/390 (100%)	348 (90%)	26 (7%)	14 (4%)	2	20
3	M	388/390 (100%)	350 (90%)	27 (7%)	11 (3%)	4	24
All	All	8453/8556 (99%)	7770 (92%)	497 (6%)	186 (2%)	7	29

All (186) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	B	64	ILE
1	C	20	ARG
1	C	67	ILE
1	d	221	PHE
1	E	221	PHE
2	h	41	ALA
2	h	128	ILE
2	h	140	THR
2	4	140	THR
2	k	30	ARG
2	l	212	ARG
2	6	139	ALA
2	n	131	ALA
3	I	237	ILE
3	I	255	THR
3	I	387	THR
3	K	124	ASP
3	K	190	LEU
3	K	191	LEU
3	K	392	LEU
3	L	118	VAL
3	L	269	LEU
3	M	131	GLU
3	M	390	PRO

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Mol	Chain	Res	Type
3	J	255	THR
3	J	270	ALA
3	J	292	ILE
3	J	387	THR
1	A	143	GLU
1	C	221	PHE
1	D	65	GLU
1	D	161	ALA
1	d	54	VAL
1	d	161	ALA
1	e	161	ALA
1	F	62	ASP
1	F	221	PHE
1	f	12	ILE
1	G	221	PHE
1	g	61	ALA
1	g	143	GLU
2	2	30	ARG
2	2	181	ALA
2	3	41	ALA
2	3	139	ALA
2	3	212	ARG
2	5	136	ASP
2	5	212	ARG
2	m	83	ARG
2	m	106	TYR
2	7	83	ARG
2	7	133	GLU
2	n	132	ILE
2	n	181	ALA
2	n	193	GLU
3	H	212	VAL
3	K	273	ASP
3	K	282	LYS
3	K	304	ASP
3	L	270	ALA
3	M	212	VAL
3	M	242	GLU
3	M	273	ASP
3	M	386	THR
3	J	269	LEU
3	J	331	ALA

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Mol	Chain	Res	Type
1	A	9	ASP
1	a	20	ARG
1	a	161	ALA
1	B	73	HIS
1	c	73	HIS
1	f	179	TYR
1	g	66	LYS
1	g	218	ASP
2	1	136	ASP
2	h	183	GLY
2	h	191	ILE
2	2	41	ALA
2	2	106	TYR
2	3	140	THR
2	j	136	ASP
2	5	83	ARG
2	1	40	LYS
2	6	19	CYS
2	6	41	ALA
2	6	102	ARG
2	m	85	PRO
2	m	183	GLY
2	7	34	GLY
2	7	185	GLY
2	7	193	GLU
2	n	35	ASN
2	n	136	ASP
3	H	136	PRO
3	H	278	ARG
3	I	122	SER
3	I	135	LYS
3	I	296	ALA
3	I	366	GLU
3	K	134	GLU
3	K	183	PRO
3	L	212	VAL
3	L	391	ASP
3	M	310	PRO
3	M	335	ASP
3	J	133	GLU
3	J	145	GLY
3	J	221	ARG

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Mol	Chain	Res	Type
3	J	275	PHE
1	a	62	ASP
1	B	221	PHE
1	b	73	HIS
1	c	62	ASP
1	e	73	HIS
1	F	9	ASP
1	G	143	GLU
2	1	212	ARG
2	i	193	GLU
2	4	35	ASN
2	4	136	ASP
2	5	133	GLU
2	l	30	ARG
2	l	41	ALA
2	n	107	LEU
2	n	137	ILE
2	n	140	THR
3	H	244	ASP
3	H	346	ALA
3	L	242	GLU
3	L	280	ASP
3	L	395	VAL
3	M	135	LYS
1	a	56	SER
1	b	161	ALA
1	C	19	GLY
1	D	9	ASP
1	E	9	ASP
1	e	14	VAL
1	g	217	ASP
1	g	221	PHE
2	4	128	ILE
2	k	181	ALA
3	H	114	ALA
3	I	202	THR
3	I	242	GLU
3	K	119	LEU
3	K	121	THR
3	K	332	GLU
3	L	310	PRO
3	L	389	ILE

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Mol	Chain	Res	Type
3	M	284	ILE
3	M	393	LYS
3	J	212	VAL
3	J	247	ALA
2	h	200	SER
2	k	135	LYS
2	5	194	ASP
2	n	30	ARG
3	I	304	ASP
3	L	113	LEU
3	L	134	GLU
3	J	135	LYS
1	a	54	VAL
2	5	191	ILE
2	6	128	ILE
2	n	200	SER
3	H	217	GLY
3	L	132	VAL
1	D	64	ILE
2	m	130	GLY
3	H	60	SER
3	I	163	LYS
3	H	246	ILE
3	K	310	PRO
3	J	310	PRO
1	d	12	ILE
2	j	185	GLY
2	5	200	SER
2	n	129	GLY
3	K	212	VAL
3	L	136	PRO
2	i	207	ILE
2	6	130	GLY
2	6	200	SER
3	K	235	PRO

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%)	190 (94%)	13 (6%)	16	37
1	B	203/203 (100%)	198 (98%)	5 (2%)	42	63
1	C	203/203 (100%)	193 (95%)	10 (5%)	22	43
1	D	203/203 (100%)	198 (98%)	5 (2%)	42	63
1	E	203/203 (100%)	192 (95%)	11 (5%)	20	41
1	F	203/203 (100%)	192 (95%)	11 (5%)	20	41
1	G	203/203 (100%)	190 (94%)	13 (6%)	16	37
1	a	199/203 (98%)	193 (97%)	6 (3%)	36	57
1	b	199/203 (98%)	187 (94%)	12 (6%)	17	39
1	c	199/203 (98%)	191 (96%)	8 (4%)	28	49
1	d	199/203 (98%)	191 (96%)	8 (4%)	28	49
1	e	199/203 (98%)	192 (96%)	7 (4%)	32	53
1	f	199/203 (98%)	189 (95%)	10 (5%)	22	43
1	g	199/203 (98%)	193 (97%)	6 (3%)	36	57
2	1	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	2	164/164 (100%)	150 (92%)	14 (8%)	10	29
2	3	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	4	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	5	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	6	164/164 (100%)	154 (94%)	10 (6%)	17	38
2	7	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	h	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	i	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	j	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	k	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	l	164/164 (100%)	159 (97%)	5 (3%)	36	57
2	m	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	n	164/164 (100%)	156 (95%)	8 (5%)	22	43
3	H	338/338 (100%)	328 (97%)	10 (3%)	36	57
3	I	338/338 (100%)	321 (95%)	17 (5%)	22	43
3	J	338/338 (100%)	329 (97%)	9 (3%)	39	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	338/338 (100%)	324 (96%)	14 (4%)	27	49
3	L	338/338 (100%)	323 (96%)	15 (4%)	25	47
3	M	338/338 (100%)	325 (96%)	13 (4%)	29	50
All	All	7138/7166 (100%)	6835 (96%)	303 (4%)	28	48

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	17	PRO
1	A	42	CYS
1	A	67	ILE
1	A	98	ILE
1	A	104	ASP
1	A	108	THR
1	A	134	VAL
1	A	144	VAL
1	A	152	PRO
1	A	201	GLU
1	A	226	PRO
1	A	229	LEU
1	a	13	THR
1	a	14	VAL
1	a	21	LEU
1	a	87	VAL
1	a	156	LEU
1	a	213	TYR
1	B	6	MET
1	B	12	ILE
1	B	56	SER
1	B	152	PRO
1	B	205	VAL
1	b	13	THR
1	b	15	PHE
1	b	28	ARG
1	b	31	VAL
1	b	59	LEU
1	b	102	THR
1	b	108	THR
1	b	109	VAL
1	b	144	VAL

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Mol	Chain	Res	Type
1	b	177	LYS
1	b	198	LEU
1	b	235	ARG
1	C	36	THR
1	C	47	ILE
1	C	66	LYS
1	C	67	ILE
1	C	68	TYR
1	C	106	PRO
1	C	124	THR
1	C	134	VAL
1	C	208	ASN
1	C	245	LYS
1	c	14	VAL
1	c	38	ILE
1	c	57	LYS
1	c	58	LEU
1	c	106	PRO
1	c	166	MET
1	c	209	ILE
1	c	213	TYR
1	D	82	VAL
1	D	102	THR
1	D	147	LEU
1	D	226	PRO
1	D	231	PRO
1	d	15	PHE
1	d	21	LEU
1	d	40	ILE
1	d	59	LEU
1	d	64	ILE
1	d	99	ASN
1	d	134	VAL
1	d	142	ASP
1	E	13	THR
1	E	33	ARG
1	E	43	LYS
1	E	46	VAL
1	E	82	VAL
1	E	98	ILE
1	E	147	LEU
1	E	162	THR

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Mol	Chain	Res	Type
1	E	164	ILE
1	E	213	TYR
1	E	220	THR
1	e	40	ILE
1	e	46	VAL
1	e	59	LEU
1	e	62	ASP
1	e	208	ASN
1	e	224	VAL
1	e	235	ARG
1	F	54	VAL
1	F	64	ILE
1	F	89	ILE
1	F	121	GLN
1	F	142	ASP
1	F	162	THR
1	F	164	ILE
1	F	166	MET
1	F	208	ASN
1	F	238	GLU
1	F	243	LEU
1	f	13	THR
1	f	21	LEU
1	f	40	ILE
1	f	57	LYS
1	f	78	THR
1	f	138	ILE
1	f	164	ILE
1	f	178	GLU
1	f	193	LEU
1	f	229	LEU
1	G	9	ASP
1	G	21	LEU
1	G	22	PHE
1	G	24	VAL
1	G	57	LYS
1	G	64	ILE
1	G	102	THR
1	G	121	GLN
1	G	144	VAL
1	G	176	GLU
1	G	206	PRO

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Mol	Chain	Res	Type
1	G	209	ILE
1	G	224	VAL
1	g	17	PRO
1	g	47	ILE
1	g	81	LEU
1	g	129	VAL
1	g	152	PRO
1	g	190	VAL
2	1	28	GLU
2	1	45	ILE
2	1	64	GLN
2	1	111	LEU
2	1	136	ASP
2	1	161	VAL
2	1	191	ILE
2	h	17	LEU
2	h	33	MET
2	h	52	MET
2	h	76	LEU
2	h	107	LEU
2	h	156	THR
2	h	189	VAL
2	h	205	GLU
2	2	14	THR
2	2	17	LEU
2	2	27	THR
2	2	32	THR
2	2	45	ILE
2	2	71	LYS
2	2	84	LYS
2	2	110	LEU
2	2	122	ILE
2	2	150	VAL
2	2	156	THR
2	2	170	ARG
2	2	201	PRO
2	2	208	LEU
2	i	45	ILE
2	i	56	THR
2	i	72	ILE
2	i	107	LEU
2	i	122	ILE

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Mol	Chain	Res	Type
2	i	137	ILE
2	i	140	THR
2	i	191	ILE
2	i	203	GLU
2	3	19	CYS
2	3	32	THR
2	3	69	ILE
2	3	161	VAL
2	3	191	ILE
2	3	213	LYS
2	j	23	VAL
2	j	45	ILE
2	j	132	ILE
2	j	148	TYR
2	j	189	VAL
2	j	190	LYS
2	4	28	GLU
2	4	128	ILE
2	4	136	ASP
2	4	140	THR
2	4	151	LEU
2	4	195	GLU
2	4	207	ILE
2	k	136	ASP
2	k	161	VAL
2	k	169	VAL
2	k	180	SER
2	5	33	MET
2	5	45	ILE
2	5	72	ILE
2	5	132	ILE
2	5	198	GLN
2	5	205	GLU
2	l	72	ILE
2	l	117	SER
2	l	136	ASP
2	l	137	ILE
2	l	146	THR
2	6	27	THR
2	6	28	GLU
2	6	45	ILE
2	6	72	ILE

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Mol	Chain	Res	Type
2	6	76	LEU
2	6	127	PRO
2	6	128	ILE
2	6	140	THR
2	6	162	ASP
2	6	202	GLU
2	m	107	LEU
2	m	108	VAL
2	m	156	THR
2	m	192	THR
2	7	28	GLU
2	7	40	LYS
2	7	64	GLN
2	7	72	ILE
2	7	108	VAL
2	7	182	SER
2	n	27	THR
2	n	87	VAL
2	n	161	VAL
2	n	170	ARG
2	n	174	SER
2	n	189	VAL
2	n	201	PRO
2	n	213	LYS
3	H	142	ASP
3	H	183	PRO
3	H	190	LEU
3	H	218	GLU
3	H	241	ASP
3	H	252	ASN
3	H	264	THR
3	H	294	ASP
3	H	327	LYS
3	H	332	GLU
3	I	10	LEU
3	I	35	LYS
3	I	41	ARG
3	I	81	SER
3	I	88	VAL
3	I	91	THR
3	I	95	ILE
3	I	116	VAL

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Mol	Chain	Res	Type
3	I	125	PRO
3	I	174	PRO
3	I	250	ARG
3	I	260	GLU
3	I	268	LEU
3	I	275	PHE
3	I	361	PHE
3	I	384	LYS
3	I	398	VAL
3	K	48	VAL
3	K	106	VAL
3	K	112	THR
3	K	127	VAL
3	K	138	VAL
3	K	140	TYR
3	K	148	VAL
3	K	165	GLU
3	K	176	LYS
3	K	190	LEU
3	K	207	VAL
3	K	250	ARG
3	K	265	MET
3	K	384	LYS
3	L	67	VAL
3	L	77	VAL
3	L	85	PRO
3	L	93	GLN
3	L	127	VAL
3	L	160	PRO
3	L	165	GLU
3	L	189	THR
3	L	200	ARG
3	L	214	LYS
3	L	255	THR
3	L	258	ASP
3	L	298	LEU
3	L	330	LEU
3	L	333	ASP
3	M	61	PRO
3	M	67	VAL
3	M	77	VAL
3	M	89	VAL

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Mol	Chain	Res	Type
3	M	90	ASN
3	M	118	VAL
3	M	149	GLN
3	M	272	LEU
3	M	283	VAL
3	M	321	PHE
3	M	327	LYS
3	M	385	LYS
3	M	390	PRO
3	J	61	PRO
3	J	79	VAL
3	J	89	VAL
3	J	106	VAL
3	J	110	GLN
3	J	122	SER
3	J	133	GLU
3	J	371	THR
3	J	381	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	97	GLN
1	A	99	ASN
1	A	121	GLN
1	a	23	GLN
1	B	169	ASN
1	B	208	ASN
1	C	23	GLN
1	C	169	ASN
1	C	237	ASN
1	c	97	GLN
1	c	99	ASN
1	c	125	GLN
1	c	237	ASN
1	D	5	GLN
1	D	121	GLN
1	D	169	ASN
1	D	208	ASN
1	d	23	GLN
1	d	122	GLN

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Mol	Chain	Res	Type
1	d	169	ASN
1	d	237	ASN
1	E	73	HIS
1	E	121	GLN
1	E	122	GLN
1	F	122	GLN
1	f	73	HIS
1	f	125	GLN
1	G	73	HIS
1	G	97	GLN
1	G	121	GLN
1	g	99	ASN
1	g	121	GLN
1	g	122	GLN
2	1	47	GLN
2	1	109	GLN
2	1	198	GLN
2	h	75	ASN
2	h	96	ASN
2	2	75	ASN
2	i	64	GLN
2	3	64	GLN
2	3	75	ASN
2	3	96	ASN
2	3	109	GLN
2	j	198	GLN
2	4	47	GLN
2	k	75	ASN
2	5	96	ASN
2	5	109	GLN
2	5	206	GLN
2	l	47	GLN
2	l	64	GLN
2	l	99	ASN
2	6	96	ASN
2	m	35	ASN
2	m	96	ASN
2	m	99	ASN
2	7	96	ASN
2	n	96	ASN
2	n	206	GLN
3	H	110	GLN

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Mol	Chain	Res	Type
3	H	149	GLN
3	H	197	ASN
3	H	213	GLN
3	I	96	ASN
3	I	197	ASN
3	I	267	GLN
3	K	90	ASN
3	K	110	GLN
3	K	198	GLN
3	K	213	GLN
3	K	228	GLN
3	K	324	HIS
3	L	111	GLN
3	L	262	GLN
3	L	319	GLN
3	L	324	HIS
3	M	90	ASN
3	M	149	GLN
3	M	197	ASN
3	M	252	ASN
3	J	90	ASN
3	J	198	GLN
3	J	288	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	3.18	6 (18%)	48,52,52	1.36	6 (12%)
4	ATP	I	401	5	32,33,33	4.12	7 (21%)	48,52,52	1.90	14 (29%)
4	ATP	L	401	5	32,33,33	3.89	8 (25%)	48,52,52	1.40	6 (12%)
4	ATP	K	401	5	32,33,33	4.43	6 (18%)	48,52,52	1.59	10 (20%)
6	ADP	M	401	5	28,29,29	1.73	7 (25%)	43,45,45	1.33	6 (13%)

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	-	5/22/38/38	0/3/3/3
4	ATP	I	401	5	-	6/22/38/38	0/3/3/3
4	ATP	L	401	5	-	9/22/38/38	0/3/3/3
4	ATP	K	401	5	-	11/22/38/38	0/3/3/3
6	ADP	M	401	5	-	6/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	401	ATP	PB-O3A	17.30	1.78	1.59
4	L	401	ATP	PB-O3B	15.71	1.76	1.59
4	K	401	ATP	PB-O3B	15.67	1.76	1.59
4	I	401	ATP	PB-O3B	14.11	1.74	1.59
4	K	401	ATP	PB-O3A	13.22	1.73	1.59
4	L	401	ATP	PB-O3A	13.05	1.73	1.59
4	J	401	ATP	PB-O3B	12.61	1.73	1.59
4	K	401	ATP	PA-O3A	12.52	1.73	1.59
4	J	401	ATP	PB-O3A	8.86	1.69	1.59
6	M	401	ADP	PA-O3A	5.75	1.65	1.59
4	J	401	ATP	PA-O3A	5.70	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	401	ATP	C5-C4	3.45	1.45	1.39
4	L	401	ATP	C2'-C1'	-3.35	1.43	1.53
4	L	401	ATP	C4-N3	-3.32	1.28	1.34
4	I	401	ATP	C4-N3	3.11	1.40	1.34
6	M	401	ADP	C5'-C4'	3.01	1.60	1.51
4	K	401	ATP	C5-N7	-2.99	1.33	1.39
4	L	401	ATP	C8-N7	-2.97	1.26	1.31
4	K	401	ATP	C2-N3	2.83	1.39	1.33
4	J	401	ATP	C5-N7	-2.79	1.34	1.39
4	K	401	ATP	O4'-C4'	2.75	1.51	1.45
6	M	401	ADP	C8-N9	-2.50	1.33	1.37
4	L	401	ATP	O4'-C1'	2.36	1.47	1.42
4	J	401	ATP	PA-O2A	-2.36	1.44	1.55
4	L	401	ATP	PA-O3A	2.30	1.62	1.59
4	I	401	ATP	C2'-C3'	-2.27	1.47	1.53
6	M	401	ADP	C6-N6	2.23	1.39	1.34
4	I	401	ATP	PA-O3A	2.21	1.61	1.59
6	M	401	ADP	C1'-N9	-2.14	1.40	1.46
6	M	401	ADP	PB-O1B	2.12	1.57	1.50
6	M	401	ADP	C2'-C3'	2.05	1.58	1.53
4	I	401	ATP	PG-O3G	-2.04	1.47	1.54
4	I	401	ATP	O2'-C2'	-2.04	1.37	1.43
4	L	401	ATP	O4'-C4'	2.04	1.49	1.45

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	401	ATP	C6-C5-C4	4.73	123.63	117.18
4	K	401	ATP	N6-C6-N1	4.49	128.38	118.38
4	I	401	ATP	N6-C6-N1	4.24	127.83	118.38
4	K	401	ATP	C4-N9-C8	-3.99	101.54	105.74
4	I	401	ATP	C5-C4-N3	-3.96	121.26	126.72
4	J	401	ATP	C6-C5-C4	3.87	122.46	117.18
4	I	401	ATP	C5'-C4'-C3'	-3.81	101.49	115.21
4	I	401	ATP	N3-C2-N1	3.75	134.26	128.58
6	M	401	ADP	C6-C5-C4	3.65	122.16	117.18
4	J	401	ATP	C5-C4-N3	-3.40	122.03	126.72
4	K	401	ATP	C6-C5-C4	3.24	121.60	117.18
4	I	401	ATP	C2'-C3'-C4'	3.23	108.85	102.61
4	L	401	ATP	O3B-PB-O1B	-3.20	101.09	110.70
4	I	401	ATP	C4'-O4'-C1'	2.93	115.94	109.47
4	L	401	ATP	C1'-N9-C8	2.82	133.34	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	401	ATP	O3A-PA-O1A	-2.77	102.37	110.70
4	K	401	ATP	O3A-PA-O1A	-2.76	102.40	110.70
6	M	401	ADP	C5-C4-N3	-2.74	122.94	126.72
4	I	401	ATP	O4'-C1'-N9	2.40	112.71	108.09
4	J	401	ATP	O5'-C5'-C4'	2.39	117.12	108.99
4	K	401	ATP	C5-C6-N6	-2.38	117.40	123.29
4	L	401	ATP	C4-N9-C1'	-2.36	121.11	126.63
6	M	401	ADP	N6-C6-N1	2.36	123.63	118.38
6	M	401	ADP	C4-C5-N7	-2.33	107.91	110.58
4	I	401	ATP	O3G-PG-O2G	2.32	116.51	107.80
4	K	401	ATP	C5-N7-C8	2.31	107.08	103.45
4	K	401	ATP	N3-C2-N1	-2.29	125.11	128.58
6	M	401	ADP	O4'-C4'-C3'	2.28	109.69	105.15
4	I	401	ATP	C5-C4-N9	2.24	108.25	105.81
4	I	401	ATP	C4-N9-C8	-2.21	103.41	105.74
4	J	401	ATP	N3-C2-N1	2.18	131.88	128.58
4	I	401	ATP	O4'-C4'-C3'	-2.17	100.85	105.15
4	L	401	ATP	O3'-C3'-C4'	2.17	117.30	111.08
4	I	401	ATP	C6-C5-N7	-2.15	127.94	132.09
4	J	401	ATP	C5-N7-C8	2.14	106.82	103.45
4	K	401	ATP	C5-C4-N9	2.11	108.11	105.81
4	J	401	ATP	N3-C4-N9	2.05	130.65	127.17
4	I	401	ATP	O2B-PB-O3A	2.04	112.78	107.27
4	K	401	ATP	C2'-C3'-C4'	2.04	106.54	102.61
6	M	401	ADP	C5-N7-C8	2.01	106.62	103.45
4	L	401	ATP	C4-C5-N7	-2.01	108.28	110.58
4	K	401	ATP	C6-C5-N7	-2.00	128.23	132.09

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	401	ATP	PB-O3B-PG-O2G
4	I	401	ATP	C5'-O5'-PA-O1A
4	I	401	ATP	C4'-C5'-O5'-PA
4	K	401	ATP	PB-O3B-PG-O2G
4	K	401	ATP	PB-O3B-PG-O3G
4	K	401	ATP	C5'-O5'-PA-O1A
4	K	401	ATP	C5'-O5'-PA-O2A
4	K	401	ATP	C5'-O5'-PA-O3A
4	L	401	ATP	PB-O3B-PG-O2G
4	L	401	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	L	401	ATP	C5'-O5'-PA-O3A
6	M	401	ADP	C5'-O5'-PA-O1A
6	M	401	ADP	C5'-O5'-PA-O2A
6	M	401	ADP	C5'-O5'-PA-O3A
4	K	401	ATP	O4'-C4'-C5'-O5'
4	K	401	ATP	C3'-C4'-C5'-O5'
6	M	401	ADP	PB-O3A-PA-O1A
4	I	401	ATP	PB-O3A-PA-O5'
4	I	401	ATP	PG-O3B-PB-O2B
4	K	401	ATP	PG-O3B-PB-O2B
4	L	401	ATP	PA-O3A-PB-O2B
4	L	401	ATP	C5'-O5'-PA-O1A
4	J	401	ATP	C5'-O5'-PA-O3A
4	L	401	ATP	C4'-C5'-O5'-PA
6	M	401	ADP	C4'-C5'-O5'-PA
4	K	401	ATP	C4'-C5'-O5'-PA
4	J	401	ATP	O4'-C4'-C5'-O5'
6	M	401	ADP	PB-O3A-PA-O2A
4	I	401	ATP	PB-O3B-PG-O3G
4	L	401	ATP	PG-O3B-PB-O1B
4	L	401	ATP	PG-O3B-PB-O2B
4	L	401	ATP	PA-O3A-PB-O1B
4	J	401	ATP	PG-O3B-PB-O2B
4	J	401	ATP	PB-O3A-PA-O2A
4	K	401	ATP	PB-O3B-PG-O1G
4	K	401	ATP	PG-O3B-PB-O1B
4	J	401	ATP	PG-O3B-PB-O1B

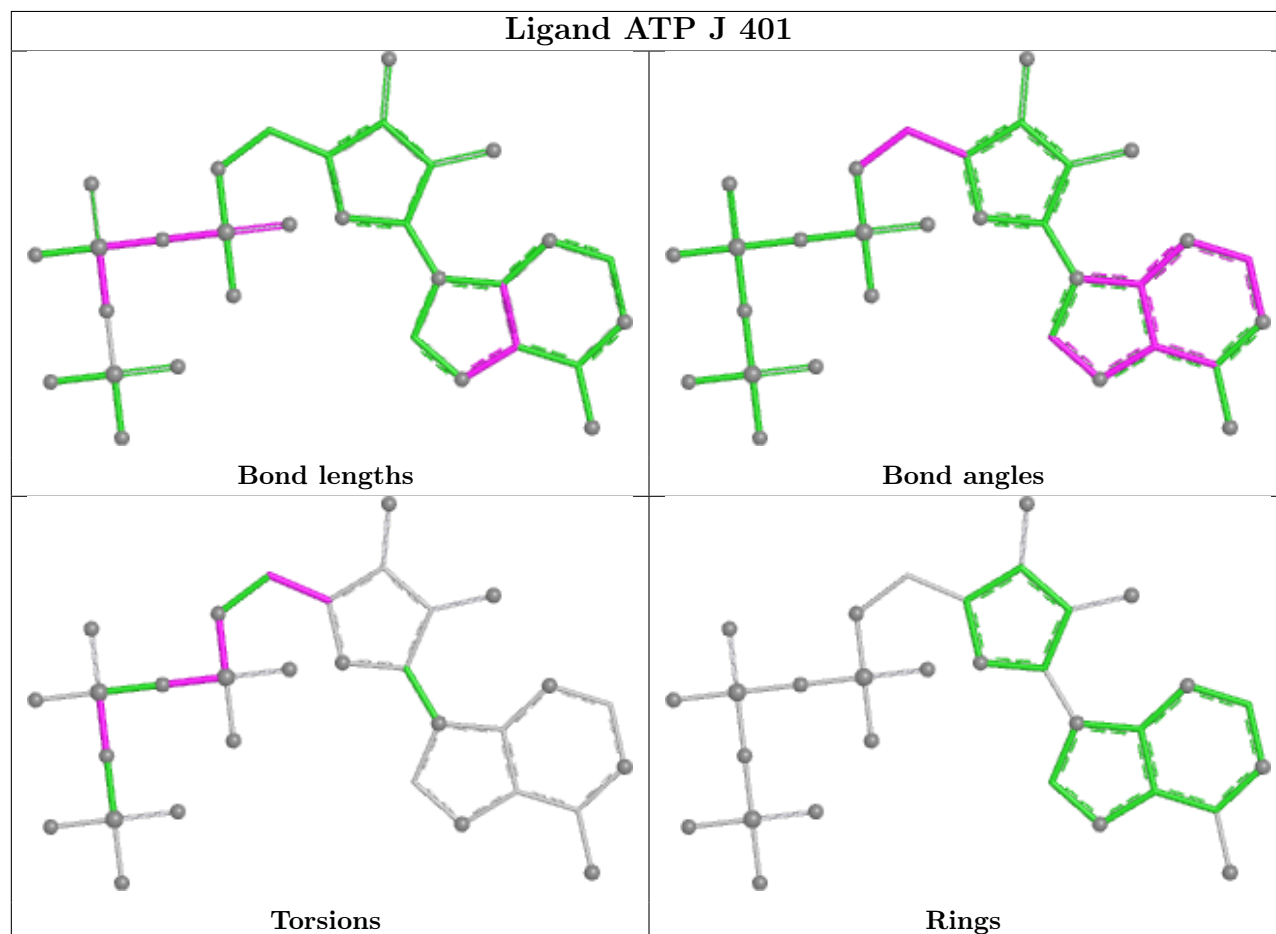
There are no ring outliers.

2 monomers are involved in 3 short contacts:

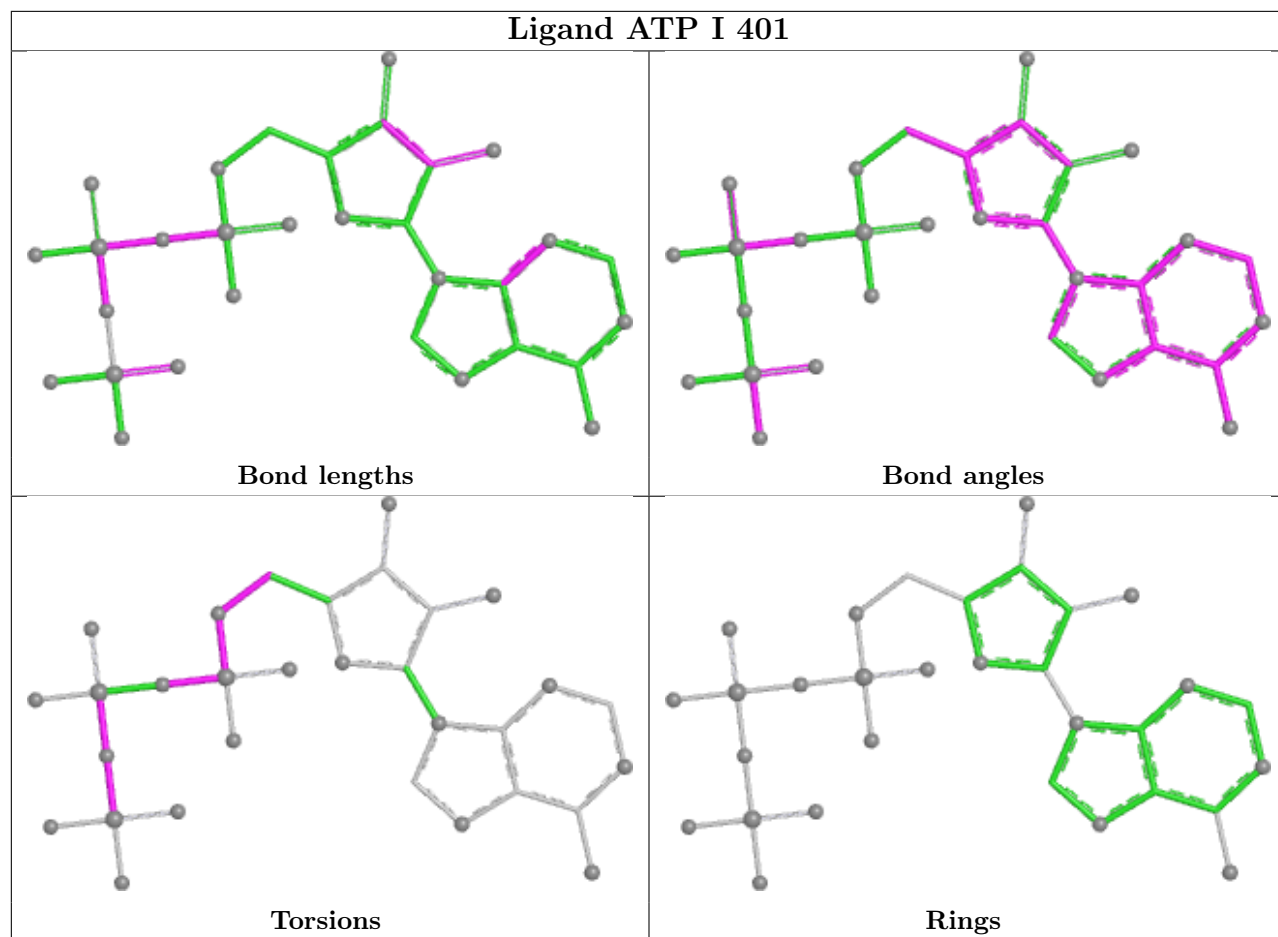
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	401	ATP	1	0
4	L	401	ATP	2	0

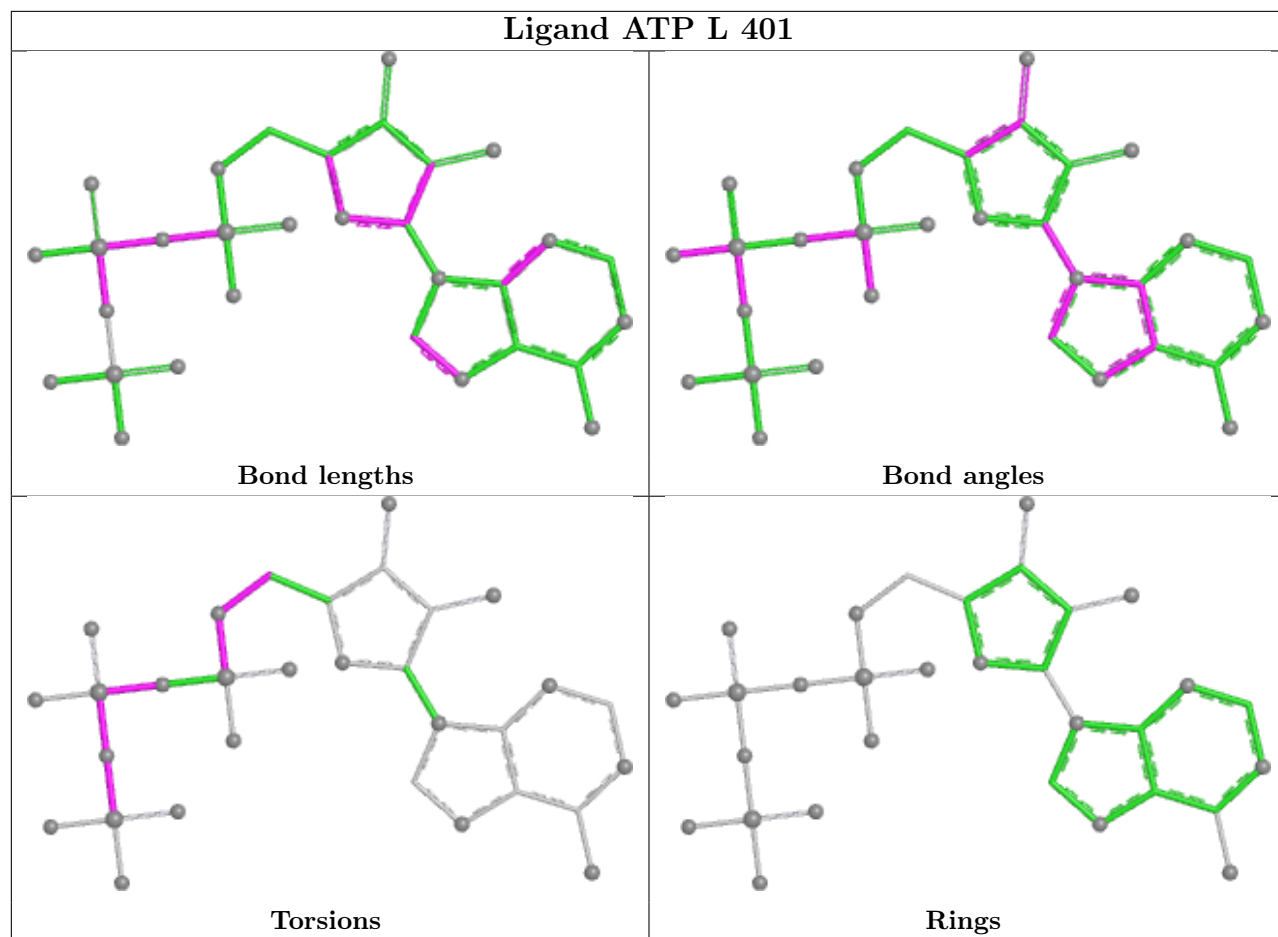
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

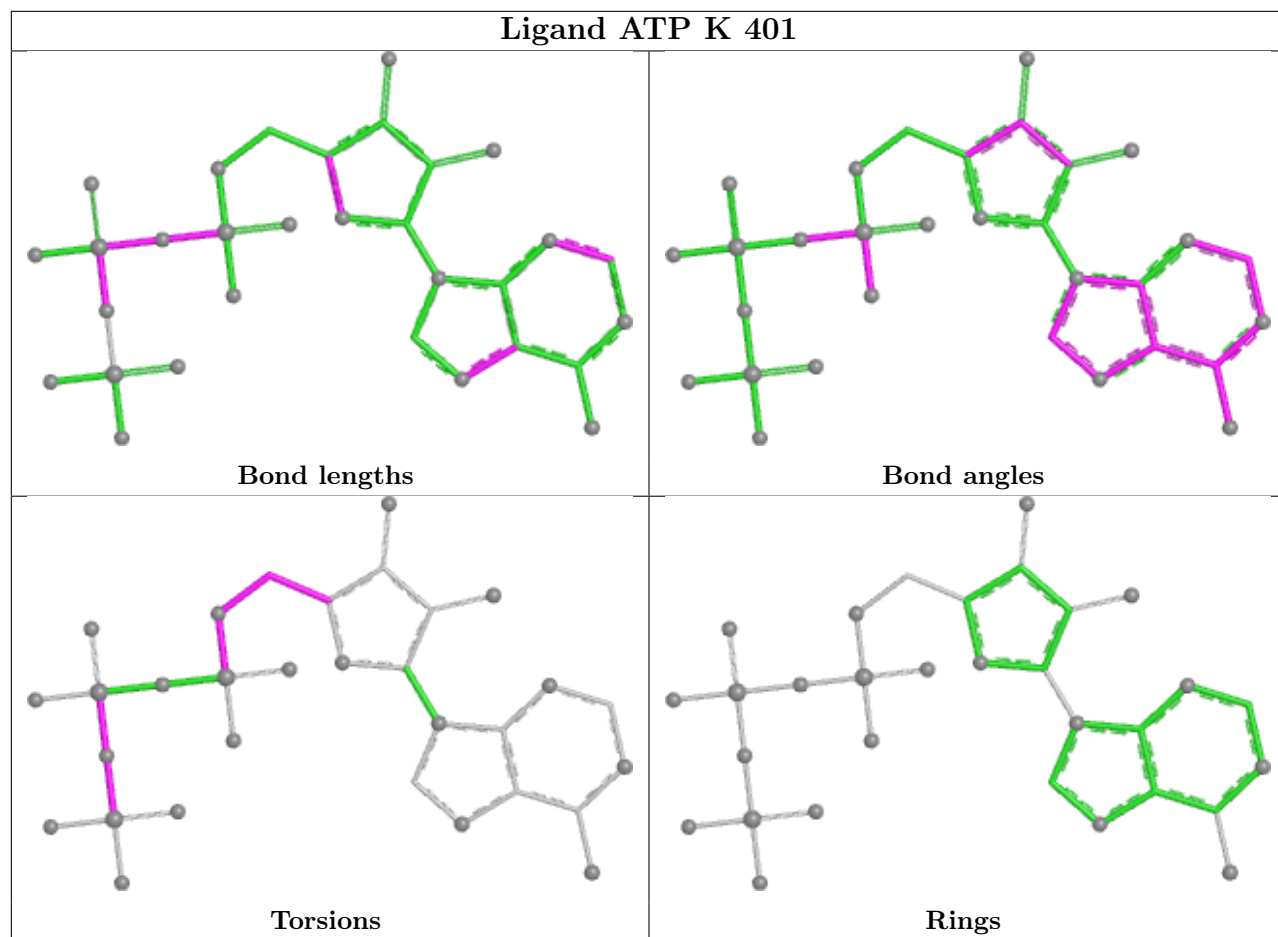


Ligand ATP I 401

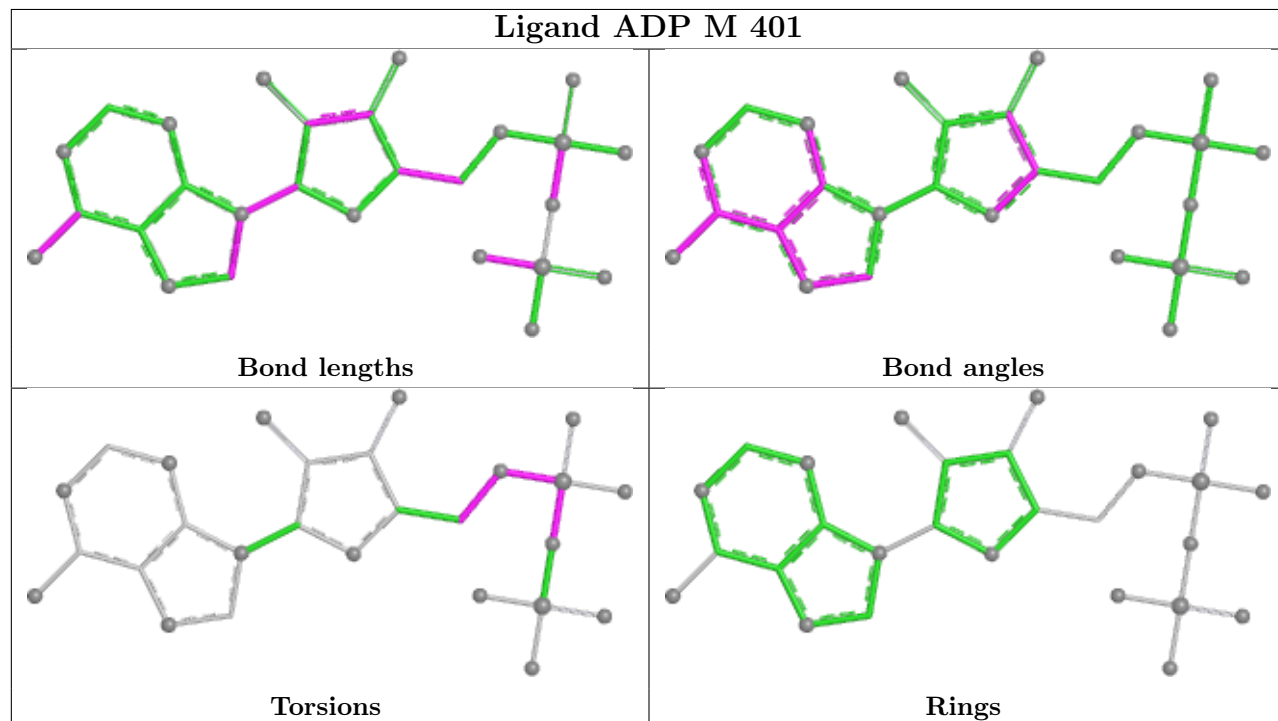




Ligand ATP K 401



Ligand ADP M 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-0212. These allow visual inspection of the internal detail of the map and identification of artifacts.

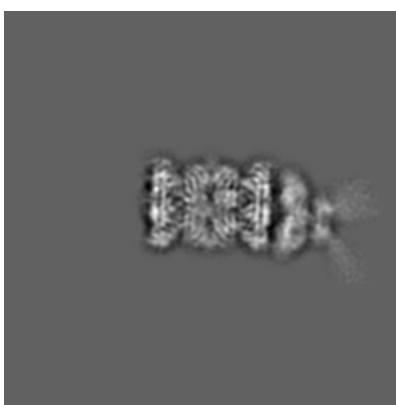
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

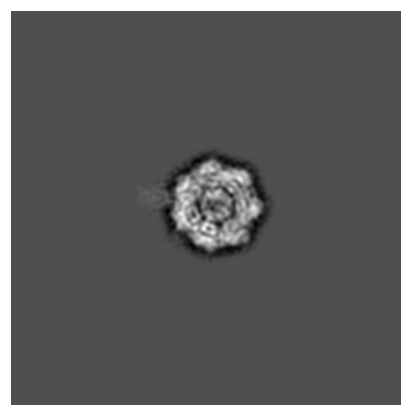
6.1.1 Primary map



X



Y



Z

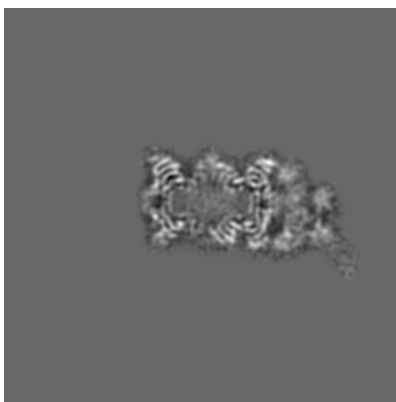
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

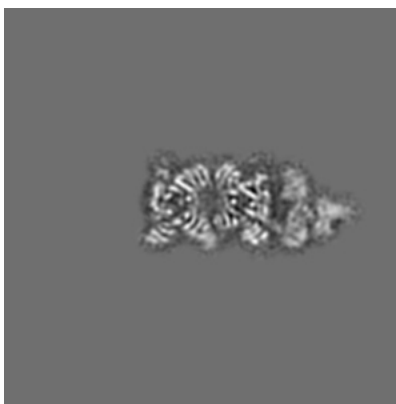
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 180

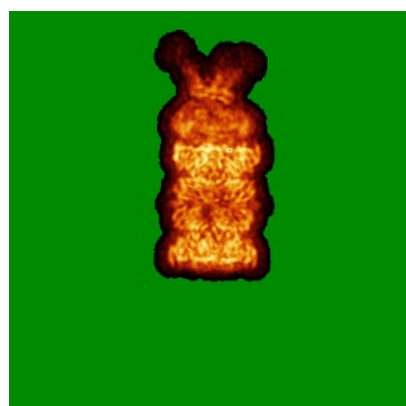


Z Index: 250

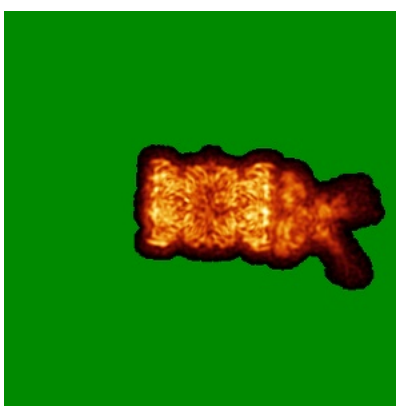
The images above show the largest variance slices of the map in three orthogonal directions.

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

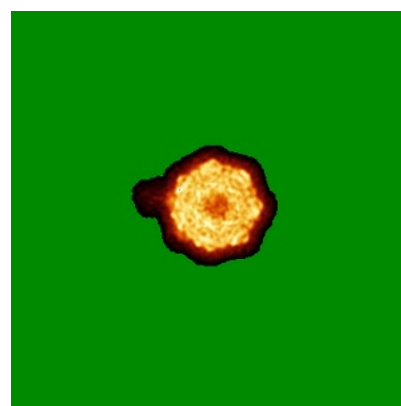
6.4.1 Primary map



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

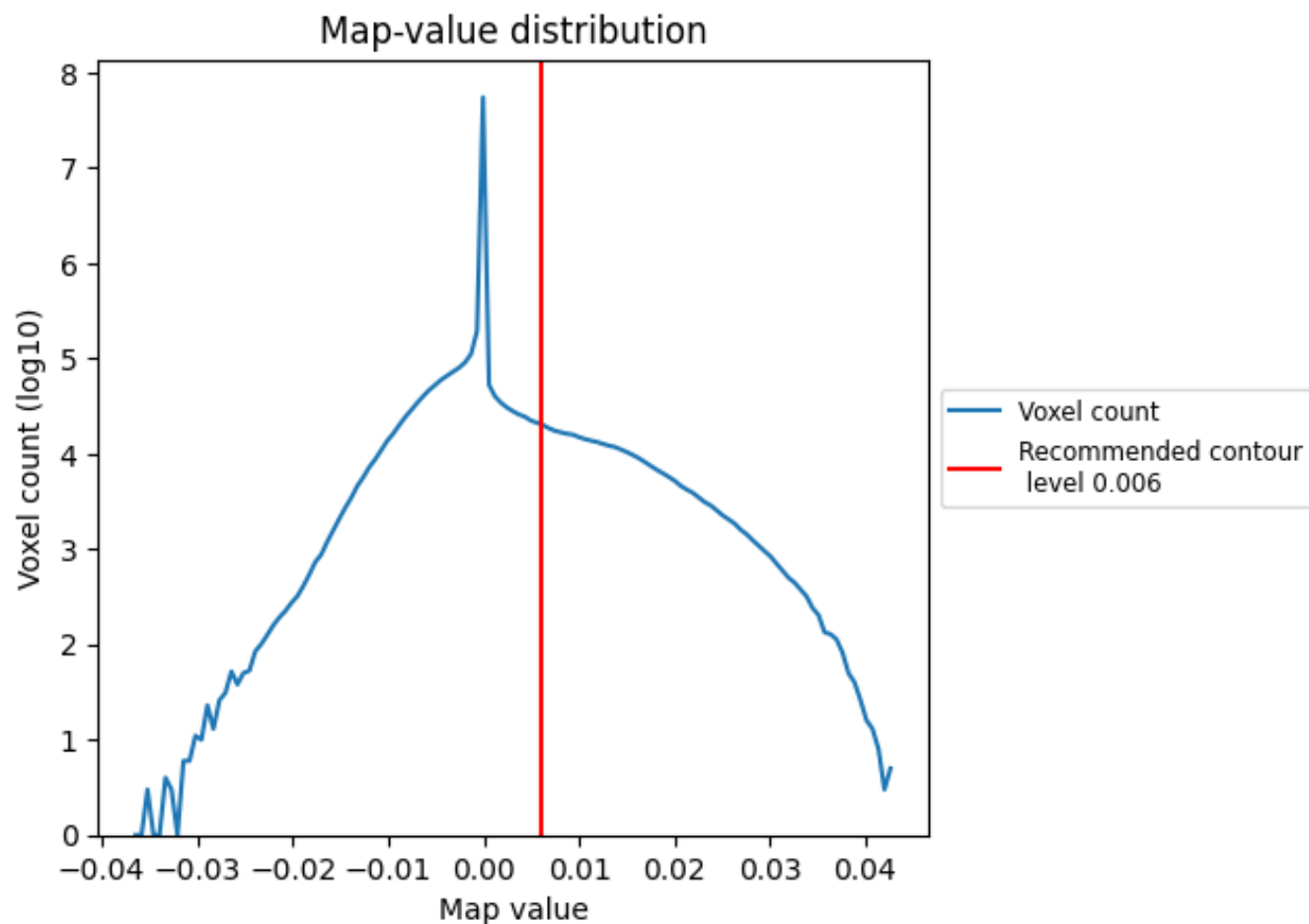
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

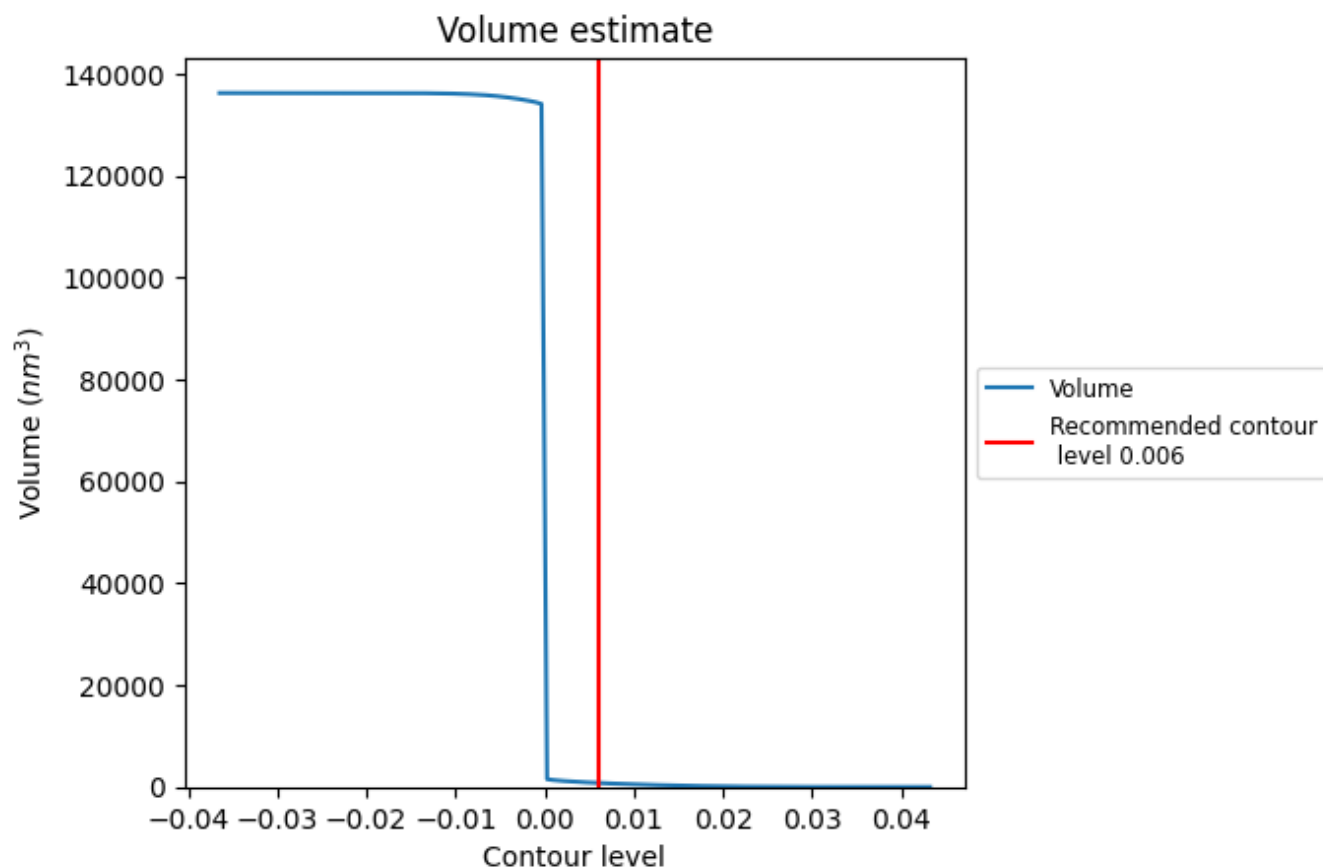
This section contains the results of statistical analysis of the map.

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.

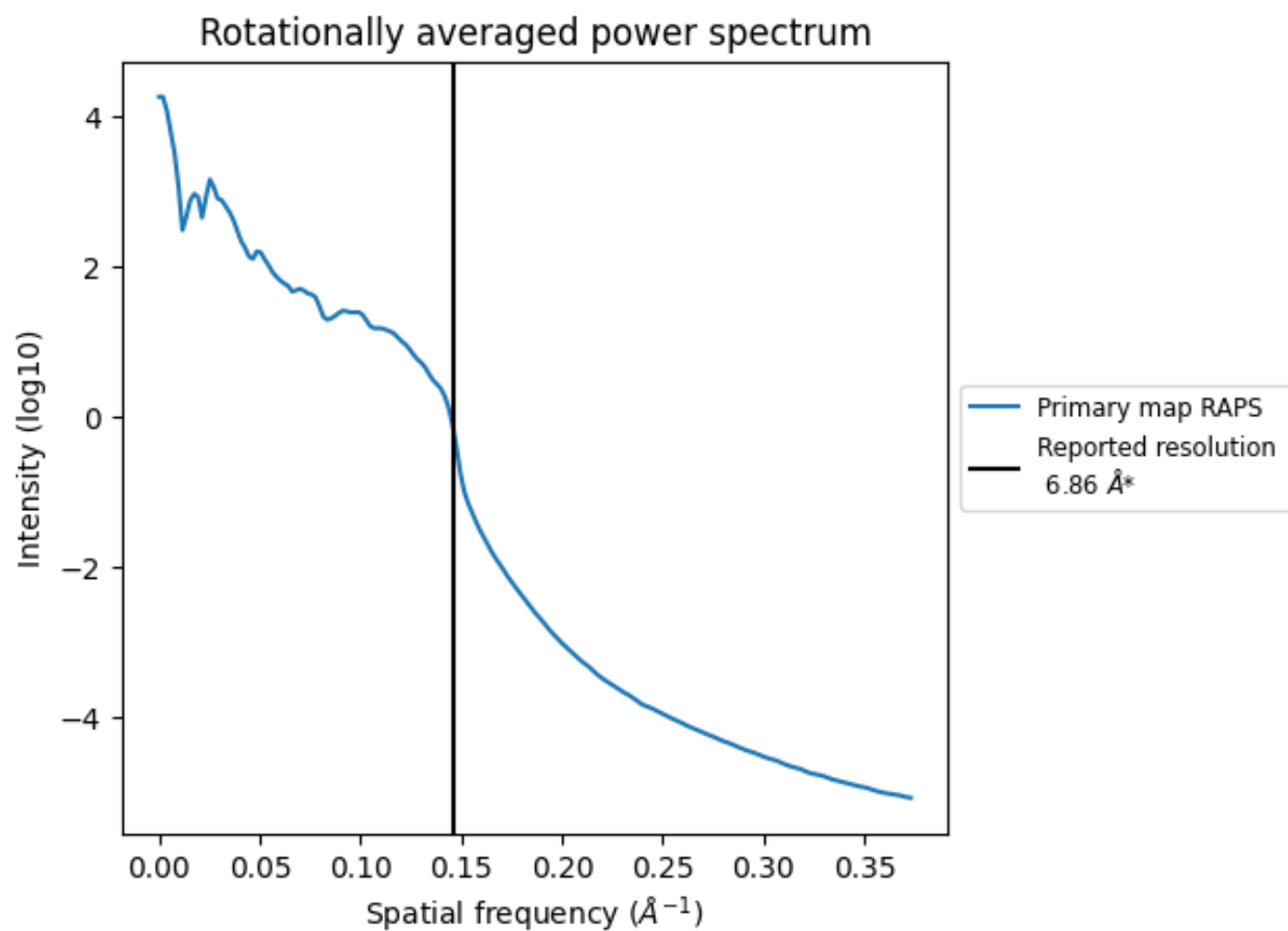
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787 nm^3 ; this corresponds to an approximate mass of 711 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 0.146 Å⁻¹

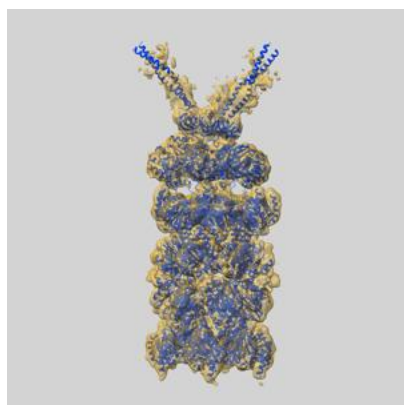
8 Fourier-Shell correlation

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

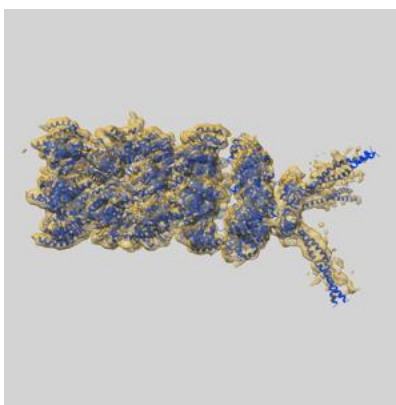
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0212 and PDB model 6HE8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

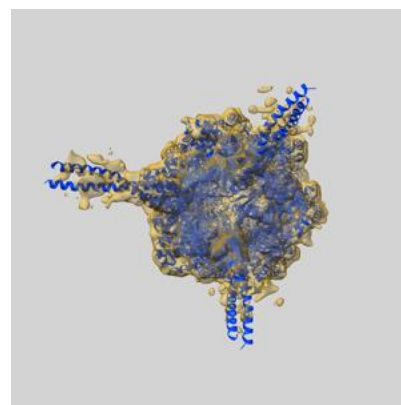
9.1 Map-model overlay [i](#)



X



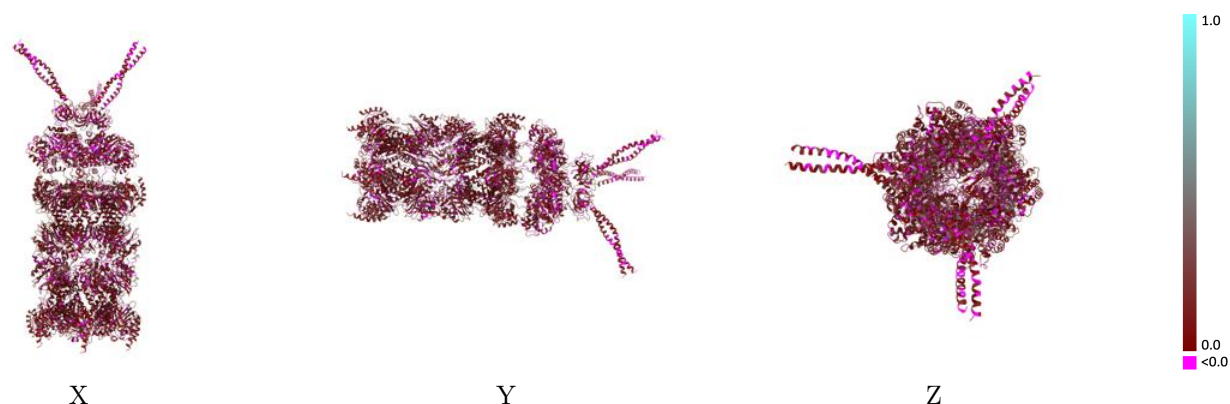
Y



Z

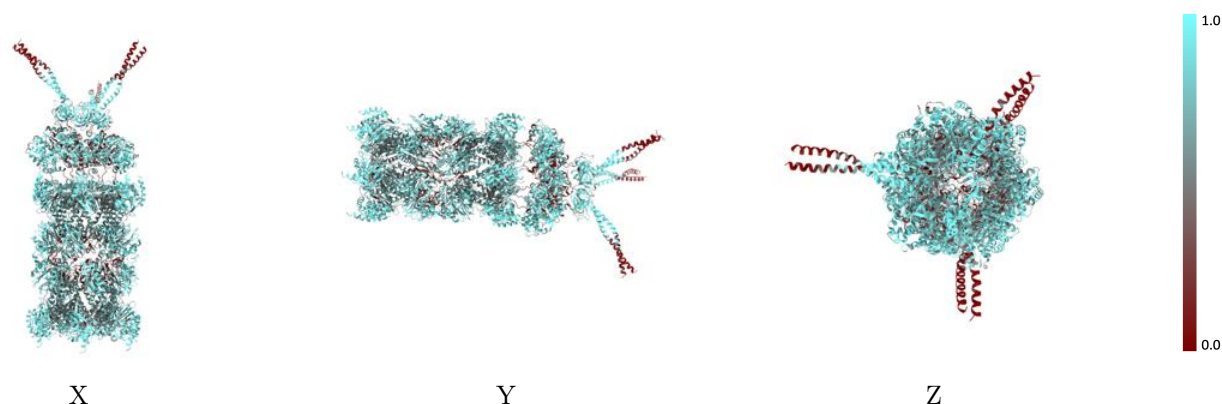
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



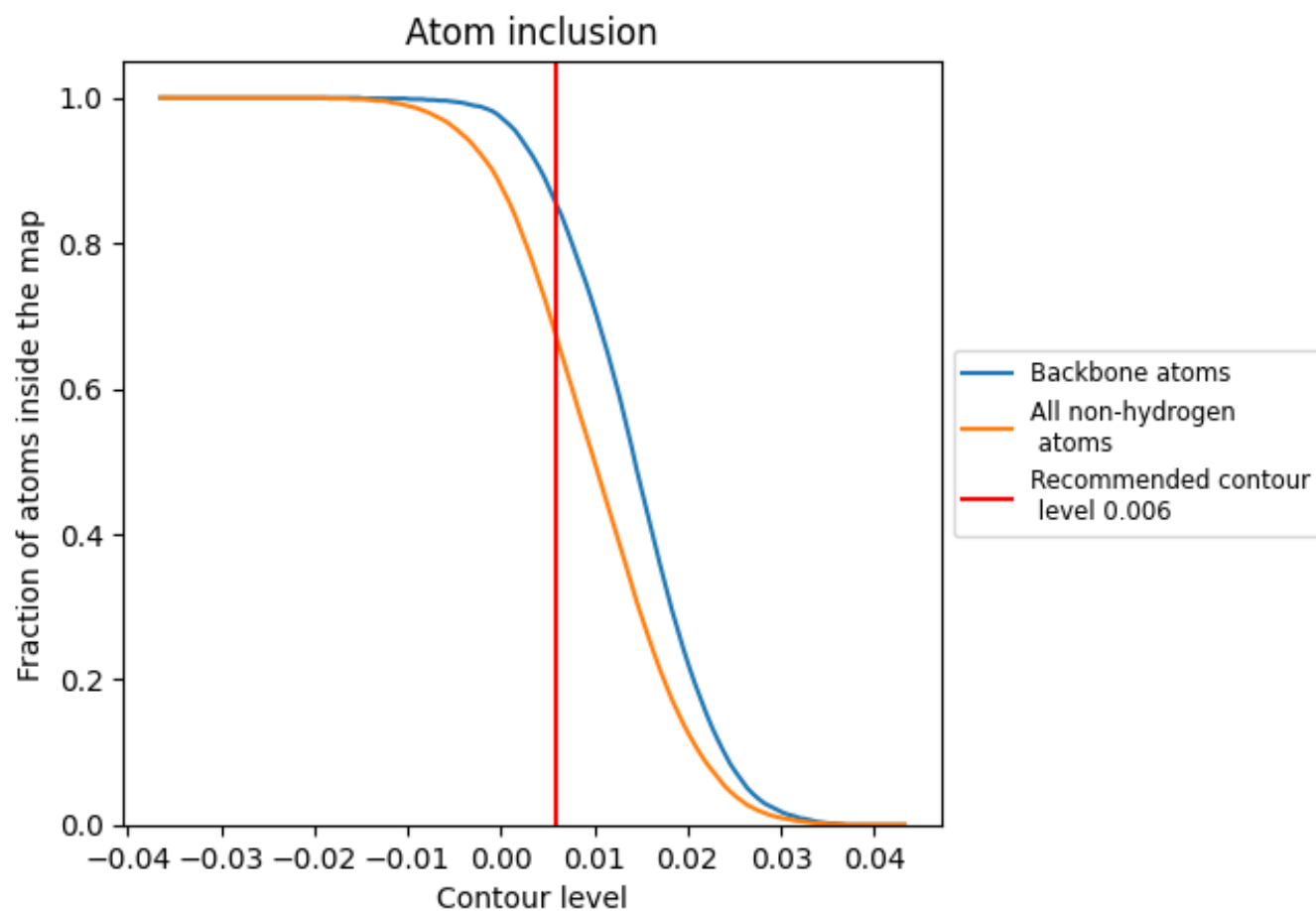
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 67% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.1150
1	 0.6470	 0.1160
2	 0.6690	 0.1270
3	 0.6520	 0.1190
4	 0.6450	 0.1220
5	 0.6520	 0.1300
6	 0.6350	 0.1220
7	 0.6420	 0.1160
A	 0.7150	 0.1320
B	 0.7220	 0.1380
C	 0.7270	 0.1340
D	 0.7070	 0.1290
E	 0.7180	 0.1370
F	 0.7210	 0.1350
G	 0.7180	 0.1330
H	 0.6060	 0.0850
I	 0.6580	 0.0950
J	 0.6580	 0.1000
K	 0.6610	 0.0950
L	 0.6160	 0.0790
M	 0.6100	 0.0830
a	 0.7090	 0.1220
b	 0.7090	 0.1250
c	 0.7050	 0.1210
d	 0.6990	 0.1250
e	 0.7230	 0.1270
f	 0.7010	 0.1200
g	 0.7220	 0.1240
h	 0.6440	 0.1130
i	 0.6620	 0.1240
j	 0.6340	 0.1140
k	 0.6250	 0.1150
l	 0.6500	 0.1180
m	 0.6520	 0.1230
n	 0.6410	 0.1120

