



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:01 AM UTC

PDB ID : 6HEC / pdb_00006hec
EMDB ID : EMD-0215
Title : PAN-proteasome in state 4
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 6.95 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:

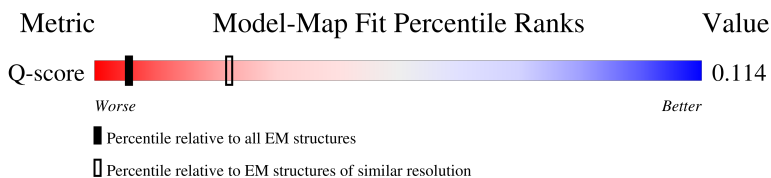
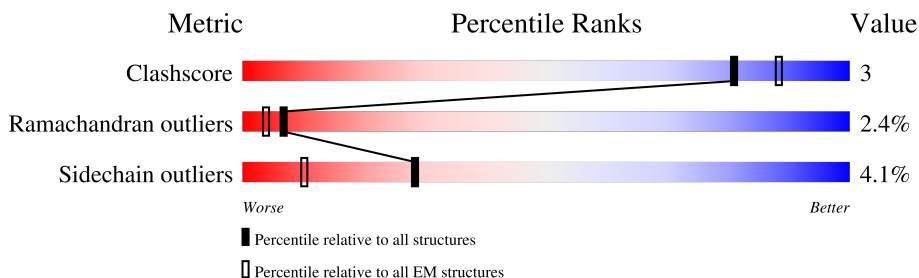
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.95 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	454 (6.45 - 7.41)

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	9% 43% 51% 6%
1	B	242	10% 39% 54% 6%
1	C	242	6% 40% 54% 5%
1	D	242	9% 40% 52% 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	
3	J	390	
3	K	390	
3	L	390	
3	M	390	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ADP	J	401	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 66909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha.

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

- Molecule 2 is a protein called Proteasome subunit beta.

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

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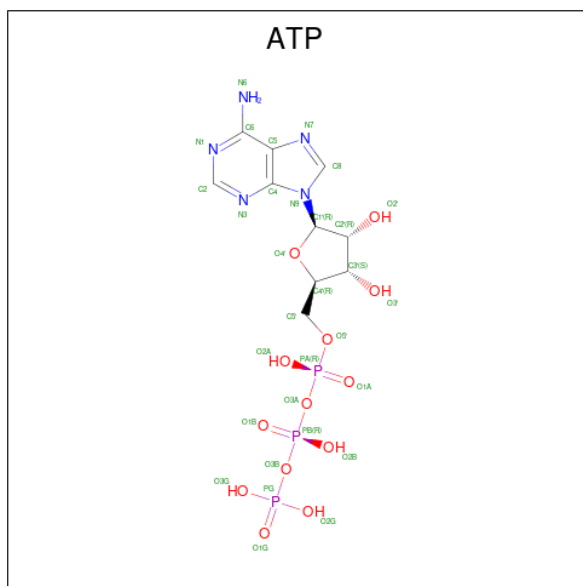
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	i	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	j	202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

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

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

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

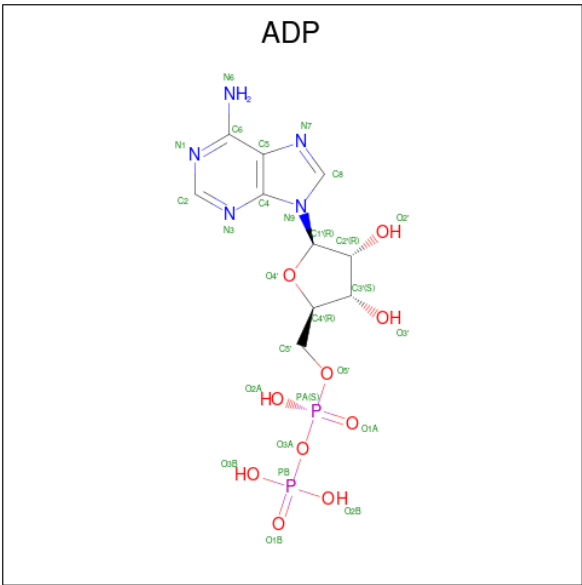


Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

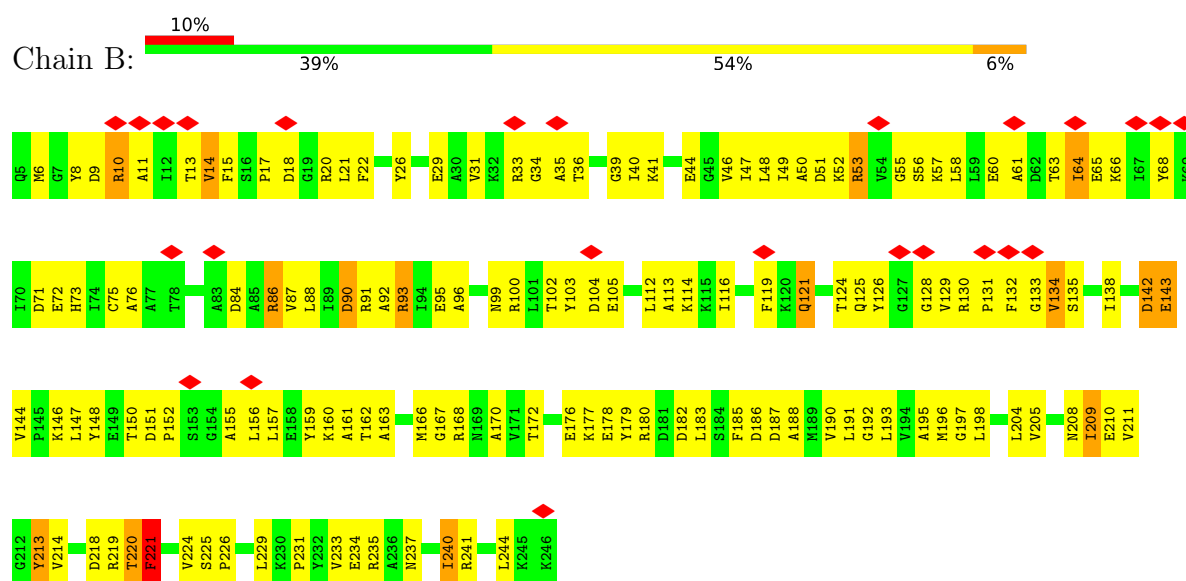
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

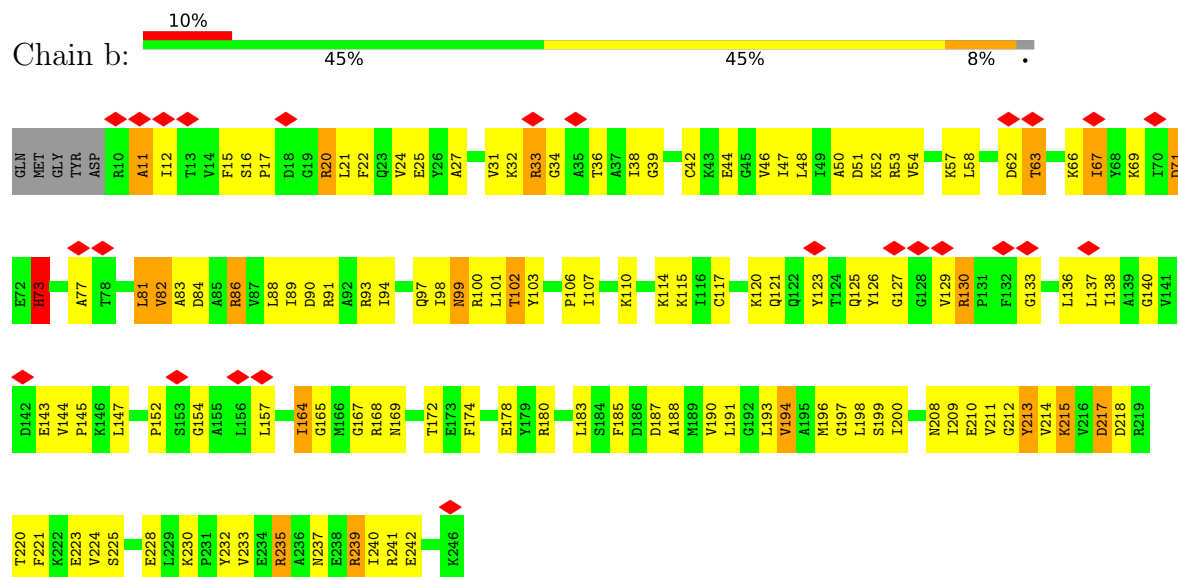
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



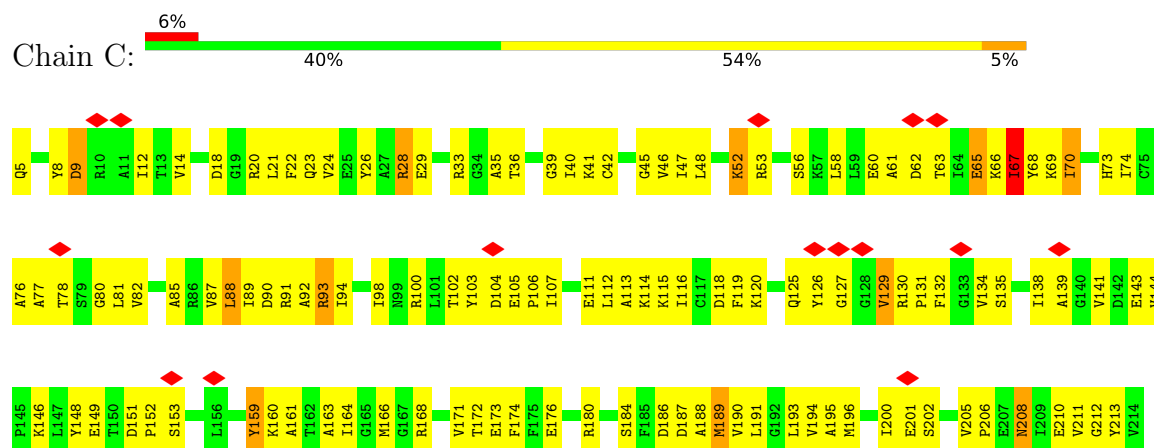
Mol	Chain	Residues	Atoms					AltConf
6	J	1	Total	C	N	O	P	0
			27	10	5	10	2	



• Molecule 1: Proteasome subunit alpha

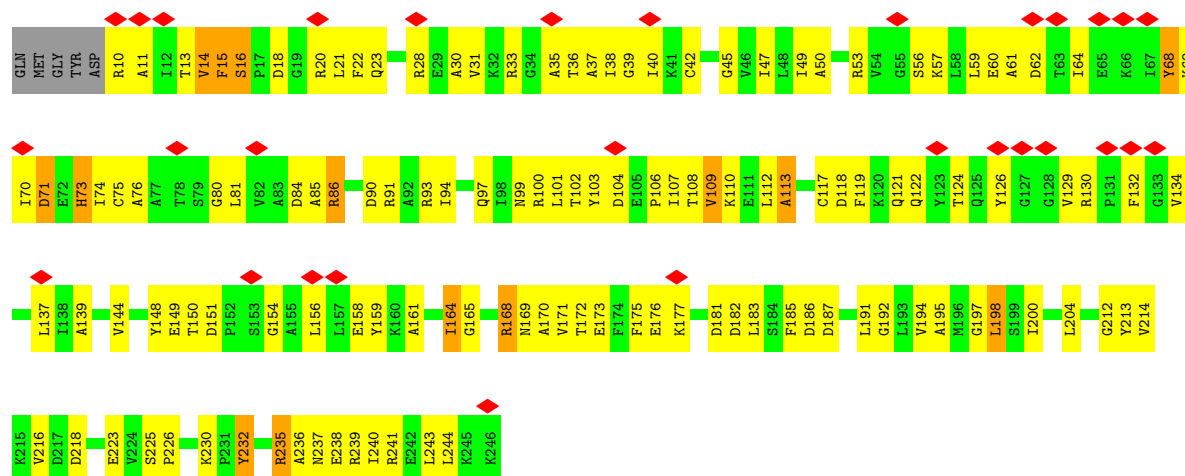


• Molecule 1: Proteasome subunit alpha

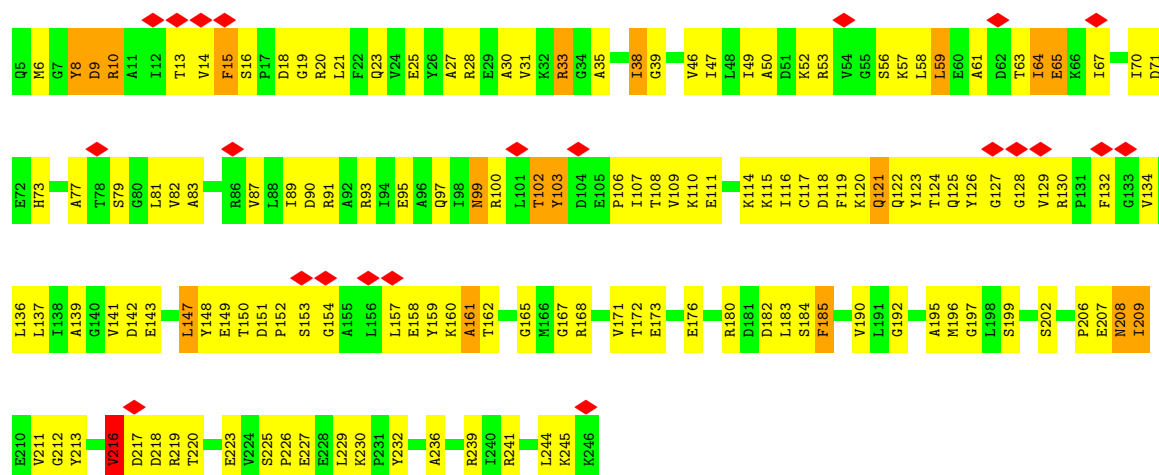




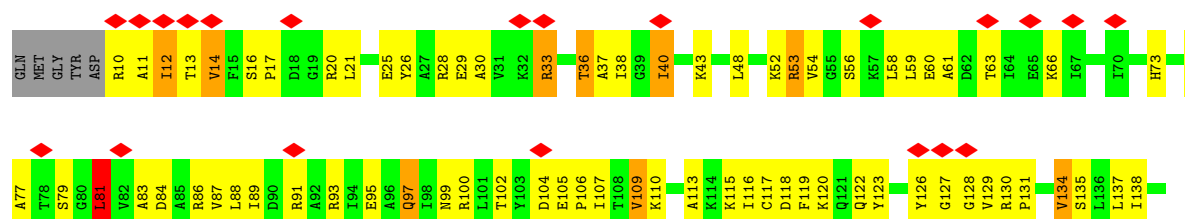
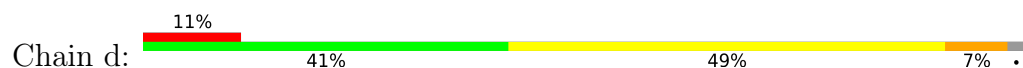
• Molecule 1: Proteasome subunit alpha

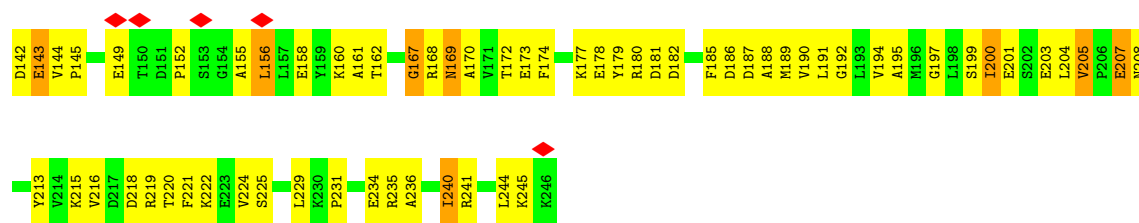


• Molecule 1: Proteasome subunit alpha

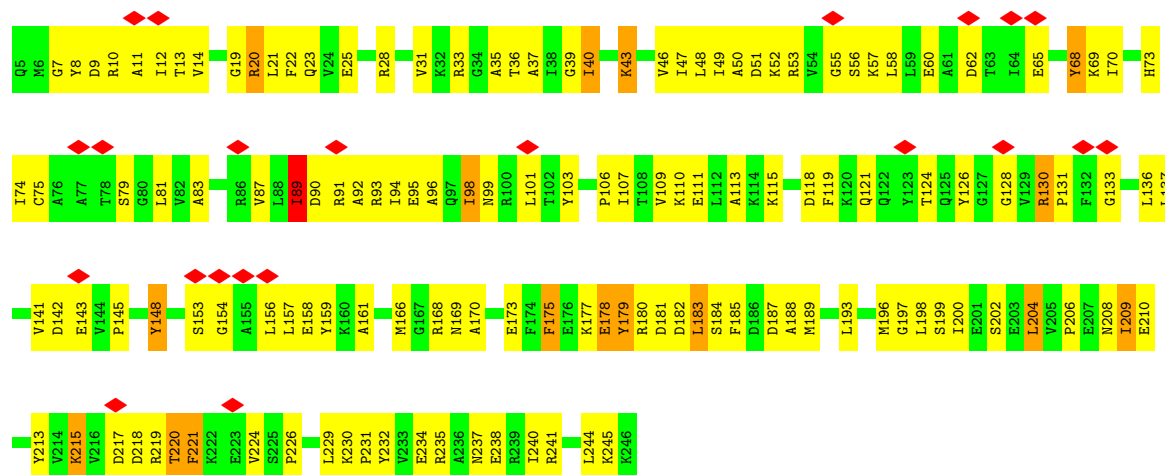
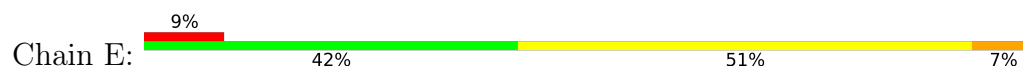


• Molecule 1: Proteasome subunit alpha

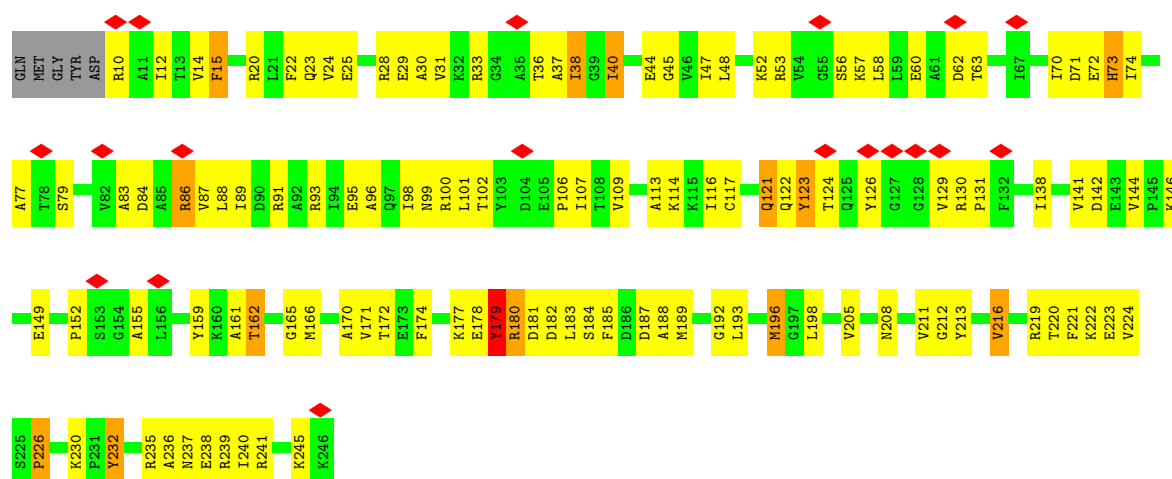




• Molecule 1: Proteasome subunit alpha

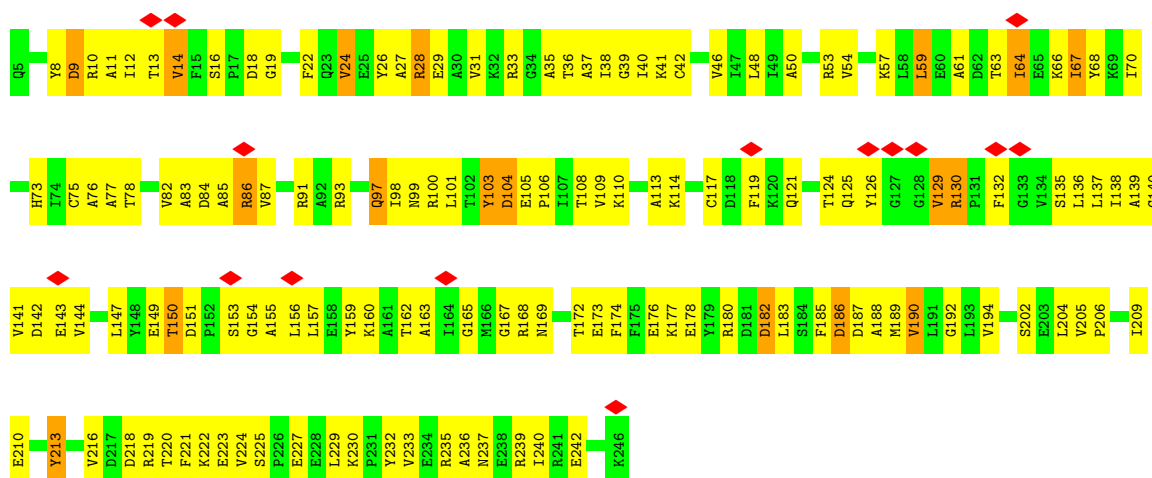


• Molecule 1: Proteasome subunit alpha

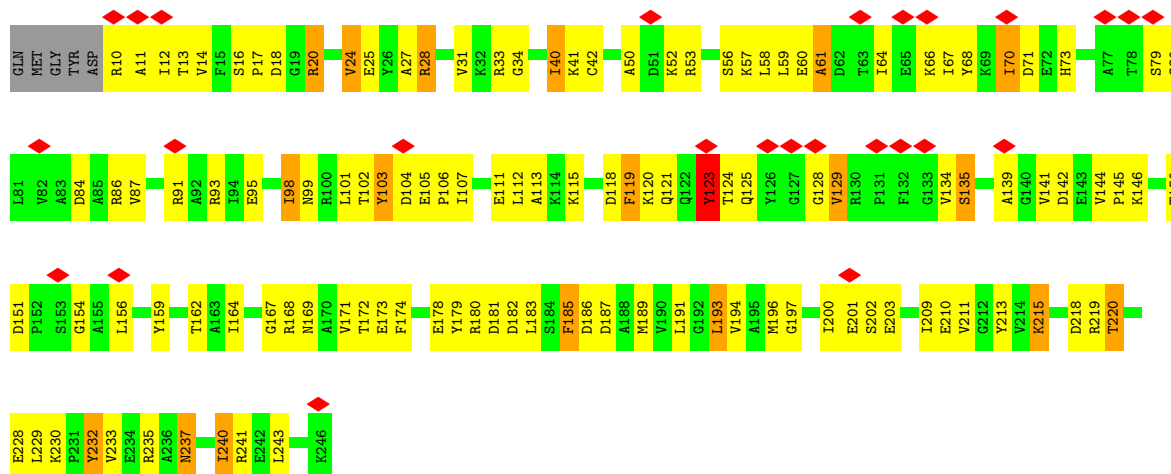


• Molecule 1: Proteasome subunit alpha

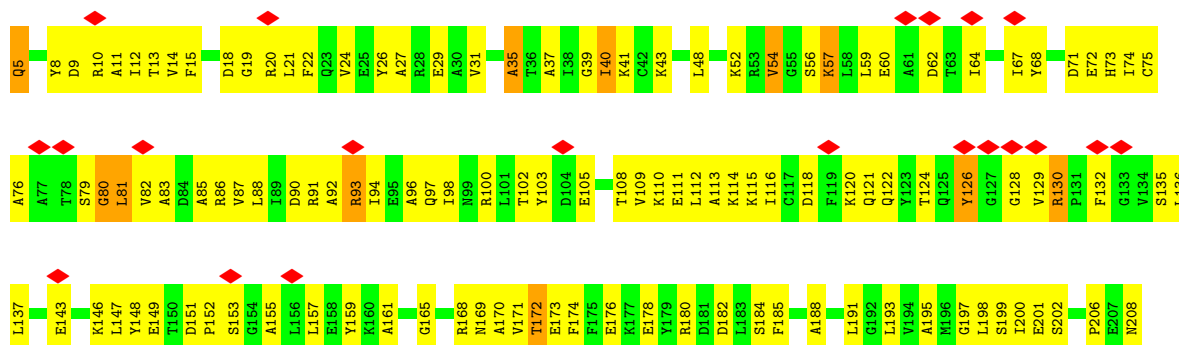




• Molecule 1: Proteasome subunit alpha

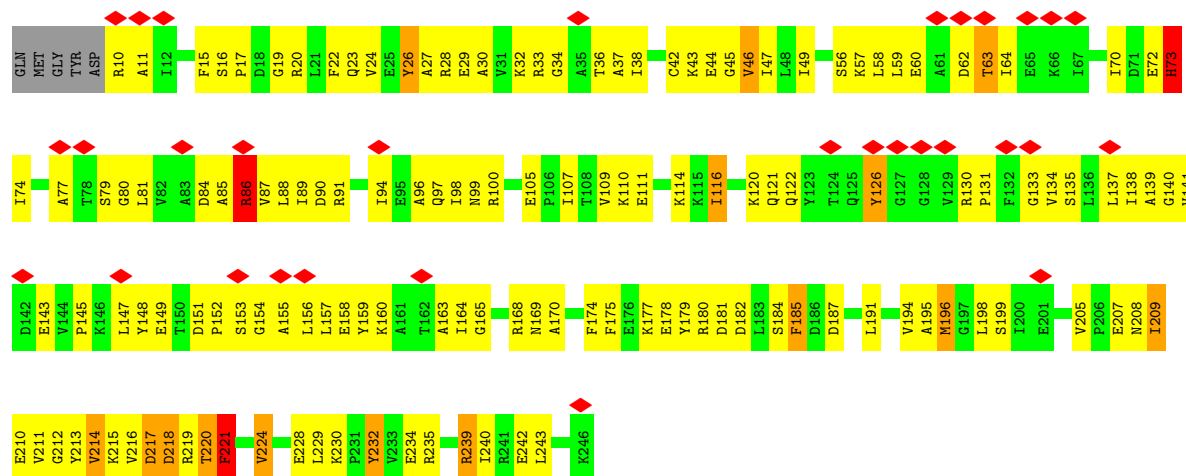


• Molecule 1: Proteasome subunit alpha





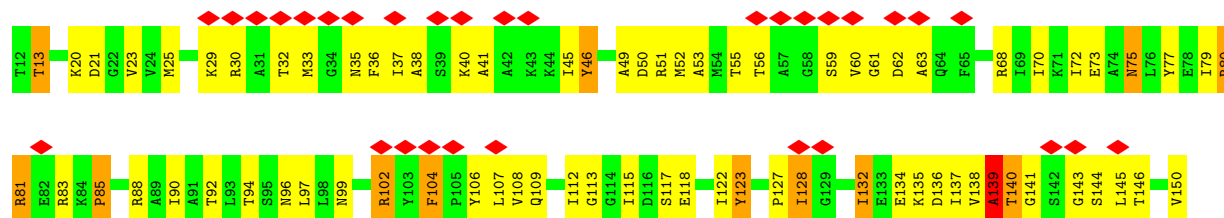
• Molecule 1: Proteasome subunit alpha

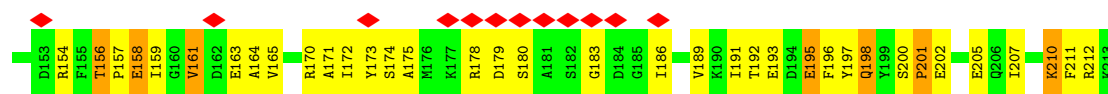


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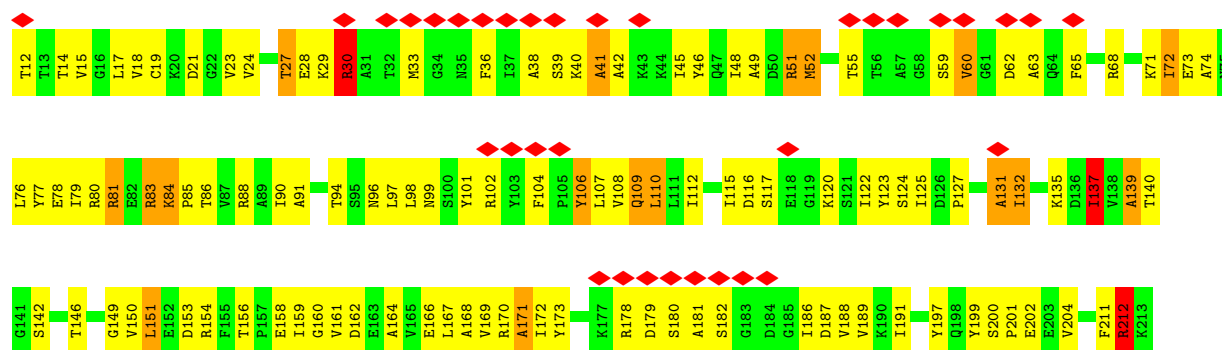
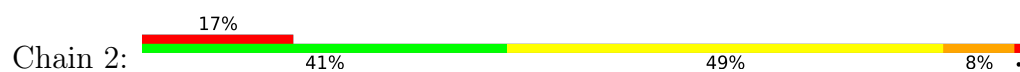


• Molecule 2: Proteasome subunit beta

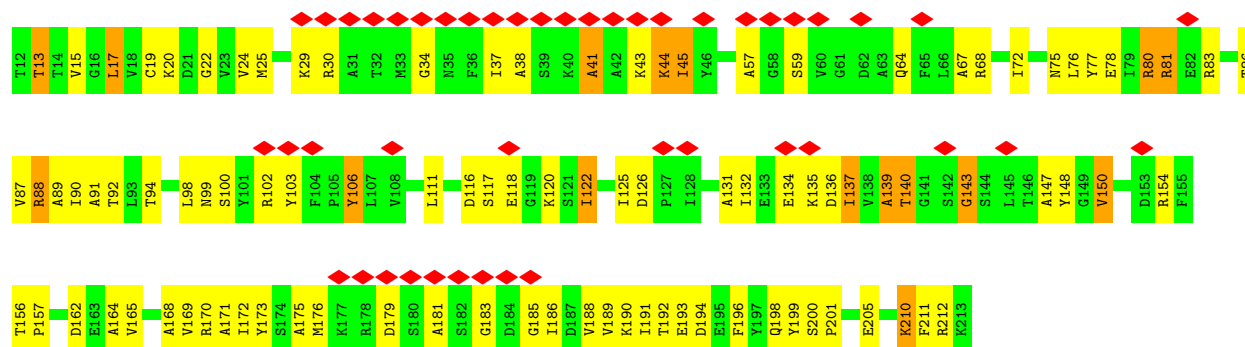




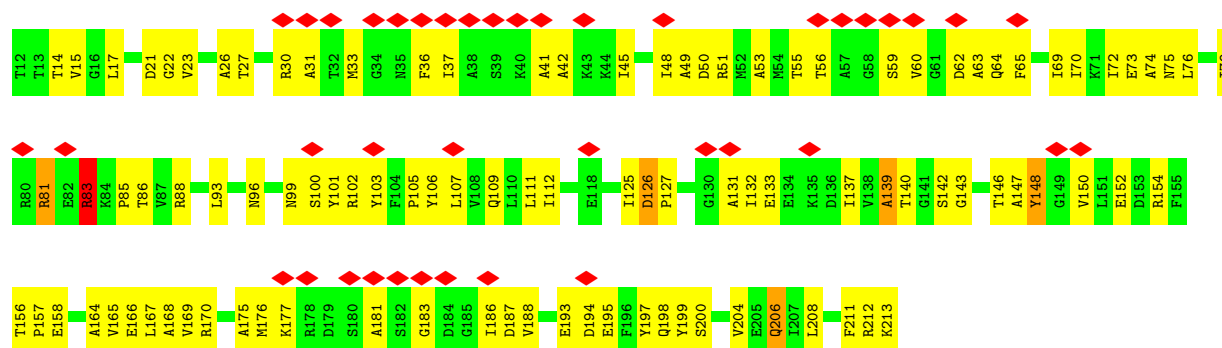
- Molecule 2: Proteasome subunit beta



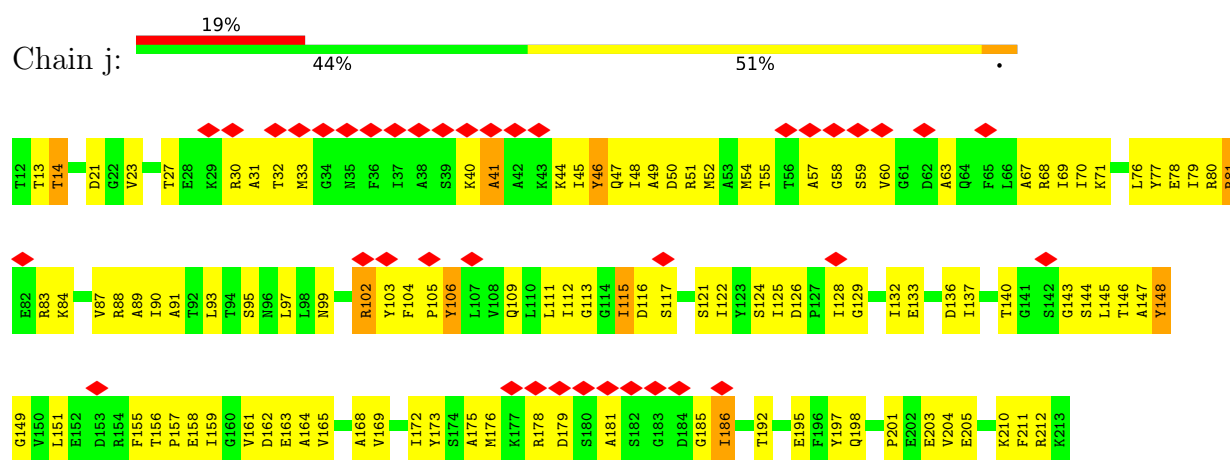
- Molecule 2: Proteasome subunit beta



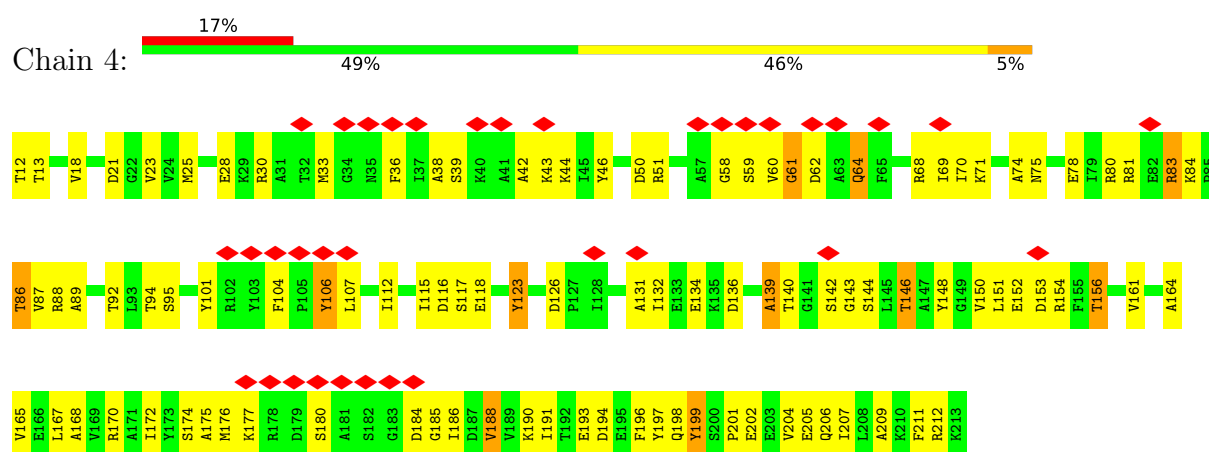
- Molecule 2: Proteasome subunit beta



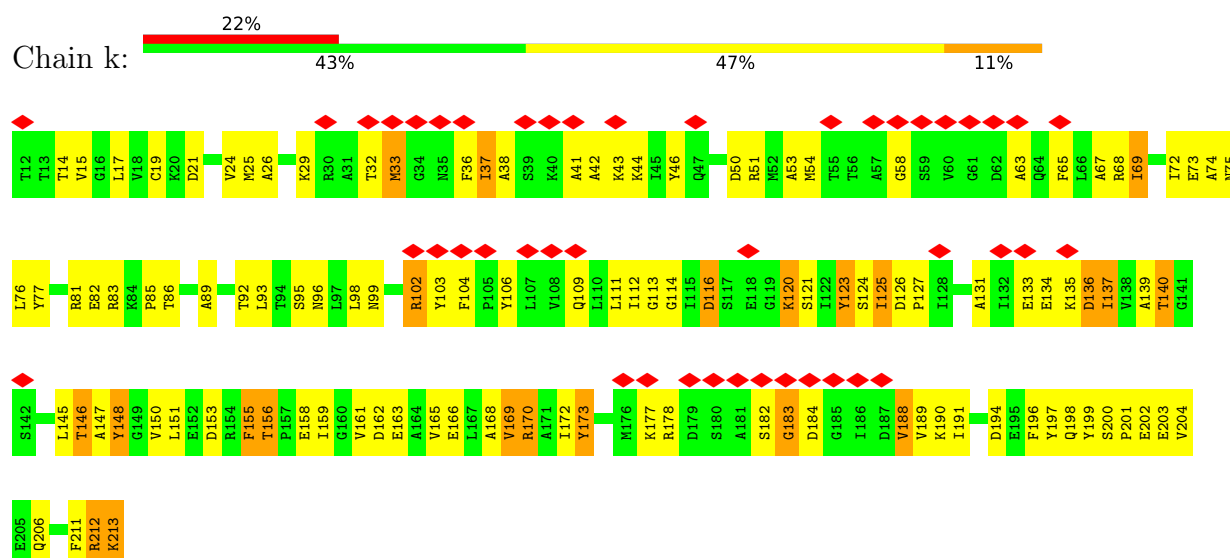
- Molecule 2: Proteasome subunit beta



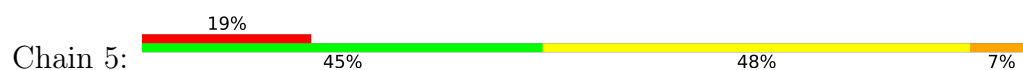
• Molecule 2: Proteasome subunit beta

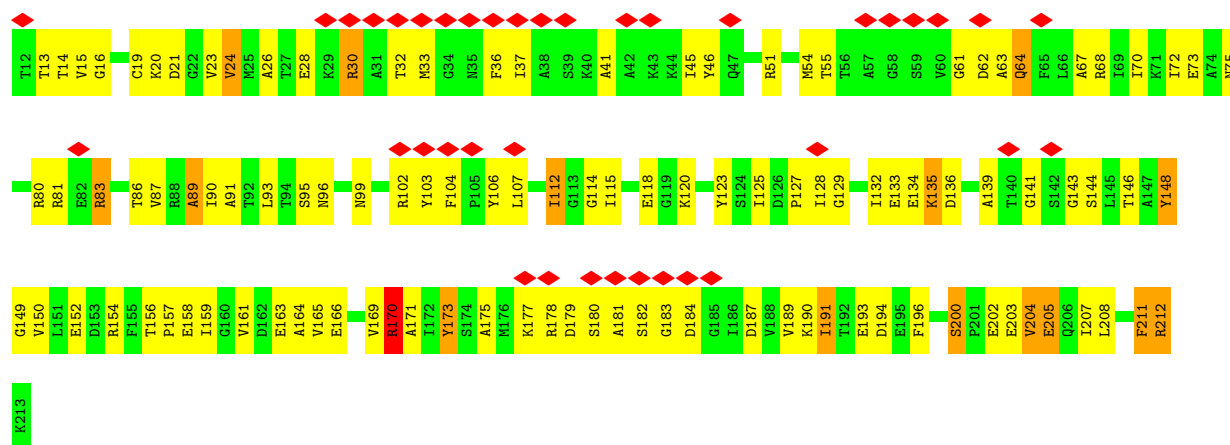


• Molecule 2: Proteasome subunit beta

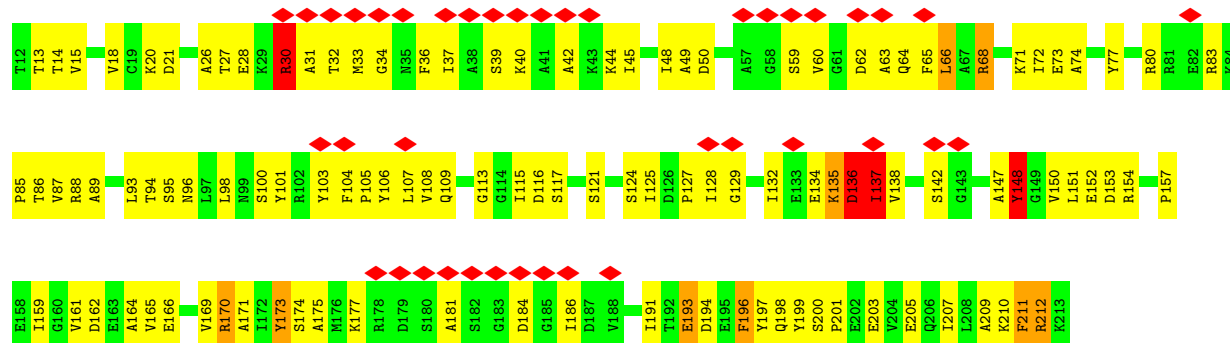


• Molecule 2: Proteasome subunit beta

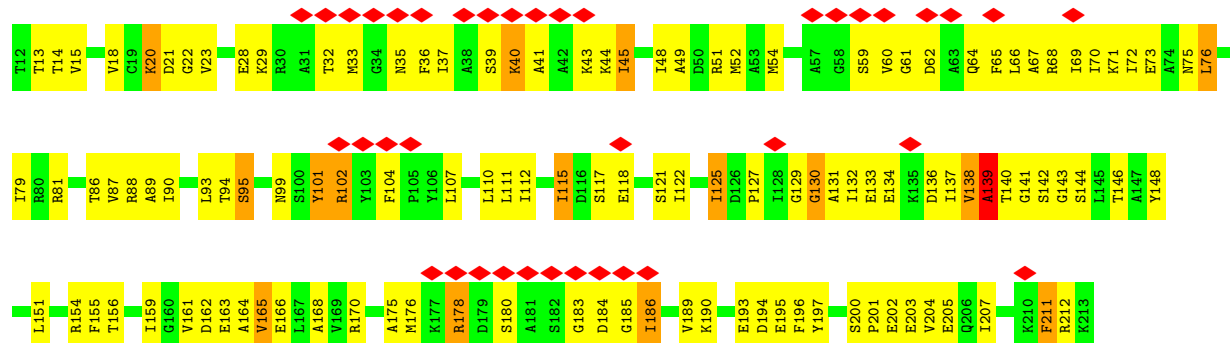
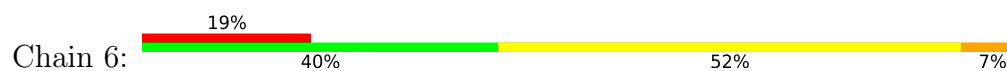




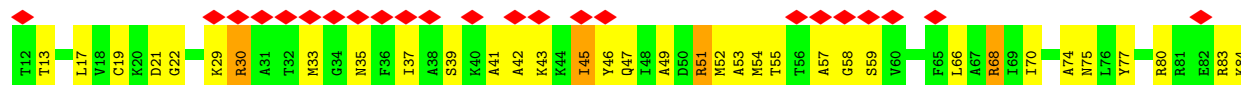
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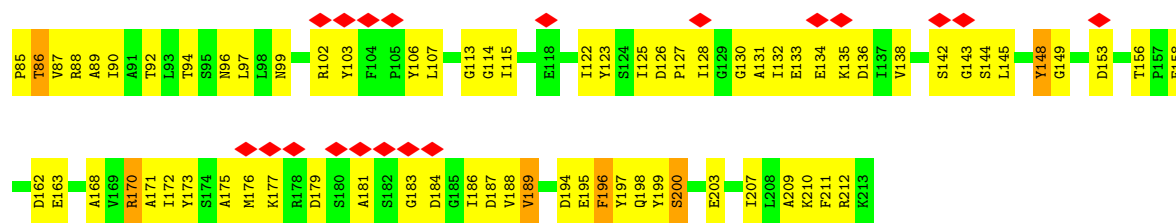


• Molecule 2: Proteasome subunit beta

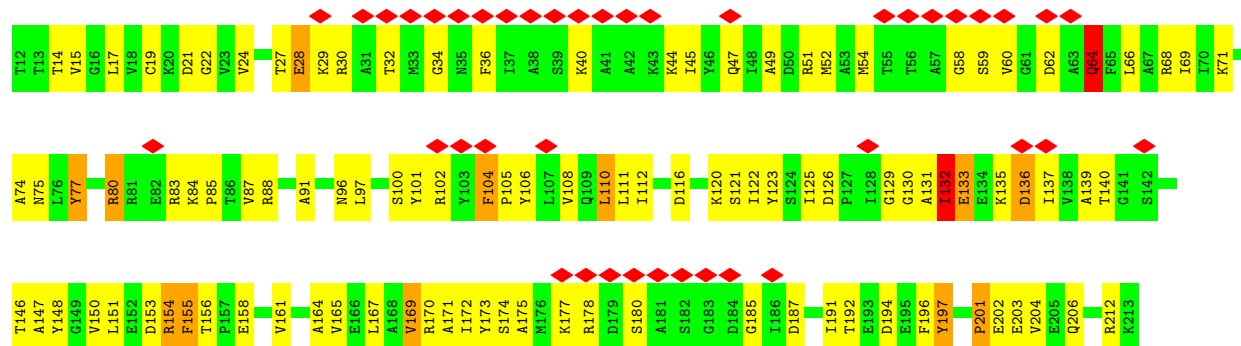


• Molecule 2: Proteasome subunit beta

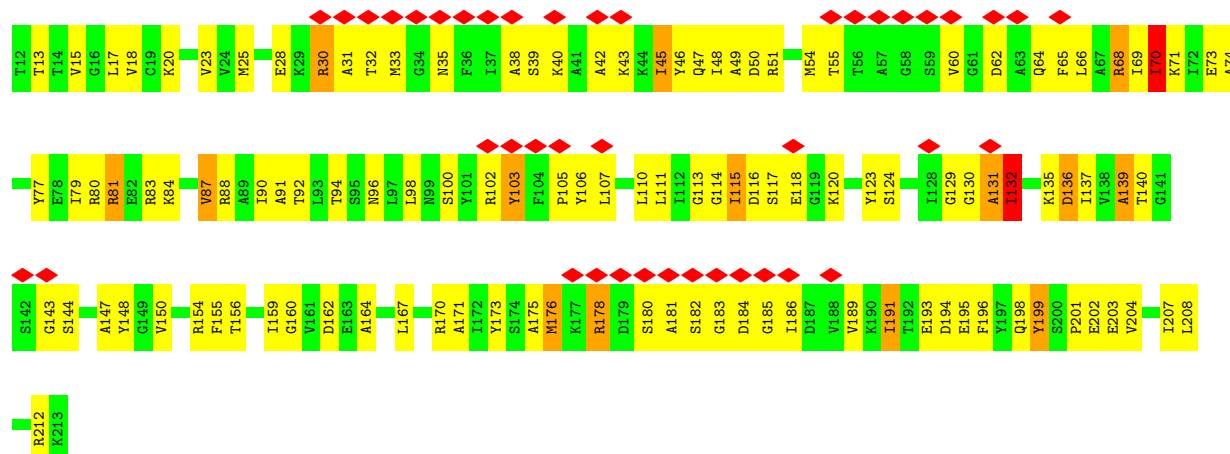




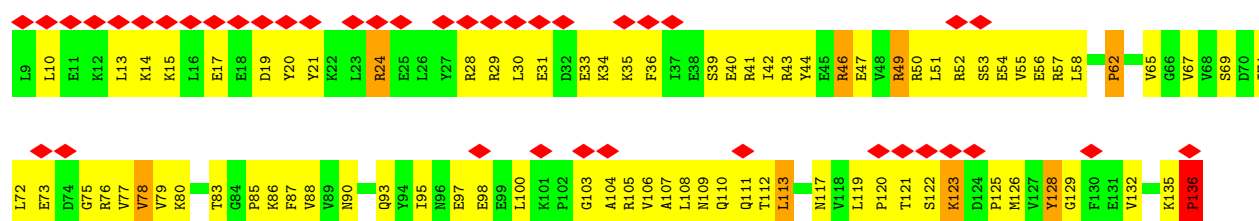
• Molecule 2: Proteasome subunit beta

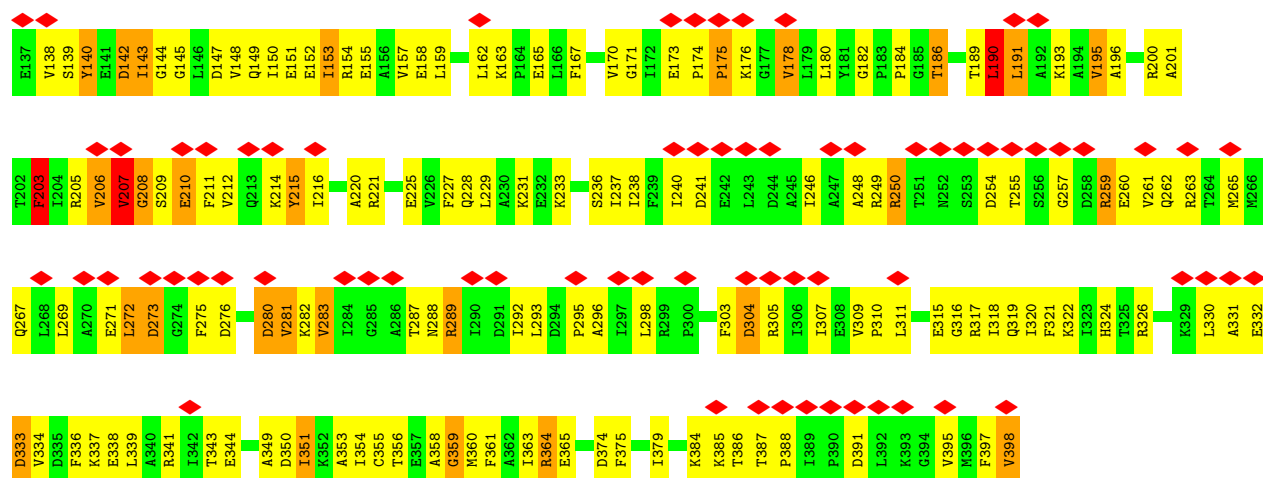


• Molecule 2: Proteasome subunit beta

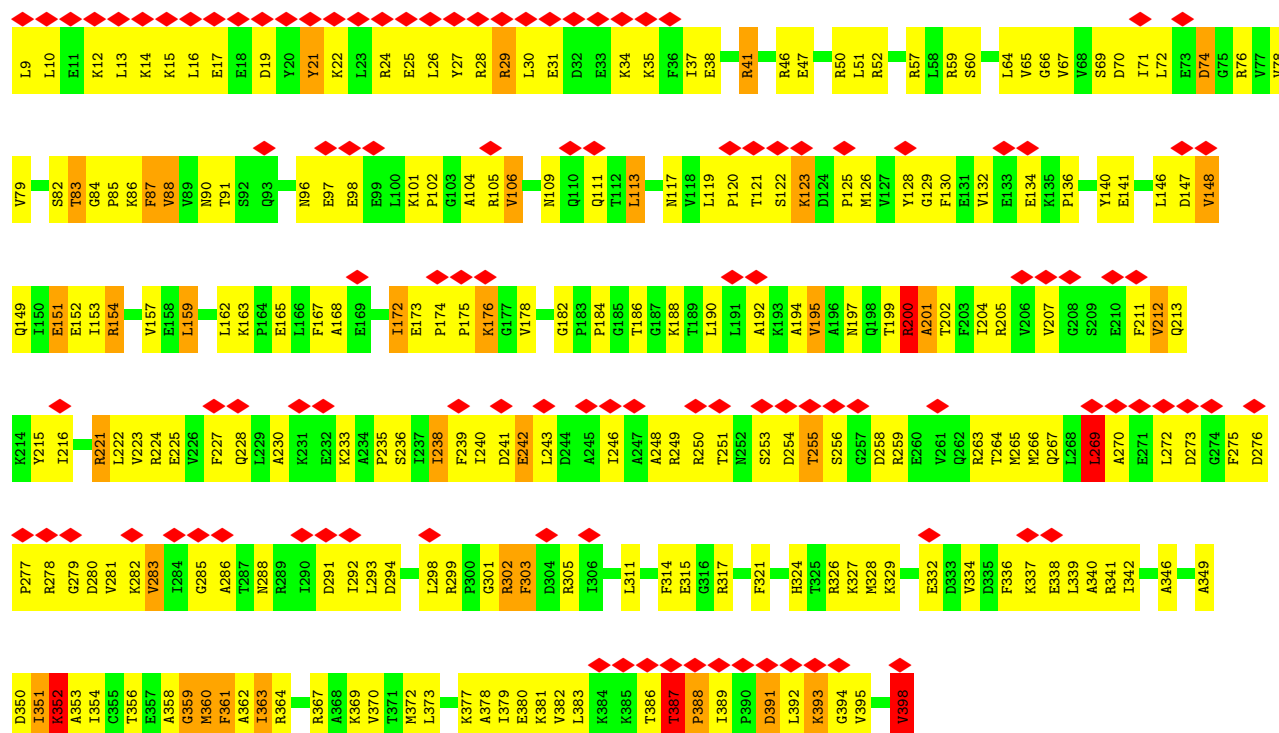


• Molecule 3: Proteasome-activating nucleotidase



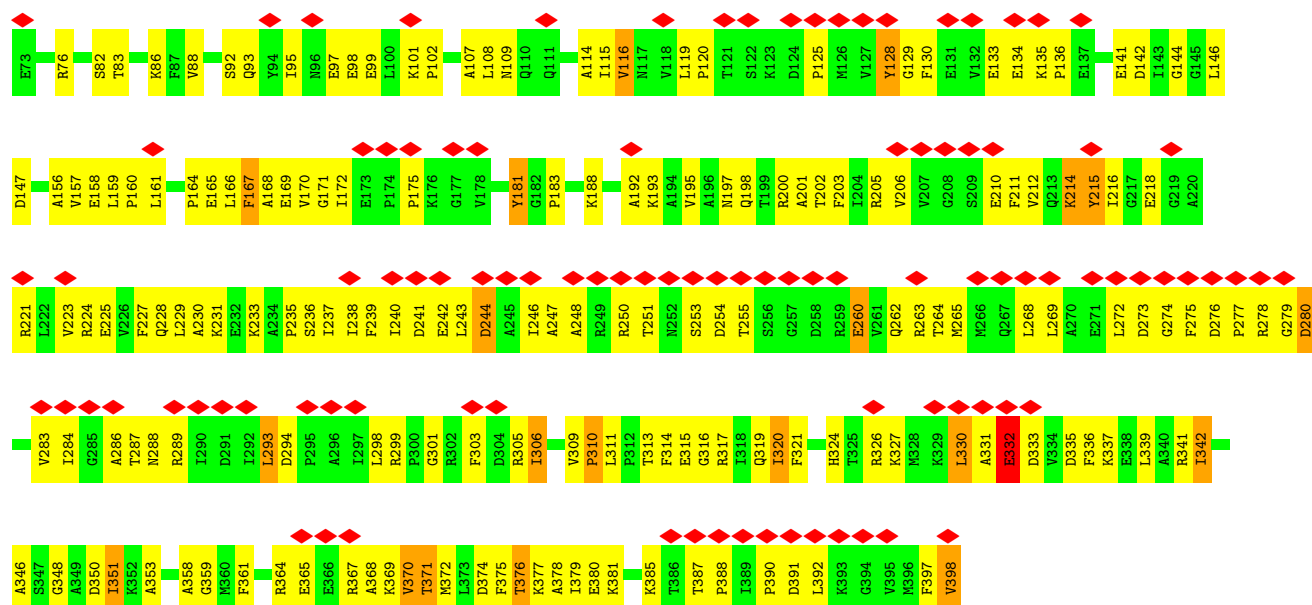


• Molecule 3: Proteasome-activating nucleotidase

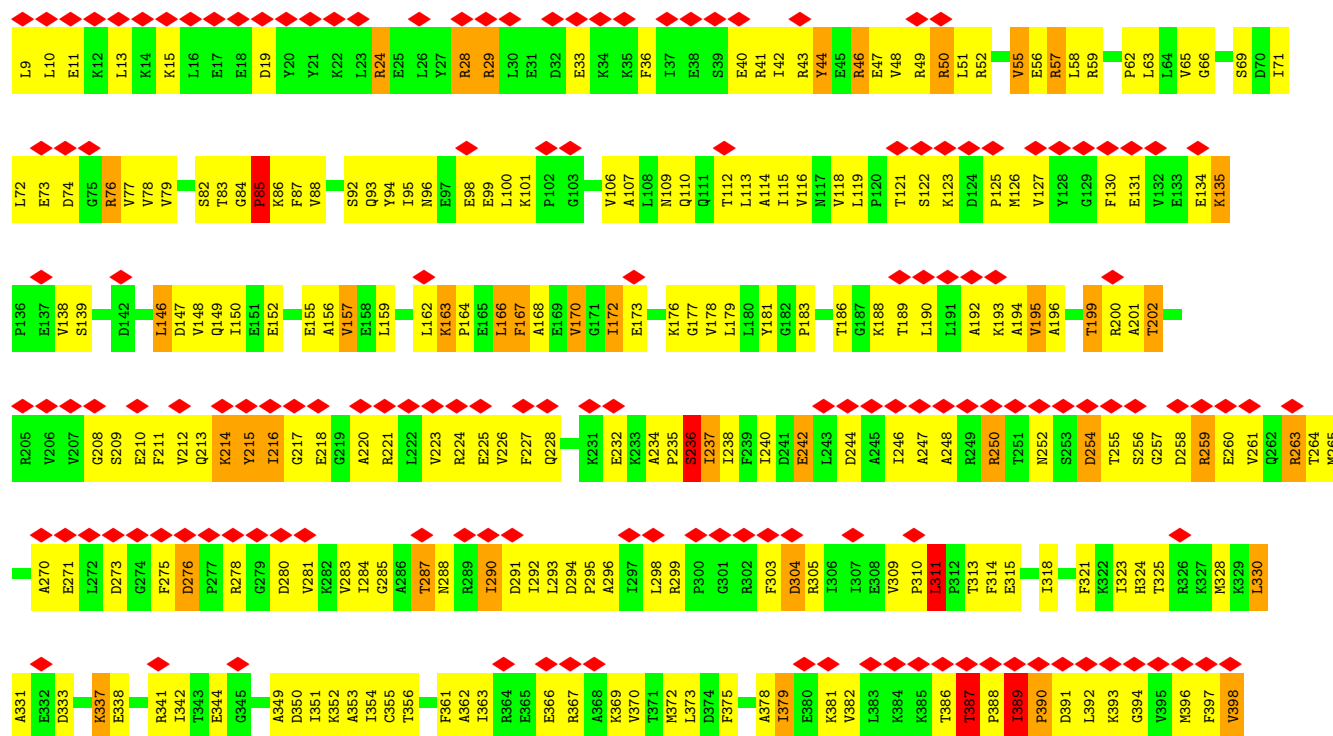


• Molecule 3: Proteasome-activating nucleotidase



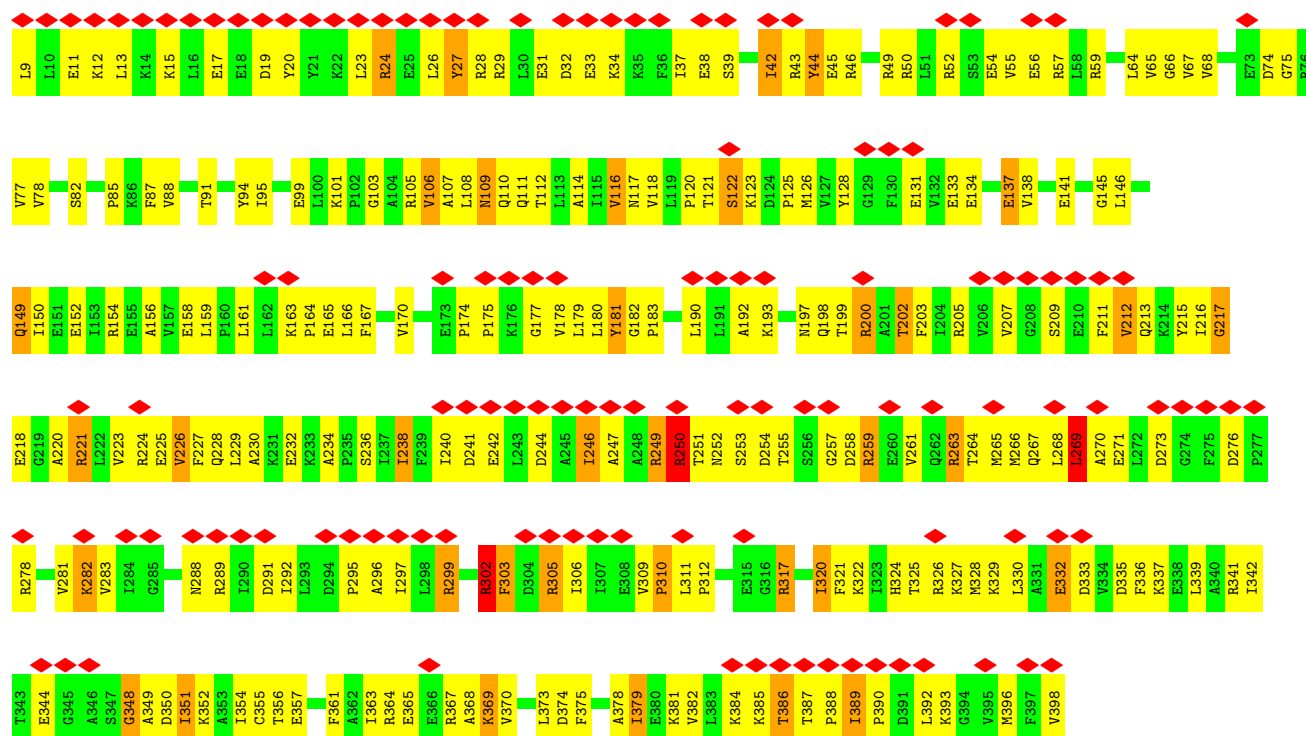


• Molecule 3: Proteasome-activating nucleotidase

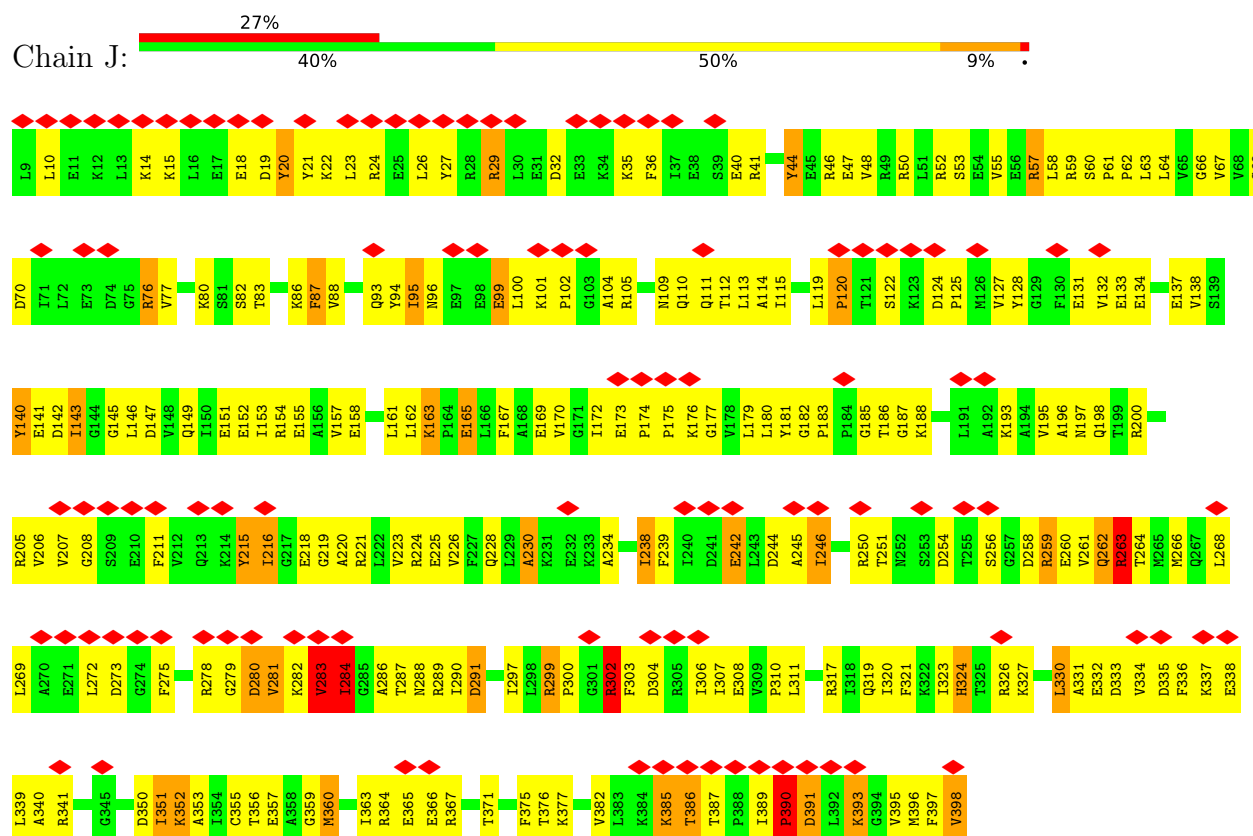


• Molecule 3: Proteasome-activating nucleotidase





• 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	36385	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	0.052	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00655	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.35	75/1934 (3.9%)	2.48	130/2605 (5.0%)
1	B	2.34	81/1934 (4.2%)	2.49	141/2605 (5.4%)
1	C	2.25	81/1934 (4.2%)	2.47	119/2605 (4.6%)
1	D	2.30	80/1934 (4.1%)	2.56	134/2605 (5.1%)
1	E	2.36	86/1934 (4.4%)	2.51	131/2605 (5.0%)
1	F	2.29	63/1934 (3.3%)	2.47	141/2605 (5.4%)
1	G	2.25	71/1934 (3.7%)	2.46	139/2605 (5.3%)
1	a	2.29	73/1892 (3.9%)	2.47	138/2549 (5.4%)
1	b	2.29	71/1892 (3.8%)	2.38	118/2549 (4.6%)
1	c	2.37	89/1892 (4.7%)	2.46	101/2549 (4.0%)
1	d	2.31	75/1892 (4.0%)	2.44	122/2549 (4.8%)
1	e	2.27	72/1892 (3.8%)	2.33	106/2549 (4.2%)
1	f	2.19	55/1892 (2.9%)	2.40	111/2549 (4.4%)
1	g	2.36	92/1892 (4.9%)	2.48	142/2549 (5.6%)
2	1	2.32	65/1573 (4.1%)	2.41	87/2121 (4.1%)
2	2	2.37	78/1573 (5.0%)	2.42	84/2121 (4.0%)
2	3	2.25	51/1573 (3.2%)	2.45	114/2121 (5.4%)
2	4	2.24	58/1573 (3.7%)	2.46	94/2121 (4.4%)
2	5	3.13	61/1573 (3.9%)	2.49	100/2121 (4.7%)
2	6	2.35	62/1573 (3.9%)	2.43	98/2121 (4.6%)
2	7	2.24	54/1573 (3.4%)	2.40	94/2121 (4.4%)
2	h	2.20	41/1573 (2.6%)	2.43	90/2121 (4.2%)
2	i	2.33	65/1573 (4.1%)	2.43	84/2121 (4.0%)
2	j	2.28	57/1573 (3.6%)	2.47	100/2121 (4.7%)
2	k	2.30	66/1573 (4.2%)	2.49	99/2121 (4.7%)
2	l	3.13	66/1573 (4.2%)	2.45	99/2121 (4.7%)
2	m	2.26	45/1573 (2.9%)	2.47	106/2121 (5.0%)
2	n	2.26	63/1573 (4.0%)	2.41	108/2121 (5.1%)
3	H	2.31	132/3146 (4.2%)	2.50	242/4240 (5.7%)
3	I	2.31	121/3146 (3.8%)	2.49	230/4240 (5.4%)
3	J	2.30	122/3146 (3.9%)	2.52	243/4240 (5.7%)
3	K	2.27	110/3146 (3.5%)	2.51	251/4240 (5.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	L	2.29	126/3146 (4.0%)	2.46	223/4240 (5.3%)
3	M	2.29	121/3146 (3.8%)	2.48	224/4240 (5.3%)
All	All	2.34	2628/67680 (3.9%)	2.46	4543/91212 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	9
1	C	0	8
1	D	0	12
1	E	0	6
1	F	0	8
1	G	0	7
1	a	0	7
1	b	0	8
1	c	0	6
1	d	0	2
1	e	0	8
1	f	0	6
1	g	0	8
2	1	0	8
2	2	0	6
2	3	0	3
2	4	0	5
2	5	0	6
2	6	0	3
2	7	0	9
2	h	0	8
2	i	0	5
2	j	0	5
2	k	0	10
2	l	0	4
2	m	0	6
2	n	0	9
3	H	0	14
3	I	0	13
3	J	0	13
3	K	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	23
3	M	0	18
All	All	0	280

All (2628) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	CZ-NH1	55.94	2.11	1.32
2	5	170	ARG	CZ-NH1	55.47	2.10	1.32
2	5	211	PHE	CG-CD2	37.15	2.16	1.38
2	1	211	PHE	CG-CD2	35.61	2.13	1.38
2	5	211	PHE	CG-CD1	33.54	2.09	1.38
2	1	211	PHE	CG-CD1	33.19	2.08	1.38
2	1	211	PHE	CE2-CZ	22.03	2.04	1.38
2	5	211	PHE	CD1-CE1	21.91	2.04	1.38
2	1	211	PHE	CE1-CZ	21.39	2.02	1.38
2	5	211	PHE	CD2-CE2	21.16	2.02	1.38
2	5	211	PHE	CE2-CZ	21.14	2.02	1.38
2	1	211	PHE	CD2-CE2	20.98	2.01	1.38
2	5	211	PHE	CE1-CZ	20.81	2.01	1.38
2	1	211	PHE	CD1-CE1	19.86	1.98	1.38
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	D	184	SER	CA-C	-11.41	1.38	1.53
1	c	16	SER	N-CA	-11.13	1.38	1.46
3	I	52	ARG	CD-NE	11.10	1.61	1.46
2	6	197	TYR	CA-C	-10.93	1.39	1.52
1	G	151	ASP	CA-CB	10.90	1.69	1.53
2	5	115	ILE	CA-C	-10.88	1.39	1.52
1	D	93	ARG	CD-NE	10.84	1.61	1.46
1	F	235	ARG	NE-CZ	10.66	1.44	1.33
2	m	125	ILE	CA-C	-10.59	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	240	ILE	CA-C	-10.32	1.44	1.53
1	F	130	ARG	CD-NE	10.30	1.60	1.46
1	D	168	ARG	NE-CZ	10.13	1.44	1.33
1	C	141	VAL	CA-C	-9.95	1.39	1.52
1	d	188	ALA	N-CA	-9.88	1.34	1.46
3	H	262	GLN	CA-C	9.82	1.66	1.52
2	l	94	THR	N-CA	-9.79	1.34	1.46
3	J	176	LYS	C-N	9.76	1.43	1.32
1	c	42	CYS	CA-C	-9.75	1.39	1.52
1	A	41	LYS	CA-C	-9.71	1.41	1.52
1	D	13	THR	N-CA	-9.68	1.34	1.46
3	H	338	GLU	CA-C	-9.67	1.40	1.52
2	n	181	ALA	N-CA	-9.66	1.38	1.47
1	e	86	ARG	CA-CB	9.66	1.68	1.53
2	m	197	TYR	CA-C	-9.63	1.40	1.52
2	1	32	THR	N-CA	-9.60	1.33	1.46
3	I	317	ARG	NE-CZ	9.59	1.43	1.33
1	G	56	SER	CA-C	9.52	1.58	1.53
1	E	175	PHE	CA-C	-9.51	1.39	1.52
2	h	113	GLY	CA-C	-9.51	1.41	1.51
3	K	76	ARG	NE-CZ	9.49	1.43	1.33
1	G	159	TYR	CA-C	-9.49	1.41	1.52
2	1	197	TYR	CA-C	-9.46	1.41	1.52
3	L	62	PRO	CA-C	-9.43	1.43	1.52
1	B	125	GLN	N-CA	-9.38	1.35	1.46
3	J	174	PRO	CA-C	-9.34	1.46	1.51
3	L	183	PRO	CA-C	9.31	1.60	1.52
1	b	53	ARG	CD-NE	9.30	1.59	1.46
2	n	154	ARG	NE-CZ	9.29	1.43	1.33
3	M	266	MET	C-N	9.28	1.46	1.33
1	F	163	ALA	N-CA	-9.27	1.34	1.45
1	c	23	GLN	N-CA	-9.27	1.35	1.46
2	l	62	ASP	CA-C	-9.26	1.40	1.52
2	m	45	ILE	N-CA	-9.23	1.35	1.46
2	4	206	GLN	C-N	9.19	1.44	1.33
3	M	389	ILE	CA-C	9.16	1.60	1.52
2	7	110	LEU	CA-C	-9.15	1.41	1.52
2	i	126	ASP	CA-CB	9.14	1.67	1.53
3	I	34	LYS	CA-C	9.14	1.65	1.52
2	3	131	ALA	CA-C	-9.14	1.41	1.52
3	J	70	ASP	C-N	9.14	1.45	1.33
2	h	102	ARG	NE-CZ	9.12	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	180	ARG	CA-C	-9.11	1.41	1.52
3	M	259	ARG	CA-C	-9.09	1.41	1.52
1	A	139	ALA	CA-C	-9.07	1.41	1.52
3	J	63	LEU	CA-C	-9.06	1.41	1.52
2	7	140	THR	CA-C	-9.06	1.42	1.52
1	f	10	ARG	NE-CZ	9.00	1.43	1.33
1	D	121	GLN	C-N	8.97	1.45	1.33
3	K	168	ALA	CA-C	-8.96	1.41	1.52
2	k	151	LEU	CA-C	-8.95	1.41	1.52
1	G	137	LEU	C-N	8.94	1.44	1.33
3	H	250	ARG	CD-NE	8.87	1.58	1.46
3	L	349	ALA	C-N	8.85	1.46	1.33
3	L	299	ARG	C-N	8.84	1.42	1.33
1	E	137	LEU	CA-C	-8.83	1.41	1.52
3	K	243	LEU	CA-CB	8.83	1.63	1.52
3	I	29	ARG	CD-NE	8.82	1.58	1.46
2	3	45	ILE	CA-CB	-8.80	1.43	1.53
2	5	150	VAL	CA-C	-8.81	1.41	1.52
2	l	31	ALA	CA-C	-8.77	1.41	1.52
1	g	44	GLU	N-CA	-8.76	1.38	1.46
2	5	180	SER	CA-C	-8.74	1.41	1.52
2	6	156	THR	CA-C	-8.74	1.43	1.52
2	3	53	ALA	CA-C	-8.73	1.41	1.52
2	6	102	ARG	NE-CZ	8.73	1.42	1.33
2	m	86	THR	CA-C	-8.71	1.41	1.52
1	B	34	GLY	CA-C	-8.71	1.43	1.52
3	M	205	ARG	CA-C	-8.68	1.42	1.52
3	I	326	ARG	CD-NE	8.66	1.58	1.46
1	G	155	ALA	CA-C	-8.66	1.42	1.52
2	3	211	PHE	N-CA	-8.65	1.35	1.46
1	B	88	LEU	CA-C	-8.64	1.41	1.52
1	b	240	ILE	N-CA	-8.63	1.36	1.46
2	k	67	ALA	CA-C	-8.59	1.41	1.52
1	c	35	ALA	CA-CB	8.59	1.66	1.53
3	I	66	GLY	CA-C	-8.58	1.45	1.52
1	E	107	ILE	CA-CB	-8.58	1.45	1.54
2	k	17	LEU	CA-CB	8.58	1.68	1.53
1	a	46	VAL	CA-CB	-8.57	1.43	1.54
3	M	163	LYS	N-CA	-8.57	1.39	1.46
1	g	239	ARG	NE-CZ	8.56	1.42	1.33
3	J	59	ARG	CA-C	-8.56	1.40	1.52
1	b	165	GLY	CA-C	-8.55	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	18	VAL	CA-C	-8.54	1.42	1.52
1	a	205	VAL	N-CA	-8.53	1.38	1.46
2	6	195	GLU	CA-CB	-8.53	1.39	1.53
2	7	68	ARG	CD-NE	8.52	1.58	1.46
1	c	214	VAL	CA-CB	-8.50	1.43	1.54
3	K	165	GLU	N-CA	-8.49	1.35	1.46
3	J	339	LEU	CA-CB	8.49	1.66	1.53
3	K	385	LYS	CA-CB	8.48	1.64	1.53
1	e	142	ASP	CA-C	-8.44	1.41	1.52
1	G	206	PRO	C-N	8.44	1.44	1.33
2	j	144	SER	CA-CB	8.43	1.67	1.53
3	H	360	MET	C-N	8.43	1.45	1.34
1	g	26	TYR	C-N	8.43	1.46	1.33
2	2	112	ILE	C-N	8.42	1.44	1.33
2	l	212	ARG	CD-NE	8.42	1.58	1.46
3	H	333	ASP	CA-CB	8.42	1.67	1.53
3	I	224	ARG	C-N	8.41	1.44	1.33
2	h	195	GLU	CA-C	-8.39	1.42	1.52
3	H	211	PHE	CA-C	-8.39	1.42	1.52
1	C	205	VAL	CA-CB	-8.37	1.48	1.54
2	7	80	ARG	NE-CZ	8.37	1.42	1.33
2	6	51	ARG	NE-CZ	8.36	1.42	1.33
2	l	45	ILE	CA-CB	-8.35	1.44	1.54
2	6	61	GLY	CA-C	8.34	1.61	1.52
3	H	140	TYR	CA-CB	8.31	1.64	1.53
2	j	176	MET	CA-CB	8.27	1.66	1.53
2	6	104	PHE	CA-C	-8.27	1.43	1.52
2	j	70	ILE	CA-C	-8.25	1.42	1.52
1	f	33	ARG	CD-NE	8.24	1.57	1.46
1	e	86	ARG	NE-CZ	8.22	1.42	1.33
3	I	151	GLU	CA-C	-8.22	1.42	1.52
3	L	94	TYR	CA-C	-8.22	1.41	1.52
2	6	64	GLN	C-N	8.21	1.45	1.33
2	2	189	VAL	CA-C	8.21	1.63	1.52
2	3	62	ASP	CA-CB	8.20	1.66	1.53
3	I	266	MET	N-CA	8.20	1.56	1.46
1	C	152	PRO	N-CD	-8.19	1.36	1.47
1	g	134	VAL	C-N	8.20	1.46	1.33
1	d	86	ARG	CD-NE	8.19	1.57	1.46
3	J	69	SER	C-N	8.19	1.43	1.33
1	G	172	THR	N-CA	-8.19	1.36	1.46
3	L	354	ILE	C-N	8.19	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	87	PHE	N-CA	-8.18	1.35	1.45
1	B	210	GLU	N-CA	-8.17	1.35	1.46
3	M	302	ARG	CD-NE	8.17	1.57	1.46
1	g	100	ARG	NE-CZ	8.17	1.42	1.33
1	c	170	ALA	CA-C	-8.15	1.42	1.52
1	E	158	GLU	N-CA	-8.15	1.36	1.46
3	M	205	ARG	NE-CZ	8.14	1.42	1.33
1	e	20	ARG	CD-NE	8.14	1.57	1.46
2	3	198	GLN	CA-C	-8.13	1.43	1.52
1	c	31	VAL	N-CA	-8.13	1.35	1.46
3	H	364	ARG	CD-NE	8.12	1.57	1.46
3	I	339	LEU	CA-C	-8.11	1.42	1.52
3	I	233	LYS	N-CA	-8.11	1.35	1.46
2	4	107	LEU	CA-CB	8.09	1.59	1.53
3	M	39	SER	N-CA	-8.09	1.36	1.46
3	M	242	GLU	CA-C	-8.08	1.43	1.52
1	G	241	ARG	NE-CZ	8.08	1.42	1.33
3	M	111	GLN	CA-C	-8.08	1.42	1.52
3	H	317	ARG	NE-CZ	8.08	1.42	1.33
1	e	180	ARG	CD-NE	8.06	1.57	1.46
1	G	209	ILE	N-CA	-8.06	1.36	1.46
1	D	244	LEU	C-N	8.06	1.44	1.33
2	1	144	SER	CA-C	-8.05	1.42	1.52
1	B	73	HIS	CA-C	-8.04	1.43	1.53
1	B	182	ASP	N-CA	-8.04	1.36	1.46
1	c	223	GLU	CA-C	-8.04	1.42	1.52
3	H	71	ILE	CA-C	-8.04	1.42	1.52
3	I	334	VAL	CA-C	8.03	1.61	1.52
1	B	68	TYR	CA-C	-8.03	1.42	1.52
2	3	112	ILE	CA-CB	8.03	1.64	1.54
2	5	156	THR	C-N	8.03	1.40	1.33
2	i	22	GLY	CA-C	-8.02	1.40	1.51
1	E	221	PHE	CA-CB	8.00	1.67	1.53
2	2	17	LEU	CA-C	-8.00	1.42	1.52
3	J	21	TYR	N-CA	-7.99	1.36	1.46
1	C	28	ARG	CD-NE	7.99	1.57	1.46
1	e	10	ARG	CD-NE	7.98	1.57	1.46
3	I	349	ALA	CA-C	-7.96	1.42	1.52
2	3	106	TYR	N-CA	-7.96	1.36	1.46
3	J	157	VAL	CA-CB	-7.95	1.46	1.55
2	5	26	ALA	CA-C	-7.94	1.42	1.52
1	c	71	ASP	N-CA	-7.93	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	40	GLU	C-N	7.93	1.44	1.33
2	7	178	ARG	N-CA	-7.92	1.40	1.47
3	M	200	ARG	NE-CZ	7.92	1.41	1.33
1	B	95	GLU	C-N	7.91	1.44	1.33
3	L	212	VAL	N-CA	-7.91	1.37	1.46
1	e	213	TYR	CA-C	-7.90	1.42	1.52
2	2	80	ARG	CD-NE	7.90	1.57	1.46
1	C	144	VAL	CA-C	-7.90	1.46	1.52
1	e	91	ARG	C-N	7.89	1.44	1.33
3	I	338	GLU	N-CA	-7.89	1.36	1.46
3	I	123	LYS	CA-C	-7.89	1.42	1.52
1	g	216	VAL	CA-C	-7.88	1.44	1.53
2	3	102	ARG	N-CA	-7.87	1.36	1.46
1	b	180	ARG	CD-NE	7.86	1.57	1.46
1	d	119	PHE	CA-CB	7.86	1.65	1.53
2	k	170	ARG	NE-CZ	7.86	1.41	1.33
1	f	111	GLU	CA-C	-7.85	1.41	1.52
1	c	28	ARG	CD-NE	7.85	1.57	1.46
1	G	100	ARG	NE-CZ	7.85	1.41	1.33
1	d	20	ARG	CD-NE	7.84	1.57	1.46
1	B	143	GLU	C-N	7.83	1.42	1.33
3	J	167	PHE	C-N	7.83	1.44	1.33
2	3	102	ARG	NE-CZ	7.81	1.41	1.33
2	j	69	ILE	C-N	7.81	1.43	1.33
3	K	221	ARG	NE-CZ	7.81	1.41	1.33
1	B	195	ALA	C-N	7.80	1.44	1.33
3	H	241	ASP	N-CA	-7.80	1.36	1.46
2	5	118	GLU	CA-C	-7.79	1.42	1.52
2	7	197	TYR	CA-C	-7.79	1.43	1.52
3	I	250	ARG	NE-CZ	7.79	1.41	1.33
1	d	14	VAL	N-CA	-7.77	1.37	1.46
2	1	212	ARG	N-CA	7.76	1.56	1.46
1	e	170	ALA	N-CA	-7.76	1.37	1.46
2	1	80	ARG	NE-CZ	7.76	1.41	1.33
1	E	231	PRO	CA-C	-7.75	1.41	1.52
2	2	171	ALA	C-N	7.75	1.42	1.33
2	m	37	ILE	CA-CB	7.74	1.63	1.54
1	F	144	VAL	N-CA	-7.73	1.37	1.46
2	l	65	PHE	CA-CB	7.73	1.65	1.53
2	3	197	TYR	CA-CB	7.73	1.64	1.53
3	H	52	ARG	NE-CZ	7.72	1.41	1.33
1	c	75	CYS	C-N	7.71	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	176	GLU	CA-C	-7.71	1.42	1.52
3	I	14	LYS	CA-CB	7.70	1.65	1.53
2	7	91	ALA	CA-C	-7.70	1.43	1.52
1	G	128	GLY	C-N	7.70	1.41	1.33
3	M	159	LEU	CA-C	7.70	1.61	1.52
3	J	216	ILE	CA-C	-7.70	1.44	1.53
1	E	237	ASN	CA-C	-7.69	1.42	1.52
1	G	244	LEU	C-N	7.69	1.44	1.33
1	a	224	VAL	CA-CB	7.69	1.62	1.54
2	l	80	ARG	NE-CZ	7.68	1.41	1.33
1	e	33	ARG	CD-NE	7.68	1.56	1.46
1	g	130	ARG	NE-CZ	7.67	1.41	1.33
3	L	338	GLU	C-N	7.66	1.44	1.33
3	M	108	LEU	CA-C	-7.65	1.43	1.52
3	H	341	ARG	NE-CZ	7.64	1.41	1.33
3	I	201	ALA	CA-CB	7.64	1.66	1.53
1	a	225	SER	CA-C	-7.64	1.45	1.53
1	g	163	ALA	N-CA	-7.63	1.36	1.46
1	D	223	GLU	N-CA	-7.63	1.37	1.46
2	n	196	PHE	N-CA	-7.62	1.36	1.47
1	A	187	ASP	CA-C	-7.62	1.43	1.52
3	M	390	PRO	CA-C	-7.62	1.44	1.52
2	m	83	ARG	CD-NE	7.61	1.56	1.46
1	f	141	VAL	CA-C	-7.60	1.42	1.52
1	G	233	VAL	CA-CB	-7.60	1.44	1.54
3	M	66	GLY	CA-C	-7.60	1.43	1.51
1	a	71	ASP	N-CA	-7.60	1.37	1.46
3	L	77	VAL	CA-C	-7.59	1.43	1.52
2	j	51	ARG	NE-CZ	7.58	1.41	1.33
1	C	90	ASP	C-N	7.58	1.43	1.33
1	c	161	ALA	CA-C	-7.56	1.43	1.52
1	A	86	ARG	NE-CZ	7.56	1.41	1.33
1	G	132	PHE	CA-CB	7.56	1.65	1.53
3	M	283	VAL	CA-C	-7.55	1.43	1.52
2	j	143	GLY	CA-C	7.55	1.61	1.51
1	e	74	ILE	CA-C	-7.54	1.43	1.52
3	H	228	GLN	C-N	7.54	1.43	1.33
2	i	212	ARG	CZ-NH1	7.53	1.43	1.32
3	J	324	HIS	CG-ND1	7.51	1.46	1.38
1	d	58	LEU	CA-C	-7.50	1.42	1.52
1	C	139	ALA	CA-C	-7.50	1.43	1.52
2	h	164	ALA	C-N	7.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	220	ALA	CA-C	-7.50	1.43	1.52
1	g	219	ARG	NE-CZ	7.50	1.41	1.33
2	j	212	ARG	CA-C	-7.50	1.43	1.53
2	i	38	ALA	CA-C	-7.50	1.43	1.52
2	1	65	PHE	C-N	7.49	1.44	1.33
1	A	51	ASP	N-CA	-7.49	1.36	1.46
3	K	309	VAL	CA-CB	-7.49	1.46	1.53
2	2	124	SER	N-CA	-7.48	1.36	1.46
1	A	156	LEU	N-CA	-7.48	1.37	1.46
2	m	122	ILE	CA-C	-7.47	1.43	1.52
3	H	56	GLU	C-N	7.47	1.43	1.33
1	A	129	VAL	CA-CB	-7.46	1.47	1.55
1	a	206	PRO	CA-C	-7.46	1.40	1.52
2	5	127	PRO	C-N	7.45	1.41	1.33
2	k	26	ALA	C-N	7.45	1.44	1.33
3	J	44	TYR	CA-C	-7.45	1.43	1.52
3	L	379	ILE	CA-C	-7.45	1.43	1.52
1	c	106	PRO	CA-CB	7.44	1.63	1.53
2	3	156	THR	N-CA	-7.44	1.39	1.46
2	4	81	ARG	C-N	7.44	1.44	1.33
3	J	163	LYS	CA-CB	7.44	1.60	1.53
1	F	46	VAL	CA-C	-7.43	1.43	1.52
3	M	52	ARG	CD-NE	7.43	1.56	1.46
1	F	235	ARG	CD-NE	7.42	1.56	1.46
2	n	124	SER	CA-C	7.40	1.61	1.52
1	A	143	GLU	C-N	7.40	1.39	1.33
2	6	189	VAL	N-CA	-7.40	1.37	1.46
1	A	60	GLU	CA-C	-7.40	1.43	1.53
2	3	30	ARG	CA-CB	7.40	1.67	1.53
1	G	15	PHE	CA-C	-7.39	1.43	1.52
3	H	384	LYS	CA-CB	7.39	1.64	1.53
1	e	57	LYS	CA-CB	7.39	1.65	1.53
1	G	60	GLU	N-CA	7.39	1.55	1.46
2	h	80	ARG	CD-NE	7.38	1.56	1.46
2	5	106	TYR	CA-C	-7.38	1.43	1.52
2	7	15	VAL	CA-C	-7.38	1.43	1.52
1	c	20	ARG	NE-CZ	7.38	1.41	1.33
2	3	199	TYR	CA-C	-7.38	1.43	1.53
1	E	142	ASP	CA-C	-7.37	1.42	1.52
1	B	58	LEU	N-CA	-7.36	1.37	1.46
1	d	192	GLY	CA-C	-7.36	1.43	1.52
1	f	194	VAL	C-N	7.36	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	52	ARG	NE-CZ	7.35	1.41	1.33
3	J	367	ARG	CZ-NH2	7.35	1.43	1.33
1	a	91	ARG	CD-NE	7.34	1.56	1.46
2	l	64	GLN	C-N	7.34	1.43	1.33
3	M	341	ARG	NE-CZ	7.34	1.41	1.33
2	l	170	ARG	CD-NE	7.33	1.56	1.46
1	A	136	LEU	C-N	7.33	1.43	1.33
2	2	36	PHE	CA-C	-7.33	1.43	1.52
1	f	144	VAL	CA-C	-7.33	1.45	1.52
1	B	91	ARG	CD-NE	7.33	1.56	1.46
2	6	138	VAL	CA-C	-7.32	1.45	1.52
2	1	187	ASP	CA-C	-7.32	1.43	1.52
3	M	299	ARG	NE-CZ	7.32	1.41	1.33
2	k	102	ARG	CZ-NH1	7.31	1.43	1.32
2	i	80	ARG	NE-CZ	7.31	1.41	1.33
2	l	174	SER	CA-C	-7.30	1.43	1.52
3	M	370	VAL	CA-C	-7.30	1.44	1.52
2	l	151	LEU	C-N	7.30	1.43	1.33
2	4	94	THR	C-N	7.30	1.43	1.33
1	d	208	ASN	N-CA	-7.30	1.37	1.46
1	E	68	TYR	N-CA	-7.29	1.37	1.45
1	G	85	ALA	N-CA	-7.29	1.37	1.46
2	2	154	ARG	CD-NE	7.29	1.56	1.46
3	M	105	ARG	CA-C	-7.29	1.43	1.52
3	M	183	PRO	C-O	-7.29	1.16	1.24
1	D	58	LEU	N-CA	7.29	1.55	1.46
2	i	83	ARG	CD-NE	7.28	1.56	1.46
3	H	321	PHE	C-N	7.28	1.43	1.33
1	f	58	LEU	CA-C	-7.27	1.43	1.52
3	L	173	GLU	C-N	7.27	1.42	1.33
1	E	115	LYS	C-N	7.26	1.43	1.33
2	1	150	VAL	N-CA	-7.26	1.38	1.46
3	L	260	GLU	C-N	7.26	1.42	1.33
1	B	33	ARG	CD-NE	7.25	1.56	1.46
3	L	273	ASP	CA-CB	7.25	1.64	1.53
1	g	121	GLN	CA-CB	7.25	1.65	1.53
1	c	33	ARG	CD-NE	7.25	1.56	1.46
2	i	190	LYS	CA-C	-7.25	1.43	1.52
2	7	108	VAL	CA-C	-7.24	1.43	1.52
3	L	29	ARG	NE-CZ	7.24	1.41	1.33
3	L	278	ARG	C-N	7.24	1.39	1.33
1	f	73	HIS	ND1-CE1	7.24	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	280	ASP	N-CA	-7.23	1.37	1.46
3	J	207	VAL	CA-CB	7.23	1.62	1.54
2	7	154	ARG	CA-CB	7.23	1.64	1.53
2	l	159	ILE	CA-C	-7.23	1.43	1.52
3	M	261	VAL	N-CA	-7.21	1.37	1.46
1	F	100	ARG	NE-CZ	7.20	1.41	1.33
1	D	83	ALA	C-O	-7.19	1.15	1.24
2	2	170	ARG	CD-NE	7.19	1.56	1.46
2	j	210	LYS	N-CA	-7.19	1.37	1.46
3	I	321	PHE	CA-C	-7.19	1.43	1.52
1	b	99	ASN	C-N	7.18	1.43	1.33
2	1	53	ALA	C-N	7.18	1.43	1.33
3	I	182	GLY	CA-C	-7.18	1.41	1.51
2	5	203	GLU	N-CA	-7.18	1.37	1.46
1	F	218	ASP	N-CA	-7.17	1.37	1.46
1	G	216	VAL	N-CA	-7.17	1.37	1.46
1	g	212	GLY	CA-C	-7.17	1.44	1.51
2	2	204	VAL	CA-CB	-7.17	1.45	1.54
2	3	188	VAL	C-O	-7.17	1.16	1.24
2	l	68	ARG	CD-NE	7.17	1.56	1.46
1	a	67	ILE	CA-CB	7.17	1.63	1.54
2	5	112	ILE	CA-C	-7.17	1.43	1.52
1	f	201	GLU	CA-C	-7.17	1.44	1.53
3	H	29	ARG	CD-NE	7.17	1.56	1.46
2	l	89	ALA	C-N	7.16	1.41	1.34
3	I	317	ARG	CD-NE	7.16	1.56	1.46
1	b	27	ALA	CA-C	-7.16	1.43	1.52
1	f	180	ARG	NE-CZ	7.16	1.41	1.33
1	C	88	LEU	CA-C	-7.16	1.43	1.52
3	K	40	GLU	N-CA	-7.16	1.37	1.46
1	C	205	VAL	N-CA	-7.15	1.39	1.46
1	c	61	ALA	N-CA	-7.15	1.39	1.46
1	d	28	ARG	CZ-NH2	7.15	1.42	1.33
2	j	125	ILE	CA-C	-7.14	1.44	1.52
1	A	223	GLU	N-CA	-7.14	1.37	1.46
3	K	330	LEU	CA-C	-7.14	1.43	1.52
1	b	164	ILE	N-CA	-7.13	1.38	1.46
2	5	154	ARG	NE-CZ	7.13	1.40	1.33
3	M	278	ARG	NE-CZ	7.12	1.40	1.33
1	E	133	GLY	CA-C	-7.11	1.41	1.51
1	f	186	ASP	CA-CB	7.11	1.64	1.53
1	A	132	PHE	CA-CB	7.11	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	130	ARG	CZ-NH1	7.11	1.42	1.32
1	G	215	LYS	C-N	7.10	1.42	1.33
2	j	149	GLY	CA-C	-7.10	1.44	1.52
1	b	154	GLY	CA-C	-7.10	1.41	1.51
1	g	169	ASN	CA-C	7.10	1.61	1.52
2	i	83	ARG	CZ-NH1	7.09	1.42	1.32
3	M	159	LEU	N-CA	-7.09	1.40	1.46
1	A	241	ARG	CD-NE	7.09	1.56	1.46
1	B	156	LEU	CA-C	-7.09	1.44	1.52
2	4	176	MET	C-N	7.09	1.43	1.33
3	J	206	VAL	C-N	7.09	1.41	1.33
3	K	391	ASP	N-CA	-7.09	1.41	1.47
2	2	72	ILE	CA-C	-7.08	1.43	1.52
1	c	124	THR	N-CA	-7.08	1.37	1.46
1	F	40	ILE	CA-C	-7.08	1.44	1.52
3	I	382	VAL	CA-C	7.07	1.61	1.52
3	J	61	PRO	CA-C	-7.07	1.45	1.52
1	A	168	ARG	CD-NE	7.06	1.56	1.46
2	5	182	SER	CA-C	-7.06	1.43	1.53
2	2	48	ILE	C-N	7.06	1.43	1.33
1	A	93	ARG	CD-NE	7.05	1.56	1.46
1	E	184	SER	C-N	7.05	1.43	1.33
1	f	164	ILE	CA-C	-7.05	1.44	1.52
2	k	69	ILE	CA-C	-7.05	1.44	1.52
2	4	118	GLU	CA-C	-7.05	1.43	1.52
1	A	208	ASN	CA-CB	7.05	1.65	1.53
1	c	112	LEU	CA-CB	-7.05	1.42	1.53
2	3	125	ILE	N-CA	-7.04	1.38	1.46
2	j	67	ALA	CA-C	-7.04	1.43	1.52
1	F	68	TYR	CA-C	-7.04	1.44	1.52
1	D	212	GLY	CA-C	-7.04	1.45	1.51
2	2	151	LEU	C-N	7.03	1.43	1.33
2	h	156	THR	CA-CB	7.03	1.64	1.54
3	I	204	ILE	CA-C	-7.03	1.43	1.52
1	a	10	ARG	NE-CZ	7.02	1.40	1.33
1	B	130	ARG	NE-CZ	7.02	1.40	1.33
3	K	201	ALA	N-CA	-7.02	1.36	1.45
1	B	208	ASN	CA-CB	7.02	1.63	1.53
2	i	13	THR	C-O	7.02	1.32	1.23
2	5	63	ALA	N-CA	-7.02	1.37	1.46
1	c	102	THR	CA-C	-7.01	1.43	1.52
1	e	165	GLY	C-N	7.00	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	22	PHE	CA-CB	7.00	1.65	1.53
2	4	46	TYR	C-N	7.00	1.43	1.33
3	K	303	PHE	CA-C	-7.00	1.44	1.52
1	e	93	ARG	CZ-NH2	6.99	1.42	1.33
1	g	177	LYS	CA-C	-6.99	1.44	1.52
2	3	177	LYS	N-CA	-6.99	1.37	1.46
2	2	137	ILE	N-CA	-6.98	1.38	1.46
2	6	54	MET	N-CA	-6.98	1.37	1.46
1	g	86	ARG	CZ-NH2	6.97	1.42	1.33
2	1	181	ALA	C-N	6.97	1.42	1.33
1	C	188	ALA	CA-C	-6.97	1.43	1.52
1	a	213	TYR	CA-C	-6.97	1.44	1.52
1	f	139	ALA	CA-C	-6.96	1.44	1.52
1	f	135	SER	N-CA	-6.96	1.37	1.46
2	k	178	ARG	CZ-NH2	6.96	1.42	1.33
2	2	160	GLY	C-N	6.96	1.41	1.34
2	j	68	ARG	NE-CZ	6.96	1.40	1.33
3	L	220	ALA	C-N	6.96	1.43	1.33
1	d	167	GLY	C-N	6.95	1.42	1.33
2	7	203	GLU	CA-CB	6.95	1.64	1.53
1	B	177	LYS	N-CA	-6.95	1.38	1.46
3	L	330	LEU	C-N	6.95	1.42	1.33
3	L	52	ARG	NE-CZ	6.94	1.40	1.33
1	b	180	ARG	NE-CZ	6.93	1.40	1.33
2	5	41	ALA	CA-C	-6.93	1.44	1.52
1	D	64	ILE	CA-C	-6.93	1.44	1.52
2	1	170	ARG	CD-NE	6.93	1.55	1.46
3	L	355	CYS	CA-C	-6.93	1.44	1.52
1	d	17	PRO	N-CD	6.93	1.57	1.47
1	C	111	GLU	CA-CB	6.92	1.64	1.53
1	c	20	ARG	CD-NE	6.92	1.55	1.46
1	b	157	LEU	CA-C	-6.92	1.44	1.52
2	i	132	ILE	CB-CG1	6.92	1.67	1.53
3	L	170	VAL	CA-C	-6.92	1.44	1.52
1	c	11	ALA	C-N	6.92	1.43	1.33
1	A	219	ARG	C-N	6.92	1.42	1.33
2	6	65	PHE	CA-C	-6.92	1.43	1.52
1	b	133	GLY	C-N	6.91	1.43	1.33
2	k	113	GLY	N-CA	-6.91	1.37	1.45
2	k	156	THR	C-N	-6.91	1.25	1.34
1	A	10	ARG	CA-C	-6.91	1.43	1.52
1	f	86	ARG	CZ-NH1	6.91	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	166	MET	N-CA	-6.90	1.37	1.46
1	g	91	ARG	CD-NE	6.90	1.55	1.46
2	3	51	ARG	NE-CZ	6.89	1.40	1.33
3	M	170	VAL	C-N	6.89	1.42	1.33
1	a	51	ASP	CA-C	6.88	1.61	1.52
1	a	156	LEU	N-CA	-6.88	1.37	1.46
1	C	187	ASP	N-CA	-6.88	1.38	1.46
2	4	33	MET	CA-CB	6.88	1.58	1.53
2	4	42	ALA	CA-CB	6.87	1.61	1.53
1	E	178	GLU	CA-C	-6.87	1.43	1.52
1	d	113	ALA	N-CA	-6.87	1.38	1.46
1	E	95	GLU	CA-C	-6.87	1.44	1.52
3	H	154	ARG	CD-NE	6.87	1.55	1.46
3	J	221	ARG	CZ-NH1	6.86	1.42	1.32
1	a	180	ARG	CZ-NH2	6.86	1.42	1.33
1	d	118	ASP	C-N	6.86	1.42	1.33
2	j	162	ASP	N-CA	-6.85	1.37	1.46
1	a	143	GLU	CA-C	-6.85	1.43	1.52
3	I	151	GLU	C-N	6.85	1.43	1.33
3	L	252	ASN	CA-C	-6.85	1.45	1.53
2	l	117	SER	C-N	6.84	1.43	1.33
1	G	147	LEU	C-N	6.84	1.42	1.33
2	6	79	ILE	N-CA	-6.84	1.38	1.46
3	K	289	ARG	NE-CZ	6.84	1.40	1.33
3	I	205	ARG	NE-CZ	6.83	1.40	1.33
3	M	252	ASN	CA-CB	6.83	1.65	1.53
1	g	96	ALA	CA-C	-6.83	1.44	1.52
3	J	48	VAL	CA-CB	6.83	1.62	1.54
2	2	38	ALA	CA-C	-6.83	1.44	1.52
3	J	264	THR	CA-C	6.83	1.61	1.52
2	k	81	ARG	NE-CZ	6.82	1.40	1.33
1	E	62	ASP	CA-C	-6.82	1.44	1.52
2	4	28	GLU	CA-C	-6.82	1.44	1.52
1	A	83	ALA	CA-C	-6.82	1.44	1.52
1	d	225	SER	CA-C	-6.82	1.46	1.53
2	i	75	ASN	CA-CB	6.82	1.64	1.53
2	k	68	ARG	NE-CZ	6.82	1.40	1.33
3	I	369	LYS	CA-CB	6.82	1.64	1.53
3	L	299	ARG	CD-NE	6.82	1.55	1.46
1	c	223	GLU	N-CA	-6.81	1.37	1.46
3	I	174	PRO	CA-CB	-6.81	1.44	1.54
1	E	130	ARG	CA-C	6.81	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	28	GLU	CA-C	-6.81	1.44	1.52
2	m	21	ASP	C-N	6.81	1.42	1.33
2	6	178	ARG	N-CA	-6.80	1.37	1.46
3	M	123	LYS	N-CA	-6.80	1.41	1.46
1	e	88	LEU	C-N	6.80	1.42	1.33
2	7	173	TYR	N-CA	-6.80	1.38	1.46
2	n	113	GLY	C-N	6.80	1.42	1.33
1	g	180	ARG	CD-NE	6.79	1.55	1.46
3	J	225	GLU	N-CA	-6.79	1.38	1.46
3	H	296	ALA	CA-C	-6.79	1.43	1.52
3	M	367	ARG	CD-NE	6.79	1.55	1.46
1	c	171	VAL	CA-CB	-6.78	1.45	1.54
2	1	154	ARG	CZ-NH2	6.78	1.42	1.33
2	i	189	VAL	CA-C	-6.78	1.44	1.52
1	B	50	ALA	C-N	6.77	1.42	1.33
2	i	94	THR	C-N	6.77	1.42	1.33
1	C	161	ALA	CA-C	-6.77	1.44	1.52
1	C	160	LYS	C-N	6.76	1.42	1.33
2	5	207	ILE	C-N	6.76	1.43	1.33
3	K	167	PHE	CA-CB	6.76	1.65	1.53
1	e	33	ARG	NE-CZ	6.76	1.40	1.33
3	H	111	GLN	CA-CB	-6.76	1.44	1.54
1	c	164	ILE	CA-C	-6.76	1.44	1.52
3	K	265	MET	N-CA	-6.75	1.38	1.46
2	2	68	ARG	CA-C	-6.75	1.44	1.52
3	I	24	ARG	CD-NE	6.75	1.55	1.46
3	K	305	ARG	N-CA	-6.75	1.37	1.45
3	M	306	ILE	N-CA	-6.75	1.38	1.46
1	d	143	GLU	C-N	6.74	1.39	1.32
3	J	393	LYS	CA-CB	6.74	1.64	1.54
1	c	216	VAL	CA-CB	-6.73	1.45	1.54
3	L	127	VAL	CA-C	-6.73	1.45	1.52
3	H	349	ALA	C-N	6.73	1.42	1.33
1	B	39	GLY	N-CA	-6.72	1.39	1.45
1	g	28	ARG	NE-CZ	6.72	1.40	1.33
1	B	53	ARG	NE-CZ	6.72	1.40	1.33
2	h	41	ALA	N-CA	-6.72	1.41	1.47
2	2	39	SER	CA-C	-6.72	1.44	1.52
2	6	134	GLU	CA-C	-6.72	1.44	1.52
3	M	15	LYS	CA-C	-6.71	1.44	1.52
1	D	225	SER	CA-CB	6.71	1.63	1.53
1	E	217	ASP	CA-C	6.71	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	111	GLU	CA-C	-6.71	1.43	1.52
2	1	47	GLN	C-N	6.71	1.39	1.33
3	H	132	VAL	CA-C	-6.71	1.44	1.52
1	b	21	LEU	CA-C	-6.70	1.44	1.52
1	c	97	GLN	C-N	6.70	1.42	1.33
1	F	239	ARG	CD-NE	6.70	1.55	1.46
2	n	65	PHE	CA-CB	6.70	1.64	1.53
1	D	28	ARG	CD-NE	6.70	1.55	1.46
1	f	56	SER	CA-C	-6.69	1.44	1.52
2	i	80	ARG	CD-NE	6.69	1.55	1.46
3	J	132	VAL	CA-CB	6.69	1.63	1.54
1	F	136	LEU	CA-C	-6.69	1.44	1.52
1	B	29	GLU	CA-CB	6.69	1.64	1.53
1	g	209	ILE	CA-C	-6.69	1.44	1.52
3	I	233	LYS	C-N	6.69	1.42	1.33
1	A	180	ARG	NE-CZ	6.68	1.40	1.33
1	a	240	ILE	CA-C	-6.68	1.44	1.52
1	b	50	ALA	CA-C	-6.68	1.44	1.52
1	D	81	LEU	CA-C	-6.68	1.44	1.52
2	m	168	ALA	CA-C	-6.68	1.44	1.52
3	M	138	VAL	CA-C	-6.68	1.44	1.52
3	H	214	LYS	C-O	-6.67	1.19	1.23
1	F	172	THR	CA-C	-6.67	1.44	1.52
1	A	16	SER	C-O	6.67	1.32	1.23
1	a	73	HIS	ND1-CE1	6.67	1.39	1.32
2	6	118	GLU	N-CA	6.67	1.53	1.46
1	B	48	LEU	CA-C	-6.67	1.44	1.52
3	L	305	ARG	NE-CZ	6.67	1.40	1.33
3	I	213	GLN	N-CA	-6.67	1.37	1.45
3	M	99	GLU	CA-C	-6.67	1.44	1.52
3	K	369	LYS	N-CA	-6.67	1.38	1.46
1	G	96	ALA	C-N	6.66	1.43	1.34
3	L	252	ASN	C-N	6.66	1.42	1.33
1	d	207	GLU	CA-C	-6.66	1.43	1.52
3	M	251	THR	N-CA	-6.66	1.37	1.46
1	d	40	ILE	CA-C	-6.66	1.44	1.52
2	7	129	GLY	N-CA	-6.66	1.36	1.44
3	H	103	GLY	CA-C	6.66	1.61	1.51
3	K	202	THR	C-N	6.66	1.43	1.33
1	g	97	GLN	C-N	6.66	1.42	1.33
3	J	205	ARG	CA-C	-6.66	1.44	1.52
1	G	76	ALA	CA-C	-6.65	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	200	ARG	CD-NE	6.65	1.55	1.46
2	j	132	ILE	CA-C	-6.64	1.44	1.52
3	M	265	MET	CA-C	-6.64	1.43	1.52
1	D	137	LEU	C-N	6.64	1.41	1.33
1	E	91	ARG	NE-CZ	6.64	1.40	1.33
2	2	107	LEU	CA-C	-6.64	1.43	1.52
2	1	64	GLN	CA-C	-6.64	1.44	1.52
3	L	263	ARG	CD-NE	6.64	1.55	1.46
1	F	186	ASP	C-N	6.63	1.43	1.33
1	g	34	GLY	N-CA	6.63	1.54	1.45
3	J	239	PHE	CA-CB	6.63	1.62	1.53
2	5	163	GLU	C-N	6.63	1.43	1.33
3	M	43	ARG	CZ-NH2	6.63	1.42	1.33
1	e	77	ALA	CA-C	-6.63	1.44	1.52
1	G	19	GLY	C-N	6.62	1.42	1.33
1	E	75	CYS	C-N	6.62	1.41	1.33
2	h	107	LEU	CA-C	-6.62	1.45	1.52
1	a	148	TYR	CA-C	-6.62	1.44	1.52
1	a	82	VAL	CA-C	-6.62	1.44	1.52
1	b	241	ARG	NE-CZ	6.62	1.40	1.33
3	I	120	PRO	CA-C	-6.62	1.44	1.52
3	L	293	LEU	CA-C	-6.62	1.44	1.52
3	J	57	ARG	CD-NE	6.62	1.55	1.46
2	1	159	ILE	CA-C	6.61	1.61	1.52
3	M	335	ASP	CA-C	-6.61	1.44	1.52
2	j	115	ILE	CA-C	-6.61	1.44	1.52
1	e	20	ARG	NE-CZ	6.60	1.40	1.33
1	e	53	ARG	CD-NE	6.60	1.55	1.46
1	c	186	ASP	C-N	6.59	1.42	1.33
1	g	198	LEU	CA-C	-6.59	1.44	1.52
2	1	66	LEU	N-CA	-6.59	1.38	1.46
2	i	170	ARG	CZ-NH1	6.59	1.42	1.32
1	b	138	ILE	N-CA	-6.59	1.38	1.46
1	F	229	LEU	CA-C	-6.59	1.44	1.52
2	i	118	GLU	C-N	6.59	1.40	1.33
3	K	231	LYS	CA-CB	6.59	1.63	1.53
2	2	142	SER	N-CA	-6.58	1.37	1.46
1	g	57	LYS	CA-C	-6.58	1.44	1.52
2	1	104	PHE	N-CA	-6.58	1.39	1.46
3	M	317	ARG	NE-CZ	6.58	1.40	1.33
2	2	97	LEU	CA-C	-6.58	1.44	1.52
2	4	143	GLY	N-CA	-6.58	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	204	LEU	CA-C	-6.58	1.44	1.52
1	d	73	HIS	C-N	6.58	1.42	1.33
1	E	106	PRO	N-CD	-6.58	1.38	1.47
2	7	212	ARG	NE-CZ	6.58	1.40	1.33
3	K	353	ALA	CA-C	6.58	1.61	1.52
2	1	49	ALA	N-CA	-6.57	1.38	1.46
3	M	116	VAL	CA-CB	6.57	1.62	1.54
1	E	180	ARG	CD-NE	6.57	1.55	1.46
1	c	243	LEU	C-N	6.57	1.41	1.33
2	h	178	ARG	C-N	6.57	1.42	1.33
1	c	241	ARG	CD-NE	6.57	1.55	1.46
2	i	29	LYS	C-N	6.57	1.42	1.33
3	H	52	ARG	CZ-NH1	6.57	1.42	1.32
3	L	95	ILE	N-CA	-6.56	1.38	1.46
1	e	146	LYS	CA-C	-6.56	1.44	1.52
2	6	168	ALA	N-CA	-6.56	1.38	1.46
1	F	36	THR	N-CA	-6.56	1.38	1.46
2	k	159	ILE	N-CA	-6.56	1.38	1.46
3	K	31	GLU	C-N	6.56	1.42	1.33
3	L	264	THR	CA-C	-6.56	1.43	1.52
1	g	79	SER	N-CA	-6.56	1.38	1.46
3	I	395	VAL	C-O	-6.55	1.17	1.24
3	M	232	GLU	CA-C	-6.55	1.43	1.52
2	m	114	GLY	CA-C	-6.55	1.43	1.52
2	6	189	VAL	C-N	6.55	1.42	1.33
3	I	129	GLY	C-N	6.55	1.42	1.33
3	M	107	ALA	N-CA	-6.55	1.38	1.46
1	B	213	TYR	N-CA	-6.55	1.38	1.46
1	D	49	ILE	C-O	-6.54	1.17	1.24
3	L	331	ALA	CA-CB	6.54	1.65	1.53
1	g	235	ARG	NE-CZ	6.54	1.40	1.33
3	M	137	GLU	C-N	6.54	1.41	1.33
1	c	71	ASP	C-N	6.54	1.42	1.33
2	i	41	ALA	C-N	6.54	1.41	1.33
2	k	103	TYR	CA-C	-6.54	1.44	1.52
1	E	213	TYR	C-N	6.54	1.42	1.33
2	i	67	ALA	CA-C	-6.54	1.44	1.52
1	C	82	VAL	CA-CB	-6.53	1.46	1.54
2	l	106	TYR	CA-C	-6.53	1.44	1.52
1	a	118	ASP	CA-C	-6.53	1.44	1.52
1	b	93	ARG	CA-C	-6.53	1.44	1.52
1	g	139	ALA	N-CA	-6.53	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	168	ALA	C-N	6.53	1.42	1.33
2	j	132	ILE	C-N	6.53	1.43	1.33
1	g	100	ARG	CZ-NH1	6.52	1.41	1.32
3	M	164	PRO	N-CA	6.52	1.56	1.47
1	D	129	VAL	CA-C	-6.52	1.44	1.52
2	m	127	PRO	N-CA	-6.52	1.39	1.47
1	a	29	GLU	C-N	6.52	1.42	1.33
1	d	170	ALA	CA-C	-6.52	1.44	1.52
1	B	147	LEU	CA-C	-6.51	1.44	1.52
1	C	220	THR	CA-C	-6.51	1.45	1.52
2	4	123	TYR	N-CA	-6.51	1.38	1.46
1	E	193	LEU	CA-C	-6.51	1.44	1.52
1	F	239	ARG	CZ-NH1	6.51	1.41	1.32
1	d	104	ASP	CA-CB	6.51	1.63	1.53
1	F	18	ASP	C-N	6.51	1.41	1.33
3	H	200	ARG	CD-NE	6.51	1.55	1.46
2	4	30	ARG	CZ-NH1	6.50	1.41	1.32
3	J	62	PRO	N-CA	-6.50	1.39	1.46
2	2	52	MET	CA-CB	6.49	1.64	1.53
1	g	110	LYS	CA-C	-6.49	1.44	1.52
2	2	101	TYR	CA-CB	6.49	1.61	1.52
3	I	79	VAL	N-CA	-6.49	1.38	1.46
1	A	188	ALA	CA-C	-6.49	1.44	1.52
2	2	172	ILE	CB-CG1	6.49	1.66	1.53
1	a	149	GLU	C-N	6.49	1.42	1.33
2	1	90	ILE	C-N	6.48	1.42	1.33
2	4	84	LYS	C-N	6.48	1.41	1.33
1	b	100	ARG	CZ-NH1	6.48	1.41	1.32
1	C	82	VAL	CA-C	-6.48	1.44	1.52
1	C	189	MET	CA-C	-6.48	1.44	1.52
2	1	139	ALA	N-CA	-6.48	1.37	1.45
2	4	153	ASP	C-N	6.48	1.42	1.33
3	L	177	GLY	N-CA	-6.48	1.38	1.45
2	i	210	LYS	N-CA	-6.48	1.37	1.46
3	J	341	ARG	CA-C	-6.48	1.44	1.52
3	K	310	PRO	CA-C	-6.48	1.43	1.52
2	h	61	GLY	C-N	6.47	1.42	1.34
2	h	81	ARG	CD-NE	6.47	1.55	1.46
3	M	310	PRO	N-CA	-6.47	1.39	1.47
1	A	69	LYS	C-N	6.46	1.40	1.33
2	1	188	VAL	CA-CB	-6.46	1.46	1.54
3	H	36	PHE	N-CA	-6.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	284	ILE	C-N	6.46	1.40	1.32
1	E	83	ALA	CA-C	-6.46	1.44	1.52
2	1	137	ILE	C-N	6.46	1.39	1.33
1	d	81	LEU	CA-CB	6.45	1.64	1.53
1	E	33	ARG	NE-CZ	6.45	1.40	1.33
2	h	29	LYS	C-N	6.45	1.42	1.33
3	I	194	ALA	CA-C	-6.45	1.44	1.52
1	c	110	LYS	N-CA	-6.45	1.38	1.46
2	k	147	ALA	CA-C	-6.45	1.44	1.52
3	H	228	GLN	CA-CB	6.45	1.63	1.53
3	J	179	LEU	CA-C	-6.45	1.44	1.52
1	d	13	THR	CA-C	-6.44	1.45	1.52
3	L	259	ARG	NE-CZ	6.44	1.40	1.33
1	c	130	ARG	NE-CZ	6.43	1.40	1.33
1	E	157	LEU	CA-C	-6.43	1.44	1.52
2	i	143	GLY	C-N	6.43	1.42	1.33
1	A	79	SER	N-CA	-6.43	1.37	1.45
1	g	156	LEU	CA-C	-6.43	1.44	1.52
1	B	93	ARG	NE-CZ	6.43	1.40	1.33
2	2	33	MET	CA-C	-6.43	1.44	1.52
3	I	71	ILE	C-O	-6.43	1.17	1.24
1	D	120	LYS	N-CA	6.43	1.54	1.46
1	d	126	TYR	C-N	6.43	1.40	1.33
1	B	229	LEU	CA-CB	6.43	1.63	1.53
1	e	138	ILE	C-N	6.43	1.42	1.33
1	a	83	ALA	CA-C	-6.42	1.44	1.52
1	e	100	ARG	NE-CZ	6.42	1.40	1.33
3	K	203	PHE	N-CA	-6.42	1.37	1.46
1	D	230	LYS	N-CA	-6.42	1.40	1.46
3	I	238	ILE	CA-C	-6.42	1.45	1.52
1	d	115	LYS	N-CA	-6.41	1.38	1.46
3	L	101	LYS	CA-C	-6.41	1.45	1.52
1	E	93	ARG	NE-CZ	6.41	1.40	1.33
1	c	53	ARG	NE-CZ	6.41	1.40	1.33
3	H	359	GLY	C-N	6.41	1.42	1.33
2	1	148	TYR	CA-CB	6.40	1.63	1.53
3	J	83	THR	C-N	6.40	1.43	1.33
1	C	134	VAL	N-CA	6.40	1.53	1.46
1	D	229	LEU	CA-C	-6.40	1.44	1.52
1	e	31	VAL	C-N	6.40	1.42	1.33
1	A	46	VAL	CA-CB	-6.40	1.46	1.54
2	4	202	GLU	CA-C	-6.40	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	309	VAL	CA-C	-6.40	1.47	1.53
1	F	91	ARG	NE-CZ	6.40	1.40	1.33
3	J	331	ALA	C-N	-6.40	1.25	1.33
3	K	70	ASP	N-CA	-6.39	1.38	1.46
3	M	238	ILE	CA-C	-6.39	1.44	1.52
1	A	142	ASP	CA-C	-6.39	1.44	1.52
3	L	224	ARG	CZ-NH2	6.39	1.41	1.33
1	a	229	LEU	N-CA	-6.39	1.38	1.46
1	G	74	ILE	N-CA	-6.39	1.38	1.46
2	4	88	ARG	NE-CZ	6.39	1.40	1.33
2	k	95	SER	C-N	6.39	1.42	1.34
1	g	155	ALA	CA-CB	6.39	1.61	1.53
1	A	205	VAL	CA-C	-6.39	1.48	1.52
2	n	28	GLU	CA-C	-6.38	1.44	1.52
3	J	251	THR	CB-OG1	-6.38	1.33	1.43
2	1	137	ILE	CA-C	-6.38	1.45	1.52
1	C	107	ILE	N-CA	6.38	1.53	1.46
2	i	165	VAL	C-N	6.38	1.42	1.33
1	b	210	GLU	CA-C	-6.38	1.44	1.52
2	j	211	PHE	N-CA	-6.38	1.39	1.46
2	4	51	ARG	CZ-NH2	6.38	1.41	1.33
3	I	46	ARG	CA-C	-6.38	1.44	1.52
1	D	14	VAL	CA-C	-6.37	1.44	1.52
2	m	149	GLY	CA-C	-6.37	1.44	1.51
3	J	250	ARG	N-CA	-6.37	1.37	1.46
1	F	143	GLU	N-CA	-6.37	1.38	1.46
2	h	170	ARG	CZ-NH2	6.37	1.41	1.33
3	H	150	ILE	CA-C	-6.37	1.44	1.52
3	I	130	PHE	CA-C	-6.37	1.44	1.52
3	J	200	ARG	NE-CZ	6.37	1.40	1.33
1	G	41	LYS	CA-CB	6.37	1.63	1.53
3	K	56	GLU	CA-CB	6.37	1.64	1.53
1	A	26	TYR	N-CA	-6.36	1.38	1.46
1	B	241	ARG	NE-CZ	6.36	1.40	1.33
2	6	180	SER	C-O	-6.36	1.17	1.24
3	L	99	GLU	N-CA	-6.36	1.38	1.46
1	B	220	THR	C-N	6.36	1.42	1.33
1	B	86	ARG	NE-CZ	6.36	1.40	1.33
2	h	37	ILE	CA-C	-6.36	1.45	1.52
1	D	20	ARG	NE-CZ	6.35	1.40	1.33
1	E	202	SER	CA-CB	6.35	1.64	1.53
1	g	10	ARG	CD-NE	6.35	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	178	ARG	CA-C	-6.35	1.43	1.52
2	i	188	VAL	CA-C	-6.35	1.45	1.52
2	k	82	GLU	CA-CB	6.35	1.62	1.53
3	I	205	ARG	CA-CB	6.35	1.62	1.53
1	b	62	ASP	C-N	6.34	1.42	1.33
1	D	114	LYS	N-CA	-6.34	1.38	1.46
2	7	130	GLY	CA-C	-6.34	1.43	1.51
1	A	91	ARG	CD-NE	6.34	1.55	1.46
1	c	244	LEU	CA-CB	6.34	1.61	1.52
2	4	175	ALA	CA-C	-6.34	1.44	1.52
2	2	197	TYR	CA-C	-6.33	1.45	1.52
1	E	20	ARG	CD-NE	6.33	1.55	1.46
3	J	333	ASP	CA-CB	6.33	1.63	1.53
3	J	52	ARG	CD-NE	6.33	1.55	1.46
1	E	70	ILE	N-CA	6.33	1.54	1.46
3	K	114	ALA	C-N	6.33	1.39	1.33
1	F	156	LEU	C-O	6.32	1.31	1.24
2	6	178	ARG	CZ-NH2	6.32	1.41	1.33
3	K	305	ARG	CA-C	-6.32	1.44	1.52
1	f	101	LEU	CB-CG	6.32	1.66	1.53
3	M	123	LYS	C-N	6.32	1.39	1.33
2	4	170	ARG	NE-CZ	6.32	1.40	1.33
2	6	110	LEU	CA-C	-6.32	1.45	1.52
1	b	103	TYR	CA-CB	6.31	1.63	1.54
1	B	235	ARG	CZ-NH1	6.31	1.41	1.32
2	5	212	ARG	NE-CZ	6.31	1.40	1.33
2	l	197	TYR	CA-C	-6.31	1.45	1.52
3	I	393	LYS	N-CA	-6.31	1.38	1.46
3	H	324	HIS	C-N	6.31	1.42	1.34
1	b	211	VAL	C-N	6.31	1.40	1.34
1	b	197	GLY	CA-C	-6.30	1.45	1.52
2	2	135	LYS	CA-C	-6.30	1.44	1.52
2	4	207	ILE	CA-CB	6.30	1.62	1.54
2	n	110	LEU	C-N	6.30	1.42	1.33
1	F	13	THR	CA-CB	6.30	1.63	1.53
1	B	166	MET	N-CA	-6.30	1.38	1.46
1	D	130	ARG	CD-NE	6.30	1.55	1.46
1	C	202	SER	C-N	6.30	1.41	1.33
3	K	57	ARG	CD-NE	6.30	1.55	1.46
3	L	162	LEU	CA-C	-6.30	1.43	1.52
2	4	212	ARG	CD-NE	6.30	1.55	1.46
3	K	324	HIS	N-CA	-6.29	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	74	ALA	CA-CB	6.29	1.63	1.53
1	C	41	LYS	C-N	6.29	1.42	1.33
1	g	130	ARG	CD-NE	6.29	1.55	1.46
2	j	105	PRO	CA-CB	6.29	1.63	1.53
3	J	300	PRO	C-N	6.29	1.41	1.33
1	E	103	TYR	N-CA	-6.29	1.38	1.46
1	F	9	ASP	C-N	6.29	1.42	1.33
1	A	180	ARG	CZ-NH1	6.28	1.41	1.32
1	C	130	ARG	CD-NE	6.28	1.55	1.46
3	I	70	ASP	CA-C	-6.28	1.45	1.52
1	a	176	GLU	CA-CB	6.28	1.63	1.53
1	G	93	ARG	NE-CZ	6.28	1.40	1.33
1	F	150	THR	CA-CB	-6.28	1.43	1.53
1	A	44	GLU	N-CA	-6.28	1.40	1.46
3	L	310	PRO	N-CA	-6.28	1.39	1.47
1	G	11	ALA	C-N	6.28	1.40	1.34
3	L	85	PRO	N-CD	-6.27	1.39	1.47
3	M	49	ARG	CD-NE	6.27	1.55	1.46
1	b	38	ILE	CA-CB	-6.27	1.46	1.54
1	d	220	THR	N-CA	-6.27	1.38	1.46
2	3	83	ARG	C-N	6.27	1.42	1.33
2	l	138	VAL	CA-C	-6.27	1.44	1.52
2	m	52	MET	C-N	6.27	1.41	1.33
2	1	110	LEU	CA-C	-6.27	1.44	1.53
2	j	30	ARG	CD-NE	6.26	1.55	1.46
3	I	25	GLU	N-CA	-6.26	1.38	1.46
1	g	228	GLU	N-CA	-6.26	1.38	1.46
2	2	120	LYS	CA-C	-6.26	1.45	1.52
3	L	59	ARG	CZ-NH2	6.26	1.41	1.33
1	f	241	ARG	NE-CZ	6.26	1.40	1.33
2	1	56	THR	CA-C	-6.26	1.45	1.52
2	5	184	ASP	N-CA	-6.26	1.38	1.46
1	g	81	LEU	CA-C	6.25	1.61	1.52
2	4	116	ASP	C-N	6.25	1.42	1.33
1	d	91	ARG	CD-NE	6.25	1.55	1.46
1	G	35	ALA	N-CA	-6.25	1.38	1.45
1	C	60	GLU	N-CA	-6.25	1.38	1.46
2	2	52	MET	N-CA	-6.24	1.38	1.46
1	a	181	ASP	N-CA	6.24	1.53	1.46
1	g	187	ASP	CA-CB	6.24	1.63	1.53
2	2	156	THR	N-CA	-6.24	1.39	1.46
2	4	25	MET	CA-C	-6.24	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	125	ILE	C-N	6.24	1.41	1.33
1	E	199	SER	N-CA	-6.24	1.38	1.46
3	M	145	GLY	CA-C	-6.24	1.43	1.51
1	C	163	ALA	C-N	6.24	1.42	1.33
1	F	100	ARG	CA-C	-6.24	1.44	1.52
3	K	277	PRO	C-N	6.24	1.42	1.33
2	i	117	SER	CA-CB	6.23	1.64	1.53
2	l	108	VAL	CA-C	-6.23	1.45	1.52
2	h	53	ALA	C-N	6.23	1.41	1.33
2	5	204	VAL	CA-C	-6.23	1.44	1.52
2	k	153	ASP	CA-CB	6.22	1.63	1.53
2	n	148	TYR	CA-CB	6.22	1.63	1.53
3	I	224	ARG	NE-CZ	6.22	1.39	1.33
3	L	63	LEU	CA-C	-6.22	1.45	1.52
2	1	144	SER	N-CA	6.22	1.53	1.46
2	j	13	THR	CA-CB	6.22	1.64	1.53
3	M	109	ASN	CA-CB	6.22	1.60	1.53
1	b	12	ILE	CA-C	6.22	1.61	1.53
2	6	117	SER	CA-CB	6.21	1.62	1.53
1	b	225	SER	C-N	6.21	1.40	1.34
2	6	130	GLY	CA-C	-6.21	1.44	1.52
3	H	283	VAL	CA-CB	6.21	1.61	1.54
3	I	377	LYS	CA-C	-6.21	1.44	1.52
3	K	275	PHE	CA-C	-6.21	1.44	1.52
3	I	364	ARG	CZ-NH1	6.21	1.41	1.32
3	L	74	ASP	C-N	6.21	1.41	1.33
1	b	33	ARG	CD-NE	6.21	1.54	1.46
1	d	26	TYR	C-N	6.21	1.42	1.34
1	E	11	ALA	C-N	6.21	1.40	1.34
1	G	219	ARG	C-N	6.21	1.41	1.33
2	4	144	SER	C-N	6.21	1.42	1.33
1	a	130	ARG	CD-NE	6.21	1.54	1.46
1	g	243	LEU	C-N	6.21	1.42	1.33
2	i	140	THR	CA-CB	6.21	1.64	1.53
3	M	15	LYS	CA-CB	6.21	1.62	1.53
2	1	112	ILE	CA-CB	-6.21	1.46	1.54
2	7	111	LEU	C-N	6.21	1.41	1.33
3	H	326	ARG	CD-NE	6.20	1.54	1.46
1	e	73	HIS	CE1-NE2	6.20	1.38	1.32
1	D	93	ARG	NE-CZ	6.20	1.39	1.33
2	j	84	LYS	CA-CB	6.20	1.62	1.53
3	M	67	VAL	N-CA	-6.20	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	99	ASN	C-O	-6.20	1.16	1.24
2	7	120	LYS	N-CA	-6.19	1.38	1.46
3	I	197	ASN	N-CA	-6.19	1.38	1.46
1	a	21	LEU	CA-C	-6.19	1.44	1.53
1	E	185	PHE	CA-C	-6.19	1.44	1.52
1	F	29	GLU	N-CA	-6.19	1.38	1.46
3	K	253	SER	C-N	6.19	1.42	1.33
1	C	65	GLU	CA-C	-6.18	1.45	1.52
1	D	239	ARG	NE-CZ	6.18	1.39	1.33
2	k	116	ASP	N-CA	-6.18	1.37	1.46
2	2	21	ASP	N-CA	6.18	1.52	1.47
2	5	16	GLY	N-CA	-6.18	1.39	1.45
1	f	201	GLU	CA-CB	6.17	1.62	1.53
1	g	235	ARG	CD-NE	6.17	1.54	1.46
2	l	15	VAL	C-N	6.17	1.41	1.32
1	A	204	LEU	C-N	6.17	1.37	1.33
2	2	132	ILE	N-CA	6.17	1.54	1.46
3	M	105	ARG	NE-CZ	6.17	1.39	1.33
3	I	305	ARG	CD-NE	6.17	1.54	1.46
1	d	131	PRO	N-CD	6.17	1.56	1.47
2	6	33	MET	CA-C	6.16	1.59	1.52
2	n	98	LEU	CA-C	-6.16	1.44	1.52
3	I	141	GLU	CA-C	-6.16	1.44	1.52
1	e	245	LYS	C-N	6.16	1.42	1.33
2	3	26	ALA	C-N	6.16	1.42	1.33
2	n	43	LYS	CA-C	-6.15	1.45	1.52
3	K	24	ARG	NE-CZ	6.15	1.39	1.33
2	h	212	ARG	CD-NE	6.15	1.54	1.46
1	d	241	ARG	C-N	6.15	1.42	1.33
3	K	11	GLU	N-CA	6.15	1.53	1.46
1	b	46	VAL	CA-CB	-6.15	1.46	1.54
1	b	63	THR	CA-C	6.14	1.60	1.52
2	4	28	GLU	C-N	6.14	1.42	1.33
1	d	168	ARG	NE-CZ	6.14	1.39	1.33
2	i	15	VAL	C-N	6.14	1.42	1.33
2	j	145	LEU	CA-CB	6.14	1.63	1.53
1	b	144	VAL	N-CA	-6.13	1.41	1.46
1	c	103	TYR	CZ-OH	6.13	1.50	1.38
2	n	69	ILE	CA-CB	-6.13	1.47	1.54
3	L	351	ILE	C-N	6.13	1.42	1.33
1	C	130	ARG	CZ-NH2	6.13	1.41	1.33
1	d	100	ARG	CA-C	-6.13	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	229	LEU	N-CA	-6.13	1.39	1.46
1	E	81	LEU	N-CA	-6.13	1.38	1.46
3	H	332	GLU	C-N	6.13	1.42	1.33
2	j	31	ALA	CA-C	-6.13	1.45	1.52
1	b	213	TYR	N-CA	-6.12	1.39	1.46
3	J	86	LYS	CA-C	-6.12	1.45	1.52
1	C	129	VAL	CA-CB	-6.12	1.46	1.54
2	i	212	ARG	CD-NE	6.12	1.54	1.46
1	b	91	ARG	N-CA	-6.12	1.39	1.46
2	n	47	GLN	CA-CB	6.12	1.61	1.53
2	6	190	LYS	N-CA	-6.12	1.38	1.46
3	I	26	LEU	CA-C	-6.12	1.45	1.52
3	K	197	ASN	CA-CB	6.12	1.62	1.53
2	j	169	VAL	CA-C	-6.11	1.45	1.52
2	6	212	ARG	NE-CZ	6.11	1.39	1.33
1	f	87	VAL	CA-C	-6.11	1.44	1.52
1	f	118	ASP	CA-CB	6.11	1.62	1.53
3	M	64	LEU	CA-C	-6.11	1.45	1.52
3	K	233	LYS	CA-C	-6.11	1.45	1.52
3	K	370	VAL	CA-C	-6.10	1.46	1.52
2	2	55	THR	CA-C	-6.10	1.45	1.52
2	7	47	GLN	CA-CB	6.10	1.61	1.53
3	J	375	PHE	N-CA	6.10	1.53	1.46
1	A	159	TYR	CA-C	-6.10	1.45	1.52
1	f	243	LEU	CA-C	-6.10	1.44	1.52
2	h	145	LEU	N-CA	-6.10	1.39	1.46
2	4	154	ARG	CD-NE	6.10	1.54	1.46
2	m	41	ALA	CA-C	-6.10	1.45	1.52
1	g	224	VAL	CA-C	-6.10	1.45	1.52
2	1	88	ARG	CA-C	-6.10	1.45	1.52
2	1	145	LEU	C-N	6.09	1.42	1.33
1	F	53	ARG	CD-NE	6.09	1.54	1.46
2	3	154	ARG	N-CA	6.09	1.53	1.46
2	7	59	SER	C-N	6.09	1.41	1.33
1	g	195	ALA	CA-C	-6.09	1.45	1.52
3	L	186	THR	CA-C	-6.09	1.45	1.52
3	J	226	VAL	CA-CB	-6.09	1.46	1.54
2	k	81	ARG	CD-NE	6.09	1.54	1.46
1	E	130	ARG	CA-CB	6.09	1.64	1.53
1	G	182	ASP	C-N	6.09	1.41	1.33
2	4	36	PHE	CA-C	-6.08	1.45	1.52
2	i	212	ARG	NE-CZ	6.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	48	ILE	C-O	-6.08	1.17	1.24
3	I	151	GLU	N-CA	-6.08	1.38	1.46
3	K	43	ARG	NE-CZ	6.08	1.39	1.33
1	c	198	LEU	CA-C	-6.08	1.44	1.52
1	E	187	ASP	CA-C	-6.08	1.44	1.52
2	h	94	THR	CA-CB	-6.08	1.43	1.53
2	l	30	ARG	NE-CZ	6.08	1.39	1.33
2	6	52	MET	CA-C	-6.08	1.45	1.52
1	c	235	ARG	C-N	6.08	1.42	1.34
2	j	186	ILE	C-N	6.08	1.41	1.33
2	l	132	ILE	CA-CB	6.08	1.61	1.53
1	c	158	GLU	CA-C	-6.07	1.44	1.52
2	i	125	ILE	C-N	6.07	1.41	1.33
2	7	175	ALA	C-O	-6.07	1.17	1.24
3	H	193	LYS	C-N	6.07	1.42	1.33
3	I	186	THR	N-CA	-6.07	1.38	1.46
1	c	60	GLU	CA-C	-6.07	1.44	1.52
1	c	69	LYS	CA-CB	6.07	1.62	1.53
1	D	227	GLU	N-CA	-6.07	1.38	1.46
3	M	65	VAL	CA-CB	-6.07	1.46	1.54
3	I	146	LEU	CA-C	-6.07	1.46	1.53
2	i	171	ALA	C-N	6.07	1.41	1.33
2	j	59	SER	CA-C	-6.07	1.44	1.52
2	m	39	SER	CA-C	-6.07	1.45	1.52
3	H	184	PRO	N-CA	-6.07	1.40	1.46
3	H	78	VAL	C-N	6.07	1.41	1.33
1	C	220	THR	N-CA	-6.06	1.39	1.46
1	e	89	ILE	C-N	6.06	1.41	1.33
2	3	101	TYR	CA-CB	6.06	1.61	1.52
1	B	20	ARG	CZ-NH1	6.06	1.41	1.32
1	C	168	ARG	CA-C	-6.06	1.44	1.52
1	D	125	GLN	CA-C	-6.06	1.45	1.52
1	F	178	GLU	N-CA	-6.06	1.38	1.46
2	7	36	PHE	CA-C	-6.06	1.45	1.52
3	H	79	VAL	N-CA	-6.06	1.38	1.46
3	J	215	TYR	CA-C	-6.06	1.44	1.52
3	K	342	ILE	C-N	6.05	1.40	1.33
2	1	132	ILE	CA-CB	-6.05	1.45	1.54
3	H	207	VAL	CA-C	-6.05	1.45	1.52
1	G	74	ILE	C-N	6.05	1.42	1.33
2	k	137	ILE	CA-CB	6.05	1.62	1.54
1	C	48	LEU	CA-C	-6.05	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	37	ILE	N-CA	-6.05	1.39	1.46
1	B	40	ILE	CA-C	-6.05	1.45	1.52
1	g	191	LEU	C-N	6.05	1.41	1.33
2	3	211	PHE	CA-C	-6.05	1.45	1.53
1	D	59	LEU	CA-C	-6.04	1.45	1.52
2	k	135	LYS	CA-C	6.04	1.59	1.52
2	5	73	GLU	CA-C	-6.04	1.44	1.52
2	n	42	ALA	C-N	6.04	1.42	1.33
2	l	54	MET	C-N	6.04	1.41	1.33
2	k	96	ASN	N-CA	-6.04	1.38	1.46
2	i	37	ILE	C-N	6.04	1.42	1.33
3	M	229	LEU	N-CA	-6.04	1.39	1.46
1	A	197	GLY	CA-C	-6.04	1.45	1.52
2	5	170	ARG	C-N	6.04	1.41	1.33
3	K	161	LEU	CA-CB	6.04	1.63	1.53
2	j	102	ARG	CD-NE	6.04	1.54	1.46
2	n	102	ARG	CD-NE	6.04	1.54	1.46
3	J	396	MET	CA-C	-6.04	1.45	1.52
3	L	192	ALA	CA-C	-6.03	1.44	1.52
1	B	21	LEU	N-CA	-6.03	1.39	1.46
3	K	32	ASP	C-O	-6.03	1.17	1.24
3	M	211	PHE	C-N	6.03	1.41	1.33
1	E	56	SER	CA-CB	6.03	1.64	1.53
2	3	105	PRO	N-CA	-6.02	1.39	1.47
1	e	183	LEU	CA-C	-6.02	1.45	1.52
1	g	158	GLU	CA-CB	6.02	1.62	1.53
2	m	30	ARG	CD-NE	6.02	1.54	1.46
1	D	217	ASP	N-CA	-6.02	1.38	1.46
2	6	87	VAL	C-N	6.02	1.42	1.33
3	L	210	GLU	CA-C	-6.01	1.44	1.52
1	e	117	CYS	CA-C	-6.01	1.45	1.52
1	e	106	PRO	C-N	6.01	1.41	1.33
2	k	125	ILE	CA-CB	-6.01	1.47	1.54
3	M	247	ALA	C-N	6.01	1.41	1.33
1	D	183	LEU	N-CA	-6.01	1.38	1.45
1	f	20	ARG	CD-NE	6.01	1.54	1.46
2	l	173	TYR	N-CA	-6.01	1.39	1.46
3	H	361	PHE	CA-C	-6.01	1.44	1.52
3	M	246	ILE	N-CA	-6.00	1.38	1.46
1	E	109	VAL	N-CA	6.00	1.53	1.46
3	H	182	GLY	CA-C	-6.00	1.43	1.51
1	G	79	SER	N-CA	-6.00	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	145	GLY	N-CA	-6.00	1.39	1.45
3	K	109	ASN	CA-CB	-6.00	1.44	1.53
1	E	154	GLY	CA-C	5.99	1.60	1.51
2	1	88	ARG	NE-CZ	5.99	1.39	1.33
3	I	338	GLU	CA-CB	5.99	1.62	1.53
1	A	178	GLU	CA-C	-5.99	1.45	1.52
1	e	180	ARG	CZ-NH2	5.99	1.41	1.33
3	L	328	MET	C-N	5.99	1.41	1.33
2	n	69	ILE	N-CA	-5.99	1.39	1.46
3	J	278	ARG	CA-CB	5.99	1.62	1.53
3	I	341	ARG	N-CA	5.99	1.53	1.46
3	L	99	GLU	CA-CB	5.99	1.62	1.53
2	n	102	ARG	CZ-NH2	5.98	1.41	1.33
2	l	199	TYR	N-CA	-5.98	1.38	1.46
2	7	87	VAL	CA-CB	-5.98	1.47	1.54
3	M	120	PRO	N-CA	-5.98	1.39	1.47
1	d	178	GLU	CA-C	-5.98	1.44	1.52
2	h	158	GLU	C-N	5.98	1.41	1.33
3	L	397	PHE	CA-C	-5.98	1.44	1.52
1	A	210	GLU	CA-C	-5.97	1.45	1.52
1	D	25	GLU	CA-C	-5.97	1.44	1.52
2	5	72	ILE	CA-C	-5.97	1.45	1.52
2	2	42	ALA	C-N	5.97	1.41	1.33
1	g	58	LEU	N-CA	-5.97	1.39	1.46
1	g	107	ILE	N-CA	-5.96	1.38	1.46
1	D	91	ARG	CD-NE	5.96	1.54	1.46
2	l	148	TYR	CA-C	-5.96	1.45	1.52
1	g	120	LYS	N-CA	-5.96	1.39	1.46
3	H	322	LYS	N-CA	5.96	1.53	1.46
2	i	68	ARG	CZ-NH2	5.95	1.41	1.33
3	H	205	ARG	CD-NE	5.95	1.54	1.46
3	M	43	ARG	NE-CZ	5.95	1.39	1.33
1	d	216	VAL	C-N	5.95	1.42	1.33
2	1	81	ARG	C-N	5.95	1.42	1.33
2	k	67	ALA	N-CA	-5.95	1.39	1.46
3	L	303	PHE	CA-C	-5.95	1.45	1.52
1	A	205	VAL	C-N	5.95	1.38	1.33
1	c	39	GLY	CA-C	-5.95	1.43	1.51
2	k	211	PHE	CA-C	-5.95	1.45	1.53
3	L	394	GLY	CA-C	5.94	1.59	1.52
1	A	147	LEU	N-CA	-5.94	1.38	1.46
1	c	86	ARG	CZ-NH1	5.94	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	20	TYR	CA-CB	5.94	1.63	1.53
3	M	253	SER	CA-CB	5.94	1.62	1.53
1	A	44	GLU	CA-C	-5.94	1.46	1.53
1	d	43	LYS	C-N	5.94	1.42	1.33
2	h	134	GLU	CA-C	-5.94	1.45	1.52
2	k	158	GLU	CA-C	5.94	1.60	1.52
1	D	111	GLU	C-N	5.94	1.41	1.33
3	H	41	ARG	NE-CZ	5.94	1.39	1.33
3	L	392	LEU	C-N	5.94	1.41	1.33
3	J	360	MET	CA-CB	5.93	1.63	1.53
3	H	49	ARG	CD-NE	5.93	1.54	1.46
1	E	131	PRO	CA-CB	5.93	1.61	1.53
2	j	128	ILE	C-N	5.93	1.42	1.33
2	n	51	ARG	CZ-NH2	5.93	1.41	1.33
3	K	30	LEU	N-CA	5.93	1.53	1.46
3	I	154	ARG	CD-NE	5.93	1.54	1.46
2	k	42	ALA	CA-CB	5.93	1.61	1.53
3	I	104	ALA	CA-C	-5.93	1.45	1.52
2	2	19	CYS	CA-C	-5.92	1.45	1.52
2	5	125	ILE	N-CA	-5.92	1.39	1.46
3	I	101	LYS	CA-CB	5.92	1.61	1.53
3	J	272	LEU	CA-C	-5.92	1.45	1.52
3	H	113	LEU	CA-CB	5.92	1.63	1.53
3	H	358	ALA	N-CA	-5.92	1.39	1.46
2	j	178	ARG	CZ-NH2	5.92	1.41	1.33
3	M	390	PRO	CA-CB	5.92	1.61	1.53
2	7	101	TYR	CA-CB	5.92	1.61	1.53
1	D	28	ARG	CZ-NH2	5.92	1.41	1.33
2	j	124	SER	N-CA	-5.92	1.39	1.46
3	H	339	LEU	C-N	5.92	1.41	1.33
1	B	21	LEU	CA-C	-5.92	1.45	1.52
2	2	68	ARG	CZ-NH2	5.92	1.41	1.33
3	J	52	ARG	CZ-NH2	5.92	1.41	1.33
2	1	146	THR	N-CA	-5.91	1.39	1.46
2	6	39	SER	C-O	5.91	1.30	1.23
3	H	332	GLU	CA-CB	5.91	1.61	1.53
3	K	246	ILE	CA-C	-5.91	1.45	1.52
2	7	191	ILE	CA-C	-5.91	1.45	1.52
1	F	138	ILE	C-O	-5.91	1.17	1.24
2	h	96	ASN	C-N	5.91	1.41	1.33
2	l	33	MET	CA-C	-5.91	1.45	1.52
2	6	69	ILE	CA-CB	-5.91	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	107	LEU	CA-C	-5.91	1.45	1.52
2	7	147	ALA	C-O	-5.91	1.17	1.24
1	b	198	LEU	CA-CB	5.90	1.62	1.53
1	E	128	GLY	C-N	5.90	1.41	1.33
1	E	111	GLU	CA-C	-5.90	1.44	1.52
1	e	193	LEU	N-CA	-5.90	1.39	1.46
1	G	243	LEU	N-CA	-5.90	1.38	1.46
2	2	76	LEU	C-N	5.90	1.41	1.33
2	4	42	ALA	C-N	5.90	1.41	1.33
2	n	164	ALA	C-N	5.90	1.41	1.33
2	7	102	ARG	CD-NE	5.90	1.54	1.46
1	e	245	LYS	C-O	-5.89	1.16	1.24
1	a	10	ARG	C-N	5.89	1.41	1.33
3	H	289	ARG	NE-CZ	5.89	1.39	1.33
1	G	201	GLU	CA-C	-5.89	1.46	1.53
2	4	75	ASN	N-CA	-5.88	1.39	1.46
1	E	141	VAL	CA-C	-5.88	1.45	1.52
1	B	209	ILE	CA-C	-5.88	1.45	1.52
2	k	54	MET	CA-C	-5.88	1.45	1.52
3	K	146	LEU	C-N	5.88	1.41	1.33
2	2	30	ARG	CD-NE	5.88	1.54	1.46
2	m	135	LYS	CA-CB	5.88	1.61	1.53
1	g	110	LYS	CA-CB	5.88	1.62	1.53
1	a	23	GLN	N-CA	-5.88	1.39	1.46
1	F	35	ALA	CA-C	-5.88	1.44	1.53
2	m	179	ASP	N-CA	-5.88	1.38	1.45
2	n	181	ALA	C-O	-5.88	1.19	1.23
1	d	83	ALA	CA-CB	5.87	1.62	1.53
1	G	71	ASP	C-N	5.87	1.41	1.33
1	A	213	TYR	CA-CB	5.87	1.63	1.53
3	J	80	LYS	C-N	5.87	1.42	1.33
1	E	244	LEU	CA-C	-5.87	1.44	1.52
1	d	10	ARG	CD-NE	5.87	1.54	1.46
3	K	130	PHE	C-N	5.87	1.41	1.33
3	L	256	SER	N-CA	5.87	1.53	1.46
1	c	169	ASN	N-CA	5.87	1.53	1.46
1	g	178	GLU	CA-C	-5.87	1.45	1.52
2	1	212	ARG	CA-C	-5.87	1.45	1.52
1	f	168	ARG	CZ-NH2	5.87	1.41	1.33
2	2	88	ARG	CZ-NH1	5.87	1.41	1.32
3	I	188	LYS	C-N	5.87	1.41	1.33
3	L	250	ARG	CA-CB	5.87	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	341	ARG	NE-CZ	5.86	1.39	1.33
3	L	95	ILE	C-N	5.86	1.41	1.33
3	L	115	ILE	CA-CB	-5.86	1.47	1.54
1	d	235	ARG	CZ-NH1	5.86	1.41	1.32
2	3	164	ALA	C-N	5.86	1.41	1.33
2	5	19	CYS	CA-C	-5.86	1.45	1.52
1	c	100	ARG	CD-NE	5.86	1.54	1.46
1	E	215	LYS	N-CA	-5.86	1.38	1.46
3	H	351	ILE	N-CA	-5.86	1.39	1.46
2	i	25	MET	C-O	-5.86	1.16	1.23
1	e	86	ARG	CD-NE	5.86	1.54	1.46
1	G	191	LEU	C-O	-5.86	1.17	1.24
2	i	116	ASP	N-CA	-5.86	1.38	1.46
3	H	103	GLY	C-N	5.86	1.41	1.33
3	H	201	ALA	CA-C	-5.85	1.45	1.53
1	a	42	CYS	N-CA	-5.85	1.37	1.46
1	a	229	LEU	CA-CB	5.85	1.63	1.53
1	b	228	GLU	CA-C	-5.85	1.45	1.52
1	E	68	TYR	C-N	5.85	1.41	1.33
1	c	76	ALA	N-CA	-5.85	1.38	1.45
2	h	189	VAL	C-O	5.85	1.29	1.24
2	n	80	ARG	CZ-NH1	5.85	1.41	1.32
1	E	202	SER	CA-C	-5.85	1.45	1.52
1	e	171	VAL	C-N	5.85	1.41	1.33
2	1	18	VAL	C-N	5.85	1.41	1.33
1	C	8	TYR	CA-C	5.85	1.59	1.53
1	C	245	LYS	CA-CB	5.84	1.62	1.53
2	5	81	ARG	C-N	5.84	1.41	1.33
2	5	146	THR	N-CA	-5.84	1.39	1.46
3	H	123	LYS	CA-C	-5.84	1.45	1.52
1	G	199	SER	CA-C	-5.84	1.44	1.52
2	6	107	LEU	N-CA	-5.84	1.39	1.46
3	M	198	GLN	C-N	5.84	1.41	1.33
1	c	64	ILE	N-CA	-5.84	1.39	1.46
1	D	49	ILE	N-CA	-5.84	1.39	1.46
1	B	135	SER	N-CA	-5.84	1.39	1.46
1	E	113	ALA	N-CA	-5.84	1.39	1.46
1	e	73	HIS	ND1-CE1	5.84	1.38	1.32
2	2	72	ILE	CA-CB	-5.83	1.46	1.54
2	4	170	ARG	CD-NE	5.83	1.54	1.46
3	J	82	SER	CA-C	5.83	1.60	1.52
2	i	99	ASN	CA-CB	5.83	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	205	VAL	N-CA	-5.83	1.39	1.46
2	2	204	VAL	C-N	5.83	1.41	1.34
3	L	299	ARG	NE-CZ	5.83	1.39	1.33
3	J	128	TYR	CZ-OH	5.83	1.50	1.38
2	4	201	PRO	C-N	5.83	1.40	1.33
3	J	131	GLU	CA-C	-5.83	1.44	1.52
3	I	165	GLU	CA-CB	5.83	1.63	1.53
3	K	116	VAL	C-N	5.83	1.41	1.33
1	D	91	ARG	CZ-NH1	5.83	1.41	1.32
2	5	41	ALA	N-CA	-5.83	1.38	1.46
1	C	76	ALA	C-N	5.83	1.41	1.33
1	E	200	ILE	C-O	5.83	1.31	1.24
2	h	79	ILE	CA-CB	-5.83	1.46	1.54
2	j	89	ALA	C-N	5.82	1.41	1.33
3	M	259	ARG	NE-CZ	5.82	1.39	1.33
1	g	60	GLU	CA-CB	5.82	1.61	1.53
2	4	115	ILE	CA-C	-5.82	1.45	1.52
3	H	57	ARG	NE-CZ	5.82	1.39	1.33
3	H	289	ARG	CA-C	-5.82	1.45	1.52
2	j	32	THR	CA-C	-5.82	1.45	1.52
3	L	130	PHE	C-N	5.82	1.40	1.33
1	F	63	THR	CA-C	-5.82	1.45	1.52
3	H	154	ARG	NE-CZ	5.81	1.39	1.33
1	g	137	LEU	CA-CB	5.81	1.61	1.53
3	H	205	ARG	N-CA	-5.81	1.39	1.46
3	M	166	LEU	CA-C	-5.81	1.45	1.52
3	L	106	VAL	N-CA	-5.81	1.39	1.46
1	F	78	THR	N-CA	-5.81	1.38	1.45
1	c	18	ASP	N-CA	5.81	1.53	1.46
3	K	68	VAL	CA-C	-5.81	1.45	1.52
2	i	91	ALA	CA-CB	5.80	1.62	1.53
3	I	250	ARG	CZ-NH2	5.80	1.41	1.33
3	L	373	LEU	CA-C	-5.80	1.45	1.52
3	M	59	ARG	CD-NE	5.80	1.54	1.46
2	n	193	GLU	CA-CB	5.80	1.62	1.54
1	B	56	SER	CA-C	-5.80	1.45	1.52
2	6	18	VAL	CA-CB	5.80	1.61	1.54
2	n	88	ARG	CZ-NH1	5.80	1.40	1.32
3	J	360	MET	CA-C	-5.80	1.45	1.52
1	f	112	LEU	CA-CB	5.80	1.62	1.53
2	4	151	LEU	CA-CB	5.80	1.62	1.53
3	J	36	PHE	C-O	-5.80	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	72	GLU	CA-CB	5.79	1.61	1.53
3	M	357	GLU	C-O	-5.79	1.17	1.24
1	e	113	ALA	C-N	5.79	1.41	1.33
2	k	166	GLU	C-N	5.79	1.41	1.33
3	K	368	ALA	CA-C	-5.79	1.45	1.52
1	E	235	ARG	CD-NE	5.79	1.54	1.46
2	6	48	ILE	CA-C	-5.79	1.45	1.52
1	c	122	GLN	C-N	5.78	1.42	1.33
3	K	41	ARG	CA-C	-5.78	1.45	1.52
2	j	158	GLU	CA-C	-5.78	1.45	1.52
3	K	364	ARG	NE-CZ	5.78	1.39	1.33
1	b	58	LEU	C-N	5.78	1.41	1.33
1	D	87	VAL	CA-C	-5.78	1.44	1.52
1	f	28	ARG	N-CA	-5.78	1.39	1.46
3	I	248	ALA	CA-C	-5.78	1.45	1.52
2	2	125	ILE	CA-C	-5.78	1.45	1.52
2	6	202	GLU	CA-CB	5.78	1.62	1.53
2	i	196	PHE	CA-CB	5.78	1.62	1.53
2	k	25	MET	CA-C	-5.78	1.45	1.52
3	H	30	LEU	CA-CB	5.78	1.62	1.53
1	B	57	LYS	C-N	5.78	1.41	1.33
2	1	122	ILE	C-N	5.78	1.41	1.33
3	L	228	GLN	CA-C	-5.78	1.45	1.52
1	a	81	LEU	N-CA	-5.77	1.39	1.46
1	c	244	LEU	CA-C	-5.77	1.45	1.53
1	E	46	VAL	C-O	-5.77	1.18	1.23
1	e	177	LYS	C-N	5.77	1.41	1.33
2	m	53	ALA	N-CA	-5.77	1.38	1.45
1	B	60	GLU	C-N	5.77	1.42	1.33
2	i	24	VAL	C-O	-5.77	1.18	1.24
2	6	104	PHE	N-CA	-5.77	1.42	1.46
1	A	101	LEU	CA-C	-5.77	1.45	1.52
2	4	80	ARG	CZ-NH2	5.77	1.41	1.33
2	m	175	ALA	CA-CB	5.77	1.62	1.53
1	a	72	GLU	N-CA	-5.76	1.39	1.46
1	b	191	LEU	C-N	5.76	1.41	1.33
1	E	124	THR	C-N	5.76	1.41	1.33
3	I	311	LEU	CA-CB	5.76	1.61	1.53
3	M	232	GLU	C-N	5.76	1.42	1.33
1	g	114	LYS	N-CA	-5.76	1.39	1.46
2	m	153	ASP	CA-CB	5.76	1.63	1.53
3	H	365	GLU	C-N	5.76	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	221	ARG	NE-CZ	5.76	1.39	1.33
1	a	232	TYR	CA-CB	5.76	1.62	1.53
1	f	68	TYR	N-CA	-5.76	1.38	1.46
2	4	81	ARG	NE-CZ	5.76	1.39	1.33
3	K	98	GLU	CA-C	-5.76	1.45	1.52
3	H	176	LYS	CA-CB	5.76	1.62	1.53
3	K	278	ARG	NE-CZ	5.76	1.39	1.33
1	e	196	MET	N-CA	-5.75	1.39	1.46
2	m	54	MET	CA-C	-5.75	1.45	1.52
3	M	78	VAL	CA-CB	5.75	1.60	1.54
2	4	154	ARG	NE-CZ	5.75	1.39	1.33
1	B	99	ASN	CA-C	5.75	1.60	1.52
2	n	208	LEU	CA-CB	5.75	1.63	1.53
3	I	26	LEU	CA-CB	5.75	1.62	1.53
1	b	71	ASP	CA-CB	5.75	1.62	1.53
1	D	121	GLN	N-CA	-5.75	1.39	1.46
2	h	138	VAL	C-O	5.75	1.29	1.23
3	M	311	LEU	N-CA	-5.75	1.36	1.46
3	J	32	ASP	N-CA	-5.75	1.39	1.46
1	B	17	PRO	C-N	5.75	1.41	1.34
3	M	26	LEU	N-CA	5.74	1.53	1.46
1	b	48	LEU	CA-CB	5.74	1.62	1.53
1	C	94	ILE	CA-CB	-5.74	1.47	1.54
1	D	110	LYS	N-CA	-5.74	1.39	1.46
1	G	232	TYR	CA-C	-5.74	1.45	1.52
2	3	154	ARG	C-N	5.74	1.41	1.33
2	k	109	GLN	CA-C	-5.74	1.45	1.52
3	H	267	GLN	CA-CB	5.74	1.62	1.53
3	K	253	SER	CA-CB	5.74	1.61	1.53
3	H	358	ALA	CA-C	5.74	1.60	1.52
3	L	200	ARG	NE-CZ	5.74	1.39	1.33
2	7	83	ARG	CZ-NH1	5.74	1.40	1.32
1	G	214	VAL	CA-CB	-5.73	1.47	1.54
3	J	308	GLU	C-N	5.73	1.39	1.33
3	J	238	ILE	N-CA	-5.73	1.39	1.46
1	B	73	HIS	ND1-CE1	5.73	1.38	1.32
2	2	51	ARG	CD-NE	5.73	1.54	1.46
2	i	170	ARG	NE-CZ	5.73	1.39	1.33
2	4	180	SER	C-N	5.73	1.41	1.33
3	M	67	VAL	CA-C	-5.73	1.45	1.52
1	A	186	ASP	CA-C	-5.73	1.45	1.52
1	b	145	PRO	C-N	5.73	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	ALA	CA-CB	5.73	1.62	1.53
2	7	96	ASN	C-N	5.72	1.41	1.33
3	L	50	ARG	CA-CB	5.72	1.62	1.53
3	L	201	ALA	C-N	5.72	1.41	1.33
3	M	317	ARG	CD-NE	5.72	1.54	1.46
2	m	113	GLY	N-CA	-5.72	1.39	1.45
2	n	66	LEU	C-O	-5.72	1.16	1.24
1	a	124	THR	CA-C	-5.72	1.44	1.52
1	D	10	ARG	NE-CZ	5.72	1.39	1.33
1	D	219	ARG	NE-CZ	5.72	1.39	1.33
3	I	278	ARG	CA-CB	5.72	1.63	1.52
3	L	325	THR	C-N	5.72	1.41	1.33
1	a	86	ARG	NE-CZ	5.71	1.39	1.33
1	G	22	PHE	C-N	5.71	1.41	1.33
1	g	24	VAL	CA-C	-5.71	1.45	1.52
2	n	114	GLY	CA-C	-5.71	1.44	1.52
3	J	155	GLU	N-CA	5.71	1.53	1.46
1	G	153	SER	C-N	5.71	1.41	1.33
2	i	150	VAL	CA-CB	-5.71	1.46	1.54
3	I	233	LYS	CA-C	-5.71	1.44	1.52
3	I	364	ARG	CD-NE	5.71	1.54	1.46
3	M	296	ALA	N-CA	5.71	1.53	1.46
1	D	147	LEU	N-CA	-5.71	1.39	1.46
3	H	67	VAL	C-O	-5.71	1.18	1.24
3	I	113	LEU	C-N	5.71	1.41	1.33
3	J	223	VAL	CA-C	-5.71	1.44	1.52
1	D	58	LEU	C-N	5.71	1.41	1.33
1	d	110	LYS	CA-C	-5.71	1.45	1.52
2	h	159	ILE	CA-CB	-5.71	1.48	1.54
2	4	39	SER	CA-C	-5.71	1.45	1.52
2	k	50	ASP	C-O	-5.71	1.17	1.24
2	k	120	LYS	C-N	5.71	1.40	1.33
1	C	191	LEU	CA-C	-5.71	1.45	1.52
2	4	106	TYR	C-N	5.71	1.40	1.33
3	I	121	THR	C-N	5.71	1.41	1.33
1	e	116	ILE	C-N	5.70	1.41	1.33
2	l	63	ALA	C-N	5.70	1.41	1.33
3	J	323	ILE	N-CA	5.70	1.53	1.46
1	A	243	LEU	CA-C	-5.70	1.45	1.52
3	M	337	LYS	CA-C	-5.70	1.45	1.52
1	a	130	ARG	CZ-NH2	5.70	1.40	1.33
1	F	104	ASP	C-O	5.70	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	166	GLU	CA-C	-5.70	1.45	1.52
3	L	156	ALA	C-N	5.70	1.41	1.33
3	M	369	LYS	CA-CB	5.70	1.61	1.53
3	J	223	VAL	CA-CB	-5.70	1.46	1.54
2	3	30	ARG	NE-CZ	5.70	1.39	1.33
1	F	125	GLN	C-N	5.70	1.41	1.33
2	k	111	LEU	N-CA	-5.70	1.39	1.46
2	m	187	ASP	C-N	5.70	1.41	1.33
3	L	149	GLN	C-N	5.70	1.41	1.33
2	5	187	ASP	CA-C	-5.69	1.45	1.52
1	a	43	LYS	N-CA	-5.69	1.38	1.46
1	B	26	TYR	N-CA	-5.69	1.38	1.46
1	F	189	MET	CA-CB	5.69	1.62	1.53
1	F	76	ALA	C-N	5.69	1.41	1.33
2	1	17	LEU	CA-CB	5.69	1.65	1.54
3	K	34	LYS	CA-C	-5.69	1.44	1.52
1	b	232	TYR	CA-CB	5.69	1.62	1.53
1	g	170	ALA	CA-C	-5.69	1.45	1.52
2	5	189	VAL	N-CA	-5.69	1.39	1.46
2	m	102	ARG	NE-CZ	5.69	1.39	1.33
1	C	67	ILE	CA-C	-5.69	1.45	1.52
1	C	176	GLU	CA-CB	5.69	1.62	1.53
1	b	152	PRO	N-CD	-5.68	1.39	1.47
1	e	62	ASP	N-CA	-5.68	1.38	1.45
2	m	177	LYS	N-CA	-5.68	1.38	1.46
1	B	240	ILE	CA-C	-5.68	1.45	1.52
1	c	139	ALA	N-CA	-5.68	1.38	1.46
1	d	130	ARG	CZ-NH1	5.68	1.40	1.32
2	i	100	SER	CA-C	-5.68	1.45	1.52
2	3	158	GLU	C-N	5.68	1.41	1.33
3	J	238	ILE	C-N	5.68	1.43	1.33
1	B	180	ARG	CA-C	-5.68	1.45	1.52
1	D	52	LYS	C-N	5.68	1.41	1.33
1	D	53	ARG	CD-NE	5.68	1.54	1.46
2	1	154	ARG	C-N	5.68	1.41	1.33
2	3	195	GLU	C-N	5.68	1.41	1.33
1	A	241	ARG	CZ-NH1	5.68	1.40	1.32
2	k	190	LYS	N-CA	5.68	1.52	1.46
3	H	85	PRO	CA-C	-5.68	1.44	1.52
1	D	182	ASP	C-O	-5.67	1.16	1.24
1	f	201	GLU	N-CA	-5.67	1.38	1.46
2	n	47	GLN	N-CA	-5.67	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	24	VAL	CA-CB	-5.67	1.47	1.54
2	7	83	ARG	NE-CZ	5.67	1.39	1.33
1	c	84	ASP	C-N	5.67	1.41	1.33
1	B	138	ILE	C-N	5.67	1.40	1.33
1	c	241	ARG	NE-CZ	5.67	1.39	1.33
3	I	283	VAL	CA-CB	-5.67	1.47	1.54
3	J	88	VAL	CA-C	5.67	1.59	1.52
2	j	137	ILE	C-N	5.67	1.38	1.33
1	a	34	GLY	C-N	5.66	1.40	1.33
1	c	186	ASP	N-CA	-5.66	1.39	1.46
1	f	145	PRO	CA-CB	-5.66	1.46	1.53
1	D	192	GLY	C-N	5.66	1.41	1.33
2	k	183	GLY	C-O	-5.66	1.16	1.23
2	5	30	ARG	CD-NE	5.66	1.54	1.46
3	J	218	GLU	CA-C	-5.66	1.45	1.52
3	H	208	GLY	C-O	-5.66	1.18	1.24
3	M	326	ARG	NE-CZ	5.66	1.39	1.33
1	B	155	ALA	CA-C	-5.65	1.46	1.52
1	g	155	ALA	N-CA	-5.65	1.39	1.46
2	7	185	GLY	N-CA	5.65	1.53	1.45
3	I	394	GLY	CA-C	5.65	1.59	1.51
1	A	22	PHE	CA-CB	5.65	1.62	1.53
1	a	171	VAL	CA-C	-5.65	1.45	1.52
1	B	134	VAL	CA-C	-5.65	1.45	1.52
3	L	47	GLU	C-N	5.65	1.41	1.33
3	L	83	THR	CA-CB	-5.65	1.44	1.53
2	m	143	GLY	CA-C	5.65	1.58	1.51
2	n	40	LYS	N-CA	5.65	1.53	1.45
1	B	86	ARG	N-CA	-5.64	1.39	1.46
2	6	101	TYR	N-CA	-5.64	1.39	1.46
1	C	184	SER	CA-C	-5.64	1.45	1.53
3	H	104	ALA	C-N	5.64	1.41	1.33
3	L	225	GLU	N-CA	-5.64	1.39	1.46
1	b	213	TYR	CA-C	-5.64	1.45	1.52
1	d	222	LYS	CA-C	-5.64	1.45	1.52
2	2	77	TYR	C-N	5.64	1.41	1.33
3	K	387	THR	CA-CB	5.64	1.62	1.52
1	c	236	ALA	N-CA	-5.64	1.39	1.46
2	4	201	PRO	CA-C	-5.64	1.44	1.52
2	k	184	ASP	C-N	5.64	1.40	1.32
3	K	372	MET	N-CA	-5.64	1.39	1.46
1	a	91	ARG	NE-CZ	5.64	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	53	ARG	C-N	5.64	1.41	1.33
1	b	94	ILE	CA-CB	-5.64	1.47	1.54
2	6	164	ALA	N-CA	-5.64	1.39	1.46
3	J	127	VAL	C-O	-5.64	1.17	1.24
1	G	91	ARG	NE-CZ	5.63	1.39	1.33
3	H	95	ILE	C-O	-5.63	1.18	1.24
1	B	41	LYS	CA-C	-5.63	1.46	1.52
1	G	83	ALA	C-O	5.63	1.30	1.24
2	n	178	ARG	NE-CZ	5.63	1.39	1.33
3	H	319	GLN	CA-CB	5.63	1.62	1.53
3	I	30	LEU	N-CA	-5.63	1.39	1.46
3	I	254	ASP	C-N	5.63	1.38	1.33
1	d	30	ALA	CA-C	-5.63	1.45	1.52
1	e	23	GLN	CA-C	-5.63	1.45	1.52
1	f	14	VAL	C-N	5.63	1.40	1.33
1	g	133	GLY	CA-C	-5.63	1.44	1.51
3	K	299	ARG	CZ-NH1	5.63	1.40	1.32
3	M	77	VAL	C-N	5.62	1.40	1.33
3	M	364	ARG	CD-NE	5.62	1.54	1.46
1	B	129	VAL	CA-C	-5.62	1.47	1.52
1	f	91	ARG	NE-CZ	5.62	1.39	1.33
2	h	175	ALA	N-CA	-5.62	1.39	1.46
2	2	107	LEU	N-CA	-5.62	1.39	1.46
2	l	113	GLY	CA-C	-5.62	1.44	1.51
2	k	170	ARG	CZ-NH1	5.62	1.40	1.32
2	6	51	ARG	CD-NE	5.62	1.54	1.46
1	B	211	VAL	CA-CB	5.62	1.61	1.54
1	f	191	LEU	CA-CB	5.62	1.62	1.53
3	L	232	GLU	N-CA	5.62	1.53	1.46
3	J	29	ARG	NE-CZ	5.62	1.39	1.33
1	C	20	ARG	NE-CZ	5.61	1.39	1.33
2	2	102	ARG	CZ-NH1	5.61	1.40	1.32
3	K	136	PRO	C-N	5.61	1.41	1.33
1	c	212	GLY	C-N	5.61	1.40	1.33
1	d	28	ARG	CD-NE	5.61	1.54	1.46
2	h	32	THR	C-N	5.61	1.40	1.33
1	e	93	ARG	NE-CZ	5.61	1.39	1.33
2	2	83	ARG	N-CA	-5.61	1.39	1.46
3	K	206	VAL	N-CA	-5.61	1.39	1.46
3	K	269	LEU	N-CA	-5.61	1.39	1.46
3	M	291	ASP	CA-CB	5.61	1.62	1.53
3	M	302	ARG	N-CA	-5.61	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	185	PHE	CA-CB	5.61	1.62	1.53
1	f	125	GLN	N-CA	-5.61	1.39	1.46
2	i	173	TYR	CA-C	-5.61	1.45	1.52
2	5	129	GLY	C-N	5.61	1.41	1.33
2	7	24	VAL	C-N	5.61	1.40	1.33
2	7	88	ARG	CD-NE	5.61	1.54	1.46
3	L	285	GLY	C-N	-5.61	1.26	1.33
1	b	224	VAL	CA-C	-5.61	1.46	1.52
1	G	86	ARG	CD-NE	5.61	1.54	1.46
1	G	211	VAL	CA-C	-5.61	1.45	1.52
1	g	46	VAL	CA-C	-5.61	1.45	1.52
3	K	361	PHE	N-CA	-5.61	1.39	1.46
1	A	43	LYS	CA-CB	5.60	1.61	1.53
1	G	18	ASP	CA-CB	5.60	1.62	1.53
2	1	19	CYS	N-CA	-5.60	1.39	1.45
2	3	133	GLU	CA-C	-5.60	1.46	1.52
1	B	198	LEU	CA-C	-5.60	1.45	1.52
1	E	89	ILE	N-CA	-5.60	1.39	1.46
2	1	141	GLY	CA-C	-5.60	1.42	1.51
2	n	60	VAL	CA-CB	5.60	1.62	1.54
3	I	250	ARG	CD-NE	5.60	1.54	1.46
3	K	76	ARG	CD-NE	5.60	1.54	1.46
3	H	298	LEU	CA-CB	5.60	1.62	1.53
3	L	93	GLN	C-N	5.60	1.41	1.33
2	l	39	SER	C-N	5.60	1.41	1.33
3	H	350	ASP	CA-CB	5.60	1.62	1.53
2	h	92	THR	C-N	5.60	1.41	1.33
1	C	120	LYS	CA-C	5.59	1.60	1.52
2	k	43	LYS	N-CA	-5.59	1.38	1.45
3	I	13	LEU	CA-C	-5.59	1.45	1.52
1	B	205	VAL	CA-C	-5.59	1.47	1.52
2	n	68	ARG	CZ-NH1	5.59	1.40	1.32
1	d	240	ILE	CA-CB	-5.59	1.47	1.54
2	5	115	ILE	C-O	5.59	1.29	1.24
2	l	177	LYS	N-CA	5.59	1.53	1.46
3	J	289	ARG	CZ-NH1	5.59	1.40	1.32
1	f	167	GLY	C-O	-5.59	1.16	1.23
1	G	68	TYR	CA-C	-5.59	1.45	1.52
1	C	47	ILE	CA-CB	-5.59	1.47	1.54
1	E	47	ILE	CA-CB	-5.59	1.47	1.54
2	2	73	GLU	N-CA	-5.59	1.39	1.46
2	n	204	VAL	CA-CB	-5.59	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	ARG	C-N	5.58	1.40	1.33
2	1	124	SER	CA-C	-5.58	1.46	1.52
2	5	170	ARG	CZ-NH2	5.58	1.40	1.33
2	n	25	MET	CA-C	-5.58	1.45	1.52
1	A	128	GLY	C-N	5.58	1.39	1.33
1	d	134	VAL	CA-C	-5.58	1.45	1.52
3	I	241	ASP	C-N	5.58	1.41	1.33
1	f	240	ILE	CA-C	-5.58	1.46	1.52
2	1	158	GLU	C-N	5.58	1.40	1.33
3	I	148	VAL	N-CA	-5.58	1.40	1.46
1	G	136	LEU	N-CA	-5.57	1.38	1.45
2	3	183	GLY	CA-C	-5.57	1.43	1.51
1	B	183	LEU	N-CA	-5.57	1.39	1.45
1	D	209	ILE	CA-C	-5.57	1.46	1.52
2	l	132	ILE	C-O	-5.57	1.17	1.24
1	B	133	GLY	N-CA	5.57	1.52	1.45
1	F	140	GLY	C-N	5.57	1.40	1.33
3	K	240	ILE	N-CA	-5.57	1.40	1.46
1	a	213	TYR	C-N	5.57	1.40	1.33
2	1	140	THR	CB-OG1	5.57	1.52	1.43
1	a	134	VAL	CA-CB	-5.56	1.45	1.55
1	C	213	TYR	CA-CB	5.56	1.63	1.53
2	7	169	VAL	CA-C	-5.56	1.46	1.52
1	F	141	VAL	CA-CB	5.56	1.61	1.54
1	g	94	ILE	CA-C	-5.56	1.45	1.52
1	B	180	ARG	N-CA	-5.56	1.39	1.45
1	f	235	ARG	CD-NE	5.56	1.54	1.46
1	g	148	TYR	CA-CB	5.56	1.63	1.53
3	L	11	GLU	CA-C	-5.56	1.45	1.52
2	i	43	LYS	CA-C	5.56	1.60	1.52
2	6	176	MET	CA-C	-5.56	1.45	1.52
1	E	56	SER	CA-C	-5.56	1.45	1.52
1	E	224	VAL	CA-C	-5.55	1.45	1.52
2	2	212	ARG	NE-CZ	5.55	1.39	1.33
1	E	240	ILE	C-N	5.55	1.41	1.33
3	H	46	ARG	CA-CB	5.55	1.61	1.53
1	f	156	LEU	N-CA	-5.55	1.39	1.46
3	H	316	GLY	C-N	5.55	1.41	1.33
2	h	73	GLU	CA-CB	5.55	1.62	1.53
3	J	163	LYS	N-CA	-5.55	1.41	1.46
1	C	135	SER	N-CA	-5.55	1.38	1.45
3	H	87	PHE	N-CA	5.55	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	281	VAL	N-CA	-5.55	1.39	1.46
1	G	75	CYS	CA-C	-5.54	1.45	1.52
3	M	327	LYS	N-CA	-5.54	1.38	1.46
2	1	81	ARG	CA-CB	5.54	1.62	1.53
2	i	80	ARG	CZ-NH1	5.54	1.40	1.32
3	L	224	ARG	C-N	5.54	1.41	1.33
3	I	90	ASN	C-N	5.54	1.41	1.33
3	L	148	VAL	CA-C	-5.54	1.45	1.52
3	L	178	VAL	C-O	-5.54	1.18	1.24
3	L	270	ALA	N-CA	-5.54	1.39	1.46
1	a	168	ARG	CD-NE	5.54	1.54	1.46
3	K	287	THR	CA-C	-5.54	1.45	1.52
1	c	68	TYR	N-CA	-5.54	1.39	1.45
1	f	209	ILE	N-CA	-5.54	1.39	1.46
3	H	72	LEU	C-N	5.54	1.40	1.33
3	J	93	GLN	CA-C	5.54	1.60	1.52
3	J	177	GLY	CA-C	-5.54	1.46	1.52
1	B	159	TYR	CA-C	-5.53	1.45	1.52
2	j	109	GLN	C-N	5.53	1.41	1.33
2	2	88	ARG	CD-NE	5.53	1.53	1.46
2	7	212	ARG	CD-NE	5.53	1.53	1.46
1	d	76	ALA	N-CA	-5.53	1.39	1.45
2	i	19	CYS	N-CA	5.53	1.53	1.45
2	3	23	VAL	N-CA	-5.53	1.39	1.46
2	m	194	ASP	C-N	5.53	1.40	1.33
3	L	126	MET	CA-C	5.53	1.60	1.52
3	J	300	PRO	N-CA	-5.53	1.40	1.46
1	f	105	GLU	C-N	5.53	1.40	1.33
2	3	22	GLY	N-CA	-5.53	1.37	1.45
2	3	206	GLN	CA-CB	5.53	1.62	1.53
3	L	341	ARG	CZ-NH1	5.53	1.40	1.32
1	F	28	ARG	CD-NE	5.52	1.53	1.46
1	g	64	ILE	C-O	5.52	1.30	1.24
2	j	41	ALA	N-CA	-5.52	1.39	1.46
1	g	30	ALA	C-N	5.52	1.40	1.33
2	2	110	LEU	CA-C	-5.52	1.45	1.52
2	3	186	ILE	N-CA	-5.52	1.39	1.46
1	c	85	ALA	CA-CB	5.52	1.61	1.53
1	g	49	ILE	C-N	5.52	1.41	1.33
2	l	108	VAL	CA-CB	-5.52	1.47	1.55
2	l	154	ARG	CD-NE	5.52	1.53	1.46
3	L	275	PHE	C-N	5.52	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	79	SER	N-CA	-5.52	1.39	1.46
1	d	17	PRO	C-N	5.52	1.40	1.33
2	4	86	THR	CA-C	-5.52	1.45	1.53
3	J	119	LEU	CA-C	-5.52	1.45	1.52
1	c	165	GLY	CA-C	-5.51	1.44	1.51
1	E	148	TYR	CA-C	-5.51	1.46	1.52
2	2	94	THR	C-N	5.51	1.40	1.33
3	J	224	ARG	NE-CZ	5.51	1.39	1.33
2	4	23	VAL	CA-CB	-5.51	1.46	1.54
2	m	99	ASN	N-CA	-5.51	1.39	1.46
2	n	91	ALA	CA-C	-5.51	1.45	1.52
3	M	178	VAL	CA-C	-5.51	1.45	1.52
1	a	188	ALA	C-N	5.51	1.41	1.33
1	f	123	TYR	N-CA	-5.51	1.38	1.46
2	l	162	ASP	CA-C	-5.51	1.45	1.52
3	I	67	VAL	CA-CB	-5.51	1.47	1.54
3	M	223	VAL	CA-C	-5.51	1.45	1.52
1	G	238	GLU	N-CA	-5.51	1.39	1.46
3	L	309	VAL	CA-C	5.51	1.57	1.53
1	c	144	VAL	CA-C	-5.51	1.47	1.52
3	J	174	PRO	C-O	-5.51	1.20	1.25
1	B	121	GLN	CA-C	-5.50	1.45	1.52
3	H	262	GLN	C-N	5.50	1.41	1.34
2	j	54	MET	CA-C	-5.50	1.45	1.52
3	L	41	ARG	N-CA	-5.50	1.39	1.46
1	E	181	ASP	C-N	5.50	1.40	1.33
1	G	188	ALA	C-N	5.50	1.41	1.33
1	g	149	GLU	N-CA	-5.50	1.39	1.46
3	I	255	THR	CA-C	-5.50	1.46	1.53
2	2	131	ALA	N-CA	-5.50	1.38	1.45
1	B	112	LEU	CA-CB	5.50	1.62	1.53
1	F	53	ARG	CZ-NH1	5.50	1.40	1.32
1	f	25	GLU	CA-CB	5.50	1.61	1.53
3	L	46	ARG	NE-CZ	5.50	1.39	1.33
3	M	126	MET	CA-C	-5.50	1.45	1.52
3	J	134	GLU	CA-C	5.50	1.59	1.52
1	F	162	THR	C-N	5.50	1.40	1.33
1	G	219	ARG	NE-CZ	5.50	1.39	1.33
2	3	49	ALA	C-O	-5.50	1.16	1.23
2	n	189	VAL	C-N	5.50	1.40	1.33
3	H	280	ASP	CA-C	-5.50	1.45	1.52
3	L	290	ILE	N-CA	-5.50	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	101	LEU	N-CA	-5.50	1.39	1.46
2	k	170	ARG	CD-NE	5.50	1.53	1.46
3	H	211	PHE	N-CA	-5.50	1.39	1.46
3	I	352	LYS	N-CA	-5.50	1.39	1.46
1	e	63	THR	C-N	5.49	1.40	1.33
1	f	154	GLY	CA-C	-5.49	1.44	1.51
2	j	117	SER	C-N	5.49	1.41	1.33
2	m	209	ALA	N-CA	-5.49	1.39	1.46
2	k	201	PRO	N-CA	-5.49	1.40	1.47
3	L	15	LYS	CA-CB	5.49	1.61	1.53
1	d	83	ALA	N-CA	-5.49	1.39	1.46
2	7	105	PRO	CA-C	5.49	1.59	1.52
1	A	184	SER	CA-C	-5.49	1.45	1.53
1	B	114	LYS	N-CA	-5.49	1.39	1.46
1	C	93	ARG	CZ-NH1	5.49	1.40	1.32
1	G	229	LEU	C-N	5.49	1.41	1.33
3	I	286	ALA	CA-C	-5.49	1.46	1.52
1	E	40	ILE	CA-CB	5.49	1.61	1.54
1	g	23	GLN	CA-C	5.49	1.59	1.52
3	L	362	ALA	CA-C	-5.48	1.45	1.52
2	h	21	ASP	N-CA	-5.48	1.42	1.47
3	M	118	VAL	CA-CB	-5.48	1.48	1.54
3	J	286	ALA	CA-C	-5.48	1.46	1.52
3	K	29	ARG	CA-C	5.48	1.59	1.52
1	D	18	ASP	CA-CB	5.48	1.62	1.53
1	f	115	LYS	CA-CB	5.48	1.61	1.53
2	h	70	ILE	CA-C	-5.48	1.45	1.52
2	5	212	ARG	N-CA	5.48	1.53	1.46
2	l	60	VAL	CA-CB	5.48	1.60	1.54
3	J	263	ARG	CZ-NH2	5.48	1.40	1.33
2	j	51	ARG	CZ-NH1	5.47	1.40	1.32
2	n	47	GLN	CA-C	-5.47	1.46	1.52
3	H	176	LYS	CA-C	-5.47	1.45	1.52
1	F	137	LEU	CA-C	-5.47	1.46	1.52
2	n	17	LEU	N-CA	-5.47	1.39	1.45
3	L	130	PHE	N-CA	-5.47	1.38	1.46
1	A	132	PHE	CG-CD1	5.47	1.50	1.38
1	b	214	VAL	N-CA	-5.47	1.38	1.46
1	f	172	THR	C-N	5.47	1.41	1.33
2	2	81	ARG	NE-CZ	5.47	1.39	1.33
1	b	83	ALA	CA-C	-5.47	1.45	1.52
1	c	104	ASP	CA-CB	5.46	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	116	ILE	C-O	-5.46	1.17	1.24
1	a	37	ALA	CA-C	-5.46	1.45	1.52
2	m	92	THR	CA-C	-5.46	1.45	1.52
1	A	120	LYS	N-CA	-5.46	1.38	1.46
2	n	105	PRO	CA-CB	-5.46	1.46	1.53
3	I	230	ALA	CA-C	-5.46	1.45	1.52
1	D	20	ARG	CZ-NH2	5.46	1.40	1.33
1	D	161	ALA	C-N	5.46	1.40	1.33
2	l	96	ASN	CA-CB	5.46	1.61	1.53
3	L	265	MET	C-N	5.46	1.41	1.33
3	L	227	PHE	C-N	5.46	1.41	1.33
2	4	83	ARG	CZ-NH1	5.45	1.40	1.32
3	L	168	ALA	C-N	5.45	1.41	1.33
3	J	165	GLU	N-CA	-5.45	1.39	1.46
2	2	79	ILE	C-N	5.45	1.41	1.33
1	b	187	ASP	C-O	-5.45	1.17	1.24
1	C	29	GLU	N-CA	-5.45	1.38	1.46
1	e	222	LYS	N-CA	-5.45	1.39	1.46
3	K	201	ALA	C-N	5.45	1.41	1.33
2	1	159	ILE	CA-CB	5.45	1.59	1.54
1	E	52	LYS	C-N	5.45	1.40	1.33
1	G	88	LEU	N-CA	-5.45	1.39	1.46
2	k	92	THR	C-N	5.45	1.41	1.33
2	l	212	ARG	NE-CZ	5.45	1.39	1.33
3	I	31	GLU	CA-C	-5.45	1.46	1.52
3	M	134	GLU	CA-C	-5.45	1.45	1.52
2	i	24	VAL	N-CA	-5.44	1.40	1.46
1	c	94	ILE	CA-CB	5.44	1.61	1.54
2	3	157	PRO	CA-CB	5.44	1.61	1.53
3	K	286	ALA	N-CA	-5.44	1.39	1.46
3	M	106	VAL	CA-C	-5.44	1.46	1.52
1	A	222	LYS	CA-CB	5.44	1.63	1.53
1	e	205	VAL	N-CA	-5.44	1.39	1.46
1	F	188	ALA	C-N	5.44	1.41	1.33
2	i	191	ILE	CA-CB	-5.44	1.47	1.53
3	K	227	PHE	C-N	5.44	1.40	1.33
1	e	31	VAL	CA-CB	-5.44	1.47	1.54
3	H	55	VAL	CA-CB	5.44	1.61	1.54
1	C	70	ILE	CA-CB	5.43	1.61	1.54
1	A	156	LEU	C-N	5.43	1.40	1.33
2	3	69	ILE	C-N	5.43	1.40	1.33
1	C	9	ASP	N-CA	-5.43	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	THR	C-N	5.43	1.40	1.33
1	c	49	ILE	CB-CG1	5.43	1.64	1.53
1	E	153	SER	C-N	5.43	1.40	1.33
1	e	48	LEU	N-CA	-5.43	1.39	1.46
1	e	126	TYR	CA-CB	5.43	1.61	1.53
2	5	144	SER	N-CA	-5.43	1.39	1.46
1	e	30	ALA	CA-C	-5.43	1.45	1.52
3	M	68	VAL	CA-C	5.43	1.58	1.52
1	A	239	ARG	NE-CZ	5.43	1.39	1.33
1	e	79	SER	C-N	5.43	1.41	1.33
3	J	310	PRO	CA-C	-5.43	1.44	1.52
1	A	235	ARG	CZ-NH2	5.42	1.40	1.33
1	E	181	ASP	N-CA	-5.42	1.38	1.46
2	2	151	LEU	N-CA	-5.42	1.39	1.46
2	i	179	ASP	CA-CB	5.42	1.59	1.52
3	I	154	ARG	NE-CZ	5.42	1.39	1.33
3	M	200	ARG	CD-NE	5.42	1.53	1.46
1	A	42	CYS	C-N	5.42	1.40	1.33
2	6	127	PRO	N-CD	-5.42	1.40	1.47
1	E	168	ARG	CD-NE	5.42	1.53	1.46
2	6	104	PHE	C-O	5.42	1.28	1.24
3	K	278	ARG	CA-C	5.42	1.59	1.52
3	J	367	ARG	CD-NE	5.42	1.53	1.46
1	E	7	GLY	CA-C	-5.42	1.43	1.51
1	e	162	THR	C-N	5.42	1.40	1.33
2	l	60	VAL	N-CA	-5.42	1.40	1.46
1	A	21	LEU	CA-C	5.42	1.59	1.52
2	7	77	TYR	CA-C	-5.42	1.45	1.52
2	n	79	ILE	CA-C	-5.42	1.46	1.52
3	I	222	LEU	C-N	5.42	1.40	1.33
1	d	190	VAL	C-O	-5.42	1.17	1.24
2	3	72	ILE	C-N	5.42	1.41	1.34
2	l	88	ARG	CZ-NH1	5.42	1.40	1.32
1	d	126	TYR	N-CA	-5.42	1.39	1.46
1	e	40	ILE	CB-CG1	5.42	1.64	1.53
2	l	100	SER	N-CA	-5.42	1.39	1.46
2	l	196	PHE	CA-C	-5.41	1.45	1.53
3	K	377	LYS	CA-C	-5.41	1.45	1.52
1	e	238	GLU	N-CA	-5.41	1.40	1.46
3	H	13	LEU	C-N	5.41	1.41	1.33
3	J	260	GLU	N-CA	5.41	1.52	1.46
1	g	86	ARG	CD-NE	5.41	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	44	TYR	C-N	5.41	1.41	1.33
1	A	187	ASP	CA-CB	5.41	1.61	1.53
1	b	239	ARG	CZ-NH1	5.41	1.40	1.32
2	h	80	ARG	CA-C	-5.41	1.46	1.52
3	H	190	LEU	C-N	5.41	1.41	1.33
1	B	150	THR	C-O	-5.40	1.17	1.24
3	K	34	LYS	N-CA	-5.40	1.39	1.46
1	A	157	LEU	N-CA	5.40	1.52	1.46
1	A	239	ARG	CD-NE	5.40	1.53	1.46
2	m	19	CYS	C-N	5.40	1.41	1.33
2	n	68	ARG	CZ-NH2	5.40	1.40	1.33
3	L	299	ARG	CZ-NH2	5.40	1.40	1.33
1	D	33	ARG	CA-C	-5.40	1.46	1.52
2	4	152	GLU	CG-CD	5.40	1.65	1.52
3	H	272	LEU	N-CA	-5.40	1.39	1.46
3	H	337	LYS	CA-CB	5.40	1.61	1.53
3	J	341	ARG	NE-CZ	5.40	1.39	1.33
2	i	59	SER	N-CA	-5.40	1.39	1.46
1	F	147	LEU	CA-C	-5.40	1.46	1.52
1	G	76	ALA	N-CA	-5.40	1.39	1.45
2	i	106	TYR	C-N	5.40	1.41	1.33
3	L	236	SER	CA-C	-5.40	1.46	1.52
2	n	180	SER	CA-CB	5.40	1.59	1.52
1	d	201	GLU	CA-CB	5.39	1.61	1.53
2	7	170	ARG	NE-CZ	5.39	1.39	1.33
1	b	114	LYS	CA-C	-5.39	1.45	1.52
1	D	91	ARG	NE-CZ	5.39	1.39	1.33
2	i	193	GLU	C-N	5.39	1.41	1.33
1	B	96	ALA	C-N	5.39	1.41	1.33
1	e	114	LYS	CA-C	-5.39	1.45	1.52
2	m	134	GLU	CA-C	-5.39	1.46	1.52
2	2	199	TYR	CA-C	-5.39	1.46	1.52
2	4	201	PRO	N-CD	5.39	1.55	1.47
2	l	193	GLU	C-N	5.39	1.41	1.33
1	C	14	VAL	CA-C	-5.38	1.45	1.52
1	G	105	GLU	N-CA	-5.38	1.37	1.45
1	C	215	LYS	N-CA	5.38	1.52	1.45
1	C	232	TYR	C-N	5.38	1.40	1.33
1	g	211	VAL	C-O	-5.38	1.18	1.24
1	g	219	ARG	CZ-NH1	5.38	1.40	1.32
1	a	120	LYS	C-N	5.38	1.41	1.34
1	G	93	ARG	CD-NE	5.38	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	81	ARG	NE-CZ	5.38	1.39	1.33
3	J	268	LEU	CA-CB	5.38	1.61	1.53
1	A	59	LEU	CA-CB	5.38	1.61	1.53
1	D	83	ALA	CA-C	-5.38	1.46	1.52
1	d	117	CYS	CA-C	-5.38	1.45	1.52
2	6	44	LYS	C-N	5.38	1.40	1.33
1	C	52	LYS	CA-C	-5.38	1.44	1.52
1	A	49	ILE	N-CA	-5.37	1.40	1.46
1	A	224	VAL	C-N	5.37	1.43	1.33
1	d	224	VAL	C-N	5.37	1.41	1.33
2	1	106	TYR	CA-CB	-5.37	1.45	1.53
3	K	62	PRO	N-CD	5.37	1.55	1.47
3	K	225	GLU	N-CA	-5.37	1.40	1.46
3	M	112	THR	CA-C	-5.37	1.45	1.52
2	7	122	ILE	N-CA	-5.37	1.39	1.46
1	D	160	LYS	C-N	5.37	1.41	1.33
1	e	172	THR	C-N	5.37	1.41	1.33
2	m	210	LYS	C-N	5.37	1.41	1.33
3	L	396	MET	CA-CB	5.37	1.62	1.53
1	b	213	TYR	CA-CB	5.37	1.62	1.53
1	C	153	SER	N-CA	-5.37	1.39	1.46
3	I	98	GLU	CA-CB	-5.37	1.44	1.53
3	K	205	ARG	CA-C	-5.37	1.46	1.52
1	d	169	ASN	C-N	5.36	1.41	1.33
1	d	224	VAL	CA-C	-5.36	1.46	1.52
1	g	196	MET	C-N	5.36	1.40	1.33
2	l	36	PHE	N-CA	-5.36	1.39	1.45
2	n	202	GLU	C-N	5.36	1.40	1.33
3	I	24	ARG	CZ-NH2	5.36	1.40	1.33
3	I	72	LEU	CA-C	-5.36	1.46	1.52
3	H	117	ASN	CA-CB	5.36	1.63	1.53
3	K	223	VAL	N-CA	5.36	1.52	1.46
3	M	258	ASP	CA-C	-5.36	1.45	1.52
1	b	228	GLU	N-CA	-5.36	1.39	1.45
2	j	33	MET	C-N	5.36	1.41	1.33
3	K	255	THR	CA-C	-5.36	1.46	1.52
3	M	125	PRO	CA-CB	-5.36	1.46	1.53
1	B	14	VAL	N-CA	-5.36	1.39	1.46
3	M	177	GLY	C-N	-5.36	1.26	1.33
2	5	80	ARG	CZ-NH2	5.35	1.40	1.33
1	A	66	LYS	N-CA	-5.35	1.39	1.46
2	m	85	PRO	CA-C	-5.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	27	ALA	C-N	5.35	1.42	1.33
3	M	215	TYR	N-CA	-5.35	1.38	1.45
1	c	124	THR	CA-C	-5.35	1.45	1.52
1	G	148	TYR	CA-C	-5.35	1.46	1.52
2	2	164	ALA	N-CA	-5.35	1.39	1.46
2	i	205	GLU	N-CA	-5.35	1.39	1.46
2	7	171	ALA	N-CA	-5.35	1.40	1.46
1	c	118	ASP	CA-C	-5.34	1.45	1.52
3	L	176	LYS	C-N	5.34	1.40	1.33
1	D	79	SER	C-N	5.34	1.40	1.32
1	f	20	ARG	NE-CZ	5.34	1.39	1.33
2	m	59	SER	C-N	5.34	1.40	1.33
3	H	86	LYS	N-CA	-5.34	1.38	1.46
3	K	283	VAL	CA-C	-5.34	1.46	1.52
3	L	134	GLU	CA-C	-5.34	1.45	1.53
3	L	150	ILE	CA-C	-5.34	1.46	1.52
3	L	341	ARG	NE-CZ	5.34	1.39	1.33
1	b	53	ARG	NE-CZ	5.34	1.39	1.33
1	C	237	ASN	N-CA	-5.34	1.39	1.46
1	G	178	GLU	C-N	5.34	1.40	1.33
2	1	39	SER	CA-C	-5.34	1.46	1.52
2	2	123	TYR	C-N	5.34	1.40	1.33
3	L	172	ILE	N-CA	-5.34	1.39	1.46
2	n	77	TYR	CA-C	-5.34	1.46	1.52
2	k	77	TYR	CG-CD1	5.34	1.50	1.39
3	H	121	THR	CB-OG1	-5.34	1.35	1.43
1	F	66	LYS	CA-CB	5.33	1.61	1.54
2	1	55	THR	CA-CB	-5.33	1.44	1.53
2	i	90	ILE	C-N	5.33	1.40	1.33
2	3	31	ALA	C-O	-5.33	1.17	1.23
2	n	132	ILE	C-N	5.33	1.40	1.33
1	a	20	ARG	CA-C	-5.33	1.45	1.52
1	C	89	ILE	C-N	5.33	1.41	1.33
2	5	54	MET	C-N	5.33	1.40	1.33
2	l	127	PRO	N-CA	-5.33	1.40	1.47
2	7	154	ARG	CZ-NH1	5.33	1.40	1.32
1	B	142	ASP	CA-C	-5.33	1.46	1.52
3	K	333	ASP	CA-CB	5.33	1.61	1.53
3	J	47	GLU	C-N	5.33	1.40	1.33
3	J	161	LEU	C-N	5.33	1.41	1.33
1	E	55	GLY	C-N	5.33	1.40	1.33
1	C	219	ARG	C-N	5.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	219	GLY	CA-C	-5.33	1.44	1.51
1	a	184	SER	CA-CB	5.32	1.60	1.53
1	B	93	ARG	CZ-NH1	5.32	1.40	1.32
1	g	149	GLU	CA-CB	5.32	1.61	1.53
2	5	107	LEU	CA-C	-5.32	1.46	1.52
3	H	155	GLU	N-CA	-5.32	1.40	1.46
2	3	81	ARG	NE-CZ	5.32	1.39	1.33
2	4	83	ARG	CD-NE	5.32	1.53	1.46
2	k	86	THR	CA-C	-5.32	1.46	1.52
1	B	134	VAL	CA-CB	5.32	1.62	1.55
1	C	149	GLU	N-CA	-5.32	1.39	1.46
1	e	60	GLU	N-CA	-5.32	1.39	1.46
1	e	149	GLU	CA-C	-5.32	1.46	1.52
3	I	83	THR	N-CA	-5.32	1.40	1.46
1	a	125	GLN	CA-C	-5.32	1.46	1.52
1	d	13	THR	N-CA	-5.32	1.40	1.46
3	L	370	VAL	C-N	5.32	1.40	1.33
1	A	106	PRO	C-N	5.32	1.40	1.33
1	A	125	GLN	C-O	-5.32	1.17	1.24
1	a	163	ALA	CA-C	-5.32	1.46	1.52
1	F	232	TYR	CE1-CZ	5.32	1.51	1.38
3	L	291	ASP	N-CA	5.32	1.53	1.46
1	D	152	PRO	N-CA	-5.32	1.40	1.47
3	L	50	ARG	CZ-NH1	5.32	1.40	1.32
3	J	259	ARG	C-O	-5.31	1.17	1.24
1	A	82	VAL	CA-CB	5.31	1.61	1.54
2	h	81	ARG	CZ-NH1	5.31	1.40	1.32
2	2	102	ARG	CD-NE	5.31	1.53	1.46
1	F	224	VAL	CA-CB	-5.31	1.47	1.53
2	m	13	THR	C-N	5.31	1.40	1.33
3	H	324	HIS	CA-CB	5.31	1.61	1.53
3	L	217	GLY	N-CA	5.31	1.53	1.45
2	h	134	GLU	C-O	-5.31	1.18	1.24
2	2	173	TYR	N-CA	-5.31	1.39	1.46
2	5	64	GLN	CA-C	-5.31	1.46	1.52
1	A	211	VAL	CA-C	-5.31	1.46	1.52
1	a	94	ILE	CA-C	-5.30	1.46	1.52
1	D	61	ALA	CA-C	-5.30	1.45	1.52
1	E	170	ALA	CA-CB	5.30	1.61	1.53
1	e	184	SER	C-N	5.30	1.41	1.33
2	j	83	ARG	CZ-NH1	5.30	1.40	1.32
2	l	198	GLN	C-N	5.30	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	74	ILE	CA-C	-5.30	1.46	1.52
3	I	167	PHE	C-N	-5.30	1.27	1.33
3	K	381	LYS	C-O	-5.30	1.18	1.24
1	b	34	GLY	CA-C	-5.30	1.46	1.52
1	C	119	PHE	CA-C	-5.30	1.46	1.52
1	c	53	ARG	CD-NE	5.30	1.53	1.46
1	d	93	ARG	CA-C	-5.30	1.46	1.52
3	K	260	GLU	CA-C	-5.30	1.46	1.52
3	L	378	ALA	C-N	5.30	1.40	1.33
2	k	103	TYR	N-CA	5.30	1.53	1.46
1	C	241	ARG	CD-NE	5.30	1.53	1.46
1	d	60	GLU	N-CA	-5.30	1.39	1.45
1	G	221	PHE	CA-C	5.30	1.59	1.52
3	I	285	GLY	CA-C	-5.30	1.47	1.52
2	h	172	ILE	C-N	5.29	1.40	1.33
1	e	57	LYS	C-N	5.29	1.41	1.33
1	g	179	TYR	CB-CG	5.29	1.63	1.51
2	l	35	ASN	N-CA	-5.29	1.39	1.46
2	6	76	LEU	N-CA	-5.29	1.40	1.46
2	n	208	LEU	C-N	5.29	1.41	1.33
1	C	213	TYR	CA-C	-5.29	1.46	1.52
3	K	381	LYS	N-CA	-5.29	1.40	1.46
2	l	112	ILE	C-N	5.29	1.40	1.33
2	n	184	ASP	C-N	5.29	1.39	1.32
2	4	196	PHE	C-N	5.29	1.41	1.33
2	k	178	ARG	NE-CZ	5.29	1.38	1.33
1	B	219	ARG	CZ-NH1	5.28	1.40	1.32
1	b	90	ASP	C-O	-5.28	1.17	1.24
1	g	100	ARG	CA-CB	5.28	1.61	1.53
2	k	68	ARG	CD-NE	5.28	1.53	1.46
3	L	324	HIS	CD2-NE2	-5.28	1.32	1.37
2	n	39	SER	CA-CB	5.28	1.65	1.54
1	a	233	VAL	N-CA	-5.28	1.40	1.46
1	G	90	ASP	CA-C	-5.28	1.46	1.52
2	l	172	ILE	N-CA	-5.28	1.39	1.46
2	2	167	LEU	N-CA	-5.28	1.40	1.46
2	4	21	ASP	N-CA	5.28	1.53	1.45
3	I	249	ARG	NE-CZ	5.28	1.38	1.33
1	A	159	TYR	CZ-OH	5.28	1.49	1.38
1	G	218	ASP	C-N	5.28	1.41	1.33
2	6	15	VAL	C-N	5.28	1.41	1.33
2	n	160	GLY	C-N	5.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	152	GLU	CA-C	-5.28	1.46	1.52
1	b	211	VAL	CA-C	-5.28	1.46	1.52
2	6	183	GLY	CA-C	-5.28	1.45	1.52
3	H	151	GLU	C-N	5.28	1.40	1.33
3	J	104	ALA	CA-C	-5.28	1.46	1.52
1	C	60	GLU	CA-CB	5.27	1.60	1.53
1	C	88	LEU	C-N	5.27	1.40	1.33
1	D	73	HIS	CA-CB	5.27	1.62	1.53
1	D	209	ILE	C-N	5.27	1.40	1.33
2	i	196	PHE	N-CA	-5.27	1.40	1.46
2	n	83	ARG	NE-CZ	5.27	1.38	1.33
1	b	185	PHE	N-CA	-5.27	1.40	1.46
1	d	219	ARG	C-N	5.27	1.40	1.33
2	j	97	LEU	N-CA	-5.27	1.40	1.46
2	5	37	ILE	C-N	5.27	1.40	1.33
2	7	167	LEU	N-CA	-5.27	1.39	1.46
3	I	82	SER	N-CA	5.27	1.52	1.46
3	J	317	ARG	NE-CZ	5.27	1.38	1.33
3	J	364	ARG	CA-CB	5.27	1.61	1.53
3	K	70	ASP	CA-CB	5.27	1.62	1.53
3	J	50	ARG	CZ-NH2	5.27	1.40	1.33
1	B	138	ILE	CA-C	-5.27	1.46	1.52
2	n	132	ILE	N-CA	-5.27	1.39	1.46
1	b	16	SER	N-CA	-5.27	1.41	1.45
1	C	129	VAL	N-CA	-5.27	1.39	1.46
2	k	133	GLU	C-N	5.27	1.40	1.33
1	c	173	GLU	CA-CB	5.26	1.61	1.53
1	d	87	VAL	CA-C	-5.26	1.46	1.52
3	H	319	GLN	CA-C	-5.26	1.46	1.52
3	M	361	PHE	N-CA	-5.26	1.39	1.46
1	A	16	SER	CA-CB	5.26	1.61	1.53
1	G	201	GLU	CA-CB	5.26	1.61	1.53
1	a	16	SER	CA-C	-5.26	1.46	1.53
2	6	170	ARG	CZ-NH1	5.26	1.40	1.32
2	7	97	LEU	CA-C	-5.26	1.46	1.52
2	6	94	THR	CA-C	-5.26	1.46	1.52
3	H	311	LEU	CA-C	-5.26	1.48	1.53
3	J	138	VAL	C-N	5.26	1.37	1.33
3	J	154	ARG	CD-NE	5.26	1.53	1.46
1	c	195	ALA	N-CA	-5.26	1.40	1.46
2	4	196	PHE	CG-CD1	5.26	1.49	1.38
1	A	232	TYR	CA-CB	5.25	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	142	SER	N-CA	-5.25	1.39	1.46
1	b	53	ARG	N-CA	-5.25	1.39	1.46
1	e	212	GLY	C-N	5.25	1.40	1.33
1	g	109	VAL	CA-CB	5.25	1.61	1.54
2	i	38	ALA	N-CA	-5.25	1.40	1.46
1	a	244	LEU	N-CA	-5.25	1.40	1.46
3	H	221	ARG	NE-CZ	5.25	1.38	1.33
2	j	80	ARG	N-CA	-5.25	1.39	1.46
2	n	115	ILE	N-CA	-5.25	1.40	1.46
3	L	65	VAL	C-N	5.25	1.41	1.33
1	B	22	PHE	C-N	-5.25	1.26	1.33
3	I	215	TYR	C-N	5.25	1.40	1.33
2	h	55	THR	CA-C	-5.25	1.46	1.52
2	h	62	ASP	N-CA	5.25	1.53	1.46
2	j	93	LEU	CA-C	5.25	1.59	1.52
2	4	212	ARG	CZ-NH2	5.25	1.40	1.33
2	7	120	LYS	CA-C	-5.25	1.46	1.52
1	a	161	ALA	C-O	-5.25	1.17	1.24
3	M	211	PHE	N-CA	-5.25	1.38	1.45
3	M	276	ASP	C-N	5.25	1.40	1.33
2	1	102	ARG	C-N	5.24	1.41	1.33
2	1	185	GLY	CA-C	5.24	1.59	1.51
1	b	178	GLU	N-CA	-5.24	1.39	1.46
2	5	51	ARG	CD-NE	5.24	1.53	1.46
2	l	32	THR	CA-C	-5.24	1.46	1.52
1	D	38	ILE	N-CA	-5.24	1.40	1.46
1	E	28	ARG	CZ-NH1	5.24	1.40	1.32
1	c	38	ILE	N-CA	5.24	1.52	1.46
1	E	28	ARG	C-N	5.24	1.41	1.34
2	4	44	LYS	CA-CB	5.24	1.62	1.53
3	K	43	ARG	CD-NE	5.24	1.53	1.46
2	n	167	LEU	C-N	5.24	1.40	1.33
1	e	230	LYS	N-CA	-5.24	1.41	1.46
2	4	193	GLU	CA-CB	5.24	1.62	1.53
3	L	138	VAL	C-N	5.24	1.41	1.33
3	J	112	THR	CA-C	-5.24	1.45	1.52
2	7	206	GLN	C-N	5.23	1.40	1.33
3	I	52	ARG	CZ-NH1	5.23	1.40	1.32
1	a	33	ARG	NE-CZ	5.23	1.38	1.33
3	I	377	LYS	CE-NZ	5.23	1.65	1.49
2	2	166	GLU	C-N	5.23	1.40	1.33
2	5	67	ALA	C-N	5.23	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	228	GLN	N-CA	-5.23	1.40	1.46
2	i	64	GLN	CA-C	-5.23	1.46	1.52
2	4	150	VAL	CA-C	5.23	1.60	1.52
2	k	177	LYS	CA-C	-5.23	1.46	1.52
3	I	38	GLU	C-O	-5.23	1.18	1.24
1	g	99	ASN	CA-C	-5.22	1.46	1.52
2	2	83	ARG	NE-CZ	5.22	1.38	1.33
3	L	127	VAL	N-CA	-5.22	1.41	1.46
3	L	381	LYS	N-CA	-5.22	1.40	1.46
1	g	10	ARG	C-N	5.22	1.39	1.33
2	1	126	ASP	CA-CB	-5.22	1.45	1.53
2	k	72	ILE	CA-CB	-5.22	1.48	1.54
1	F	202	SER	C-N	5.22	1.41	1.33
2	5	205	GLU	C-N	5.22	1.41	1.33
1	C	212	GLY	N-CA	5.22	1.50	1.45
1	g	49	ILE	C-O	-5.22	1.18	1.24
1	c	172	THR	N-CA	-5.22	1.40	1.46
2	k	127	PRO	N-CA	5.22	1.53	1.47
1	E	238	GLU	N-CA	5.22	1.52	1.46
2	k	83	ARG	CA-C	-5.22	1.46	1.52
3	H	384	LYS	C-N	5.22	1.42	1.33
1	d	100	ARG	CD-NE	5.21	1.53	1.46
1	f	73	HIS	C-N	5.21	1.40	1.33
2	h	83	ARG	CZ-NH2	5.21	1.40	1.33
3	K	169	GLU	CA-CB	5.21	1.61	1.53
3	K	205	ARG	CD-NE	5.21	1.53	1.46
3	M	363	ILE	C-O	-5.21	1.18	1.24
1	f	219	ARG	CD-NE	5.21	1.53	1.46
2	1	108	VAL	N-CA	-5.21	1.40	1.46
2	k	75	ASN	CG-ND2	5.21	1.44	1.33
3	L	109	ASN	N-CA	-5.21	1.39	1.46
3	J	352	LYS	CA-CB	5.21	1.61	1.53
1	G	27	ALA	CA-C	5.21	1.59	1.52
2	7	24	VAL	N-CA	5.21	1.52	1.46
3	H	324	HIS	ND1-CE1	5.21	1.37	1.32
3	I	346	ALA	CA-C	-5.21	1.46	1.52
1	B	53	ARG	CZ-NH2	5.21	1.40	1.33
1	b	147	LEU	CA-C	-5.21	1.46	1.52
1	g	28	ARG	CZ-NH2	5.21	1.40	1.33
2	5	159	ILE	CA-C	5.21	1.58	1.52
1	c	204	LEU	C-N	5.21	1.37	1.32
1	F	235	ARG	CZ-NH1	5.21	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	149	GLY	C-O	5.21	1.30	1.23
3	K	195	VAL	N-CA	-5.21	1.40	1.46
3	J	338	GLU	CA-CB	5.21	1.61	1.53
2	3	103	TYR	CZ-OH	5.21	1.49	1.38
2	2	80	ARG	CZ-NH1	5.20	1.40	1.32
1	F	205	VAL	CA-C	5.20	1.58	1.52
1	F	22	PHE	CA-CB	5.20	1.61	1.53
2	3	111	LEU	N-CA	-5.20	1.39	1.46
2	4	30	ARG	CD-NE	5.20	1.53	1.46
2	7	180	SER	CA-C	-5.20	1.45	1.52
1	f	68	TYR	C-N	5.20	1.40	1.33
2	j	163	GLU	N-CA	5.20	1.52	1.46
2	l	200	SER	CA-CB	5.20	1.61	1.53
3	L	194	ALA	C-N	5.20	1.40	1.33
3	J	244	ASP	CA-CB	5.20	1.61	1.53
2	6	67	ALA	CA-C	-5.20	1.46	1.52
3	H	374	ASP	CA-CB	5.20	1.61	1.53
1	E	48	LEU	N-CA	-5.19	1.40	1.46
1	e	141	VAL	N-CA	-5.19	1.40	1.46
2	i	68	ARG	CZ-NH1	5.19	1.40	1.32
2	l	125	ILE	CA-CB	5.19	1.60	1.54
1	b	143	GLU	C-O	-5.19	1.18	1.24
1	b	183	LEU	CA-C	-5.19	1.46	1.52
2	1	157	PRO	C-N	5.19	1.41	1.33
3	H	76	ARG	NE-CZ	5.19	1.38	1.33
1	g	130	ARG	CZ-NH1	5.19	1.40	1.32
2	j	60	VAL	CA-C	-5.19	1.46	1.52
3	J	340	ALA	C-O	5.19	1.30	1.24
1	A	95	GLU	CA-CB	-5.19	1.44	1.53
1	g	28	ARG	CD-NE	5.19	1.53	1.46
1	a	68	TYR	N-CA	-5.19	1.39	1.45
1	c	15	PHE	C-O	-5.19	1.17	1.24
1	E	92	ALA	CA-CB	5.19	1.61	1.53
2	2	49	ALA	N-CA	-5.19	1.38	1.46
2	l	87	VAL	CA-CB	-5.19	1.48	1.54
1	C	80	GLY	C-N	5.19	1.40	1.33
1	c	99	ASN	C-N	5.19	1.41	1.34
2	2	79	ILE	N-CA	-5.18	1.40	1.46
2	4	59	SER	CA-C	-5.18	1.46	1.52
2	l	95	SER	N-CA	-5.18	1.40	1.46
2	6	212	ARG	N-CA	-5.18	1.39	1.46
3	I	57	ARG	CZ-NH1	5.18	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	69	SER	CA-C	-5.18	1.45	1.52
1	D	149	GLU	N-CA	-5.18	1.40	1.46
2	6	141	GLY	C-N	5.18	1.40	1.33
3	J	186	THR	CA-C	-5.18	1.46	1.52
2	3	175	ALA	CA-CB	5.18	1.61	1.53
3	K	367	ARG	CD-NE	5.18	1.53	1.46
1	E	101	LEU	CB-CG	5.18	1.63	1.53
1	F	177	LYS	N-CA	-5.18	1.40	1.46
2	j	88	ARG	NE-CZ	5.18	1.38	1.33
1	c	47	ILE	CA-CB	-5.17	1.48	1.54
1	g	20	ARG	CZ-NH2	5.17	1.40	1.33
2	6	20	LYS	N-CA	-5.17	1.39	1.46
1	a	162	THR	N-CA	-5.17	1.40	1.46
2	h	154	ARG	NE-CZ	5.17	1.38	1.33
1	D	150	THR	N-CA	-5.17	1.39	1.46
2	6	88	ARG	NE-CZ	5.17	1.38	1.33
1	e	219	ARG	NE-CZ	5.17	1.38	1.33
1	f	119	PHE	CA-C	-5.17	1.46	1.52
1	g	91	ARG	CA-C	-5.17	1.46	1.52
2	m	97	LEU	CA-CB	5.17	1.61	1.53
3	J	86	LYS	C-N	5.17	1.41	1.33
2	j	197	TYR	N-CA	-5.17	1.39	1.46
2	l	136	ASP	CA-C	-5.17	1.46	1.52
2	7	150	VAL	N-CA	-5.17	1.40	1.46
1	d	122	GLN	N-CA	5.16	1.52	1.46
3	I	59	ARG	CA-CB	5.16	1.62	1.53
3	I	59	ARG	CD-NE	5.16	1.53	1.46
3	M	263	ARG	CZ-NH2	5.16	1.40	1.33
3	J	289	ARG	NE-CZ	5.16	1.38	1.33
1	b	107	ILE	C-N	5.16	1.40	1.33
1	C	106	PRO	CA-C	-5.16	1.46	1.52
1	D	91	ARG	CA-C	-5.16	1.46	1.52
1	g	158	GLU	N-CA	-5.16	1.39	1.46
2	k	178	ARG	CZ-NH1	5.16	1.40	1.32
3	H	108	LEU	CA-C	-5.16	1.46	1.52
1	c	192	GLY	CA-C	-5.16	1.45	1.51
3	H	318	ILE	C-N	5.16	1.40	1.33
1	a	105	GLU	CA-C	-5.16	1.48	1.52
1	E	234	GLU	C-N	5.16	1.40	1.33
1	F	10	ARG	CA-C	-5.16	1.45	1.52
1	f	93	ARG	CZ-NH2	5.16	1.40	1.33
2	l	107	LEU	CA-C	-5.16	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	367	ARG	NE-CZ	5.16	1.38	1.33
1	c	117	CYS	C-N	5.15	1.40	1.33
1	g	15	PHE	CA-C	-5.15	1.46	1.52
3	H	98	GLU	C-N	5.15	1.40	1.33
2	2	146	THR	C-N	5.15	1.40	1.33
3	H	69	SER	CA-C	5.15	1.59	1.52
3	K	98	GLU	C-N	5.15	1.41	1.33
3	K	101	LYS	CA-CB	5.15	1.61	1.54
1	g	11	ALA	CA-C	-5.15	1.46	1.52
1	g	239	ARG	C-N	5.15	1.40	1.33
2	7	156	THR	CA-C	5.15	1.58	1.52
3	H	57	ARG	CZ-NH2	5.15	1.40	1.33
3	I	19	ASP	C-N	5.15	1.41	1.33
3	K	214	LYS	C-N	5.15	1.40	1.33
1	A	91	ARG	C-N	5.15	1.40	1.33
1	E	177	LYS	C-N	5.15	1.41	1.33
1	E	53	ARG	CD-NE	5.15	1.53	1.46
3	I	69	SER	C-N	5.15	1.40	1.33
3	K	50	ARG	CA-C	-5.15	1.46	1.52
1	D	124	THR	C-N	5.15	1.41	1.33
1	g	145	PRO	C-N	5.15	1.40	1.33
3	H	109	ASN	CA-C	-5.15	1.46	1.52
3	J	284	ILE	C-N	5.15	1.41	1.33
1	D	47	ILE	C-O	-5.14	1.19	1.24
2	i	188	VAL	N-CA	-5.14	1.40	1.46
1	G	102	THR	CA-CB	5.14	1.61	1.53
2	i	137	ILE	CA-CB	-5.14	1.48	1.54
2	j	33	MET	CA-C	-5.14	1.47	1.53
3	H	110	GLN	CA-CB	5.14	1.61	1.53
2	6	122	ILE	N-CA	-5.14	1.40	1.46
3	H	205	ARG	CA-C	-5.14	1.46	1.52
1	B	241	ARG	CD-NE	5.14	1.53	1.46
1	e	178	GLU	CA-C	-5.14	1.46	1.52
2	i	86	THR	C-N	5.14	1.40	1.33
3	K	46	ARG	NE-CZ	5.14	1.38	1.33
1	c	237	ASN	CA-CB	5.14	1.61	1.53
1	G	219	ARG	CD-NE	5.14	1.53	1.46
1	g	42	CYS	CA-C	-5.14	1.45	1.52
2	k	54	MET	N-CA	-5.14	1.39	1.46
3	M	224	ARG	NE-CZ	5.14	1.38	1.33
2	n	47	GLN	C-O	-5.13	1.17	1.24
3	H	281	VAL	C-N	5.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	238	ILE	N-CA	-5.13	1.39	1.46
3	L	276	ASP	CA-CB	5.13	1.59	1.53
1	C	241	ARG	CA-C	-5.13	1.46	1.52
1	g	213	TYR	C-N	5.13	1.39	1.33
2	l	73	GLU	N-CA	5.13	1.52	1.46
1	c	216	VAL	N-CA	-5.13	1.40	1.46
2	k	73	GLU	C-N	5.13	1.41	1.33
3	I	239	PHE	N-CA	-5.13	1.39	1.46
1	c	93	ARG	CZ-NH2	5.13	1.40	1.33
1	c	74	ILE	C-N	5.13	1.40	1.33
1	d	53	ARG	CZ-NH1	5.13	1.40	1.32
2	n	33	MET	CA-C	-5.13	1.46	1.52
3	H	267	GLN	C-N	5.13	1.40	1.33
3	K	294	ASP	CA-C	-5.13	1.47	1.53
1	G	48	LEU	C-N	5.13	1.40	1.33
2	4	212	ARG	CA-C	-5.13	1.46	1.52
3	J	52	ARG	N-CA	-5.13	1.39	1.46
1	B	73	HIS	CB-CG	5.12	1.57	1.50
3	J	258	ASP	CG-OD2	5.12	1.35	1.25
1	a	49	ILE	CA-C	-5.12	1.46	1.52
2	j	201	PRO	CA-CB	-5.12	1.46	1.53
2	k	203	GLU	N-CA	-5.12	1.40	1.46
3	L	100	LEU	C-N	5.12	1.39	1.33
1	D	115	LYS	CA-C	-5.12	1.46	1.52
2	k	196	PHE	N-CA	-5.12	1.39	1.46
1	C	111	GLU	N-CA	-5.12	1.39	1.46
1	c	36	THR	CA-C	-5.12	1.46	1.52
3	I	52	ARG	NE-CZ	5.12	1.38	1.33
2	3	167	LEU	CA-CB	5.12	1.61	1.53
3	I	15	LYS	CA-C	5.12	1.59	1.52
3	M	12	LYS	CA-CB	5.12	1.61	1.53
1	a	119	PHE	N-CA	-5.12	1.40	1.46
2	5	68	ARG	CZ-NH2	5.12	1.40	1.33
1	A	100	ARG	CZ-NH2	5.12	1.40	1.33
1	a	31	VAL	CA-C	-5.12	1.45	1.52
1	F	192	GLY	CA-C	-5.12	1.45	1.51
1	F	210	GLU	C-N	5.12	1.40	1.33
2	5	102	ARG	C-N	5.12	1.41	1.33
2	m	184	ASP	N-CA	-5.12	1.39	1.46
1	a	19	GLY	C-O	5.11	1.29	1.23
1	B	132	PHE	N-CA	-5.11	1.39	1.45
1	G	118	ASP	C-N	5.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	132	ILE	CA-CB	-5.11	1.47	1.54
2	7	40	LYS	CA-CB	5.11	1.61	1.53
1	b	51	ASP	N-CA	-5.11	1.39	1.46
1	E	47	ILE	N-CA	-5.11	1.40	1.46
1	d	21	LEU	N-CA	-5.11	1.39	1.46
2	l	77	TYR	C-N	5.11	1.40	1.33
3	I	367	ARG	CA-CB	5.11	1.62	1.53
3	M	55	VAL	CA-CB	5.11	1.60	1.54
3	M	393	LYS	C-N	5.11	1.41	1.33
1	B	88	LEU	C-N	5.11	1.40	1.33
1	C	39	GLY	CA-C	5.11	1.56	1.51
2	2	18	VAL	CA-CB	-5.11	1.48	1.54
2	i	20	LYS	CA-C	-5.11	1.45	1.52
1	d	160	LYS	N-CA	-5.11	1.38	1.45
1	g	49	ILE	CA-C	-5.11	1.46	1.52
2	n	74	ALA	N-CA	-5.11	1.40	1.46
1	f	11	ALA	N-CA	-5.11	1.39	1.46
2	1	193	GLU	N-CA	5.11	1.52	1.46
3	H	43	ARG	CZ-NH2	5.11	1.40	1.33
3	H	334	VAL	CA-C	-5.11	1.46	1.52
3	I	125	PRO	N-CA	-5.11	1.43	1.47
2	2	106	TYR	CA-CB	5.10	1.62	1.53
2	2	12	THR	C-N	5.10	1.39	1.33
3	I	380	GLU	CA-C	-5.10	1.46	1.52
2	j	106	TYR	N-CA	-5.10	1.39	1.45
2	l	171	ALA	C-N	5.10	1.39	1.33
1	B	148	TYR	CA-CB	5.10	1.62	1.54
2	2	109	GLN	CA-C	-5.10	1.46	1.52
2	5	175	ALA	C-N	5.10	1.40	1.33
2	m	99	ASN	C-N	5.10	1.40	1.33
3	J	100	LEU	CA-CB	5.10	1.61	1.53
1	c	194	VAL	C-N	5.10	1.40	1.33
2	j	81	ARG	CD-NE	5.10	1.53	1.46
3	H	120	PRO	N-CD	-5.10	1.40	1.47
1	f	146	LYS	N-CA	-5.10	1.39	1.46
1	A	161	ALA	CA-C	5.09	1.59	1.52
1	C	236	ALA	C-N	5.09	1.40	1.33
2	k	65	PHE	CA-C	-5.09	1.45	1.52
2	7	69	ILE	CA-C	-5.09	1.46	1.52
1	d	195	ALA	CA-CB	5.09	1.61	1.53
1	F	192	GLY	N-CA	-5.09	1.39	1.45
3	I	12	LYS	CA-CB	5.09	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	149	GLN	C-N	5.09	1.40	1.33
1	b	20	ARG	N-CA	-5.09	1.40	1.45
1	C	5	GLN	C-N	5.09	1.40	1.33
2	2	59	SER	CA-C	-5.09	1.46	1.52
2	2	86	THR	C-N	5.09	1.40	1.33
2	j	50	ASP	CA-CB	5.09	1.61	1.53
2	n	136	ASP	C-N	5.09	1.40	1.33
3	K	272	LEU	CA-CB	5.09	1.61	1.53
3	L	388	PRO	C-N	5.09	1.39	1.33
1	B	144	VAL	CA-CB	5.09	1.60	1.54
1	D	159	TYR	C-N	5.09	1.40	1.33
1	E	241	ARG	NE-CZ	5.09	1.38	1.33
3	K	337	LYS	CA-CB	5.09	1.61	1.53
1	A	241	ARG	CZ-NH2	5.09	1.40	1.33
1	C	40	ILE	C-N	5.09	1.40	1.33
2	i	148	TYR	CA-CB	5.09	1.61	1.53
2	j	146	THR	N-CA	-5.09	1.40	1.46
2	n	167	LEU	N-CA	-5.09	1.40	1.46
2	n	199	TYR	N-CA	-5.09	1.40	1.46
3	J	278	ARG	NE-CZ	5.09	1.38	1.33
2	m	207	ILE	CA-C	-5.08	1.46	1.52
3	K	313	THR	N-CA	5.08	1.52	1.45
1	b	233	VAL	CA-CB	-5.08	1.48	1.54
1	c	37	ALA	C-N	5.08	1.40	1.33
1	d	189	MET	CA-C	-5.08	1.46	1.52
1	e	239	ARG	NE-CZ	5.08	1.38	1.33
3	H	162	LEU	CA-CB	5.08	1.61	1.53
3	I	117	ASN	CA-C	-5.08	1.46	1.52
3	L	313	THR	N-CA	-5.08	1.39	1.46
3	J	162	LEU	CA-C	-5.08	1.46	1.52
1	E	182	ASP	C-N	5.08	1.40	1.33
1	F	53	ARG	CA-C	-5.08	1.46	1.52
2	i	201	PRO	C-N	5.08	1.40	1.33
3	H	52	ARG	CD-NE	5.08	1.53	1.46
3	H	305	ARG	CA-CB	5.08	1.60	1.52
1	g	46	VAL	C-N	5.08	1.41	1.33
1	e	38	ILE	C-O	5.08	1.29	1.24
1	f	210	GLU	N-CA	-5.08	1.39	1.46
2	5	102	ARG	NE-CZ	5.08	1.38	1.33
3	H	42	ILE	CA-C	-5.08	1.46	1.52
1	a	205	VAL	C-N	5.08	1.39	1.34
2	6	176	MET	CA-CB	5.08	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	168	ALA	CA-CB	5.08	1.61	1.53
3	H	50	ARG	CZ-NH1	5.07	1.39	1.32
3	I	46	ARG	NE-CZ	5.07	1.38	1.33
1	D	39	GLY	N-CA	-5.07	1.40	1.46
1	E	62	ASP	N-CA	-5.07	1.40	1.46
1	E	110	LYS	CA-CB	5.07	1.61	1.53
2	7	100	SER	CA-C	5.07	1.59	1.52
3	L	315	GLU	C-N	5.07	1.40	1.33
3	M	325	THR	CA-C	-5.07	1.46	1.52
3	I	200	ARG	NE-CZ	5.07	1.38	1.33
3	M	34	LYS	N-CA	5.07	1.52	1.46
1	b	125	GLN	CA-CB	-5.07	1.45	1.53
1	D	127	GLY	CA-C	-5.07	1.47	1.52
3	L	209	SER	N-CA	-5.07	1.39	1.46
3	L	291	ASP	CA-CB	5.07	1.61	1.53
3	L	328	MET	CA-CB	5.07	1.61	1.53
3	M	57	ARG	NE-CZ	5.07	1.38	1.33
3	J	180	LEU	C-N	5.07	1.40	1.33
1	D	148	TYR	CA-C	-5.07	1.46	1.52
2	1	171	ALA	C-N	5.07	1.40	1.33
3	H	152	GLU	N-CA	-5.07	1.40	1.46
3	M	28	ARG	CD-NE	5.06	1.53	1.46
3	K	86	LYS	N-CA	-5.06	1.39	1.46
2	3	56	THR	C-N	5.06	1.40	1.33
1	C	159	TYR	CA-C	-5.06	1.46	1.52
1	D	136	LEU	CA-C	-5.06	1.46	1.52
1	F	99	ASN	N-CA	-5.06	1.40	1.46
2	7	54	MET	C-N	5.06	1.40	1.33
1	F	33	ARG	CD-NE	5.06	1.53	1.46
2	5	171	ALA	CA-C	-5.06	1.46	1.52
3	H	315	GLU	N-CA	-5.06	1.39	1.46
3	K	288	ASN	N-CA	-5.06	1.40	1.46
3	L	146	LEU	CA-C	-5.06	1.46	1.52
3	L	324	HIS	N-CA	-5.06	1.40	1.46
3	M	306	ILE	CA-C	-5.06	1.47	1.52
1	C	127	GLY	CA-C	5.06	1.60	1.51
2	3	109	GLN	CA-C	-5.06	1.46	1.52
3	H	275	PHE	CA-CB	5.06	1.61	1.54
1	a	93	ARG	CZ-NH2	5.05	1.40	1.33
2	i	102	ARG	NE-CZ	5.05	1.38	1.33
2	l	174	SER	CA-CB	5.05	1.61	1.53
1	g	17	PRO	C-N	5.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	76	ARG	CZ-NH2	5.05	1.40	1.33
1	b	144	VAL	C-O	5.05	1.28	1.24
1	D	8	TYR	N-CA	-5.05	1.39	1.46
1	d	204	LEU	C-N	5.05	1.39	1.33
2	k	51	ARG	CD-NE	5.05	1.53	1.46
3	J	246	ILE	C-O	-5.05	1.18	1.24
1	b	47	ILE	CA-C	-5.05	1.46	1.52
2	1	122	ILE	N-CA	5.05	1.52	1.46
2	j	71	LYS	CA-C	-5.05	1.46	1.52
2	l	173	TYR	N-CA	-5.05	1.40	1.46
2	6	115	ILE	CA-C	-5.05	1.46	1.52
1	a	36	THR	C-N	5.05	1.40	1.33
1	E	96	ALA	C-N	5.05	1.40	1.33
1	f	145	PRO	N-CA	-5.05	1.41	1.47
3	J	311	LEU	CA-CB	5.05	1.61	1.53
1	a	97	GLN	N-CA	-5.05	1.39	1.46
1	c	169	ASN	C-O	-5.05	1.18	1.24
1	d	115	LYS	C-N	5.05	1.39	1.33
2	2	168	ALA	C-N	5.05	1.40	1.33
3	I	28	ARG	CD-NE	5.05	1.53	1.46
1	C	224	VAL	CA-CB	-5.04	1.48	1.53
1	F	39	GLY	N-CA	5.04	1.50	1.45
1	f	113	ALA	CA-C	-5.04	1.46	1.52
2	4	185	GLY	N-CA	-5.04	1.39	1.45
2	m	57	ALA	CA-C	-5.04	1.46	1.52
2	n	185	GLY	CA-C	-5.04	1.46	1.52
3	H	293	LEU	CA-C	-5.04	1.46	1.53
3	H	309	VAL	CA-CB	-5.04	1.49	1.54
1	e	52	LYS	N-CA	-5.04	1.39	1.46
2	n	135	LYS	CA-CB	5.04	1.61	1.53
2	5	68	ARG	CZ-NH1	5.04	1.39	1.32
3	I	60	SER	C-O	5.04	1.30	1.23
1	g	63	THR	CA-CB	5.04	1.61	1.53
1	g	138	ILE	C-N	5.04	1.40	1.33
3	J	319	GLN	CA-CB	5.04	1.61	1.53
1	d	205	VAL	CA-CB	-5.04	1.47	1.54
1	C	28	ARG	CZ-NH1	5.04	1.39	1.32
1	D	239	ARG	CZ-NH2	5.04	1.40	1.33
1	d	186	ASP	N-CA	-5.04	1.40	1.46
2	n	70	ILE	CA-CB	5.04	1.60	1.54
3	H	201	ALA	C-N	5.04	1.40	1.33
3	M	27	TYR	N-CA	-5.04	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	124	THR	C-N	5.03	1.41	1.33
1	D	154	GLY	C-N	5.03	1.40	1.33
2	3	170	ARG	C-N	5.03	1.40	1.33
2	5	46	TYR	C-O	5.03	1.30	1.23
2	l	34	GLY	C-N	5.03	1.39	1.33
2	6	112	ILE	C-O	-5.03	1.18	1.24
3	I	221	ARG	NE-CZ	5.03	1.38	1.33
3	K	390	PRO	CA-CB	5.03	1.60	1.53
1	D	46	VAL	N-CA	-5.03	1.40	1.46
3	H	355	CYS	C-N	5.03	1.40	1.33
2	6	201	PRO	C-O	5.03	1.30	1.24
2	7	154	ARG	CZ-NH2	5.03	1.40	1.33
1	c	200	ILE	CA-CB	-5.03	1.48	1.54
1	E	37	ALA	N-CA	-5.03	1.40	1.46
1	g	210	GLU	N-CA	-5.03	1.39	1.46
3	H	271	GLU	C-N	5.03	1.40	1.33
3	J	376	THR	CA-CB	5.03	1.61	1.53
1	F	219	ARG	CZ-NH1	5.03	1.39	1.32
2	1	81	ARG	CZ-NH1	5.03	1.39	1.32
3	K	52	ARG	CZ-NH1	5.03	1.39	1.32
1	c	149	GLU	CA-CB	5.02	1.62	1.53
3	I	339	LEU	C-N	5.02	1.40	1.34
1	E	173	GLU	N-CA	-5.02	1.40	1.46
3	L	259	ARG	CZ-NH2	5.02	1.40	1.33
1	b	110	LYS	C-N	5.02	1.40	1.33
1	C	60	GLU	CA-C	-5.02	1.46	1.52
1	C	151	ASP	C-N	5.02	1.40	1.34
1	C	201	GLU	CA-CB	5.02	1.60	1.53
1	c	235	ARG	CZ-NH2	5.02	1.40	1.33
2	k	203	GLU	CA-CB	5.02	1.61	1.53
1	a	241	ARG	NE-CZ	5.02	1.38	1.33
1	B	73	HIS	N-CA	-5.01	1.41	1.46
2	3	37	ILE	N-CA	-5.01	1.40	1.46
2	k	131	ALA	CA-C	-5.01	1.46	1.52
2	6	36	PHE	C-N	5.01	1.39	1.33
2	6	133	GLU	N-CA	-5.01	1.39	1.45
3	H	140	TYR	N-CA	-5.01	1.40	1.46
3	M	320	ILE	C-O	-5.01	1.18	1.24
3	J	20	TYR	C-O	-5.01	1.18	1.24
3	H	195	VAL	CA-C	5.01	1.59	1.52
3	M	356	THR	N-CA	-5.01	1.40	1.46
1	C	28	ARG	C-N	5.01	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	81	ARG	CZ-NH2	5.01	1.40	1.33
2	7	71	LYS	CA-CB	5.01	1.61	1.53
3	J	88	VAL	C-O	-5.01	1.18	1.24
3	J	230	ALA	CA-C	-5.01	1.46	1.52
1	D	67	ILE	CA-C	-5.01	1.48	1.53
1	e	100	ARG	N-CA	-5.01	1.40	1.46
1	g	73	HIS	N-CA	-5.01	1.39	1.46
2	m	90	ILE	CA-CB	5.01	1.60	1.54
2	h	186	ILE	C-O	-5.01	1.18	1.24
2	l	184	ASP	C-O	-5.01	1.17	1.23
1	a	86	ARG	CD-NE	5.01	1.53	1.46
1	c	53	ARG	CA-C	-5.01	1.46	1.52
1	c	214	VAL	CA-C	5.01	1.58	1.52
1	F	77	ALA	C-N	5.01	1.40	1.33
2	k	38	ALA	CA-C	-5.01	1.46	1.52
2	k	134	GLU	CA-C	-5.01	1.46	1.52
2	n	77	TYR	CA-CB	5.01	1.61	1.53
3	H	171	GLY	C-N	5.01	1.40	1.33
3	J	76	ARG	NE-CZ	5.01	1.38	1.33
1	d	174	PHE	CA-C	5.00	1.59	1.52
1	a	208	ASN	CG-ND2	5.00	1.43	1.33
2	l	199	TYR	CA-C	5.00	1.59	1.52
2	h	77	TYR	CA-CB	5.00	1.61	1.53
2	j	198	GLN	N-CA	-5.00	1.40	1.46
2	6	70	ILE	CA-CB	5.00	1.60	1.54
3	I	224	ARG	CA-C	-5.00	1.46	1.52
3	M	158	GLU	N-CA	5.00	1.52	1.46
1	d	100	ARG	C-N	5.00	1.40	1.33
1	F	42	CYS	N-CA	-5.00	1.39	1.45
2	5	55	THR	N-CA	-5.00	1.40	1.46
3	M	209	SER	CA-C	5.00	1.59	1.52

All (4543) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	170	ARG	NE-CZ-NH2	-23.57	97.98	119.20
2	5	170	ARG	NE-CZ-NH2	-22.71	98.76	119.20
3	L	246	ILE	N-CA-C	-15.16	98.35	112.90
1	C	143	GLU	N-CA-C	-13.13	99.65	114.62
1	C	196	MET	CA-C-N	12.79	134.35	120.03
1	C	196	MET	C-N-CA	12.79	134.35	120.03
3	M	261	VAL	N-CA-C	-12.72	98.48	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	395	VAL	N-CA-C	-12.52	99.79	113.43
3	I	167	PHE	CA-CB-CG	-12.47	101.33	113.80
3	I	386	THR	CA-C-N	12.22	143.70	121.70
3	I	386	THR	C-N-CA	12.22	143.70	121.70
2	4	156	THR	O-C-N	-11.94	112.93	121.65
1	E	22	PHE	CA-CB-CG	-11.90	101.90	113.80
3	J	175	PRO	CA-C-N	11.84	135.83	120.44
3	J	175	PRO	C-N-CA	11.84	135.83	120.44
2	3	99	ASN	CA-CB-CG	-11.76	100.84	112.60
3	M	87	PHE	CA-CB-CG	-11.63	102.17	113.80
1	c	230	LYS	CA-C-O	-11.56	107.58	118.44
1	G	62	ASP	CA-CB-CG	-11.52	101.08	112.60
3	J	261	VAL	CA-C-N	11.50	135.69	120.28
3	J	261	VAL	C-N-CA	11.50	135.69	120.28
1	g	181	ASP	CA-CB-CG	-11.46	101.14	112.60
1	B	187	ASP	CA-C-N	11.44	135.60	120.28
1	B	187	ASP	C-N-CA	11.44	135.60	120.28
1	e	96	ALA	CA-C-N	11.43	135.59	120.28
1	e	96	ALA	C-N-CA	11.43	135.59	120.28
2	k	156	THR	CA-C-O	-11.37	109.62	120.19
1	C	12	ILE	N-CA-C	-11.32	102.12	113.10
3	J	101	LYS	CA-C-N	11.24	133.90	119.84
3	J	101	LYS	C-N-CA	11.24	133.90	119.84
2	2	62	ASP	CA-CB-CG	-11.19	101.42	112.60
2	7	153	ASP	CA-CB-CG	-11.18	101.42	112.60
3	H	358	ALA	CA-C-N	11.11	132.22	120.00
3	H	358	ALA	C-N-CA	11.11	132.22	120.00
1	d	63	THR	N-CA-C	-10.96	100.65	114.56
2	4	126	ASP	CA-C-O	-10.95	111.00	120.19
2	2	40	LYS	N-CA-C	-10.93	100.48	114.04
1	e	239	ARG	NE-CZ-NH2	10.84	128.96	119.20
1	a	22	PHE	CA-C-N	10.76	134.43	120.44
1	a	22	PHE	C-N-CA	10.76	134.43	120.44
1	D	13	THR	N-CA-C	10.75	123.00	111.28
3	K	255	THR	CA-C-N	10.70	134.35	120.44
3	K	255	THR	C-N-CA	10.70	134.35	120.44
2	1	48	ILE	N-CA-C	-10.64	102.66	111.81
3	H	395	VAL	N-CA-C	-10.59	102.74	112.90
2	7	58	GLY	CA-C-O	10.55	129.86	120.79
1	b	215	LYS	CA-C-N	10.54	134.06	120.56
1	b	215	LYS	C-N-CA	10.54	134.06	120.56
2	l	170	ARG	NH1-CZ-NH2	10.53	132.98	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	389	ILE	N-CA-C	-10.51	100.57	109.19
2	6	18	VAL	N-CA-CB	10.47	122.13	110.72
2	3	139	ALA	CA-C-N	10.46	140.54	121.70
2	3	139	ALA	C-N-CA	10.46	140.54	121.70
3	M	281	VAL	CA-C-N	10.42	140.45	121.70
3	M	281	VAL	C-N-CA	10.42	140.45	121.70
3	I	272	LEU	N-CA-C	-10.41	97.87	112.13
2	m	83	ARG	NE-CZ-NH1	-10.40	111.10	121.50
2	h	165	VAL	N-CA-CB	10.38	123.85	110.57
2	h	96	ASN	CA-CB-CG	-10.37	102.23	112.60
2	h	112	ILE	N-CA-C	-10.36	93.61	108.11
2	1	83	ARG	NE-CZ-NH2	10.32	128.49	119.20
1	D	9	ASP	CA-CB-CG	10.29	122.89	112.60
3	K	159	LEU	O-C-N	-10.28	111.05	120.71
3	J	283	VAL	O-C-N	-10.25	112.47	123.03
1	g	217	ASP	CA-CB-CG	10.22	122.83	112.60
3	K	159	LEU	CA-C-N	10.21	129.86	119.24
3	K	159	LEU	C-N-CA	10.21	129.86	119.24
2	l	207	ILE	N-CA-C	-10.20	98.32	112.50
1	A	79	SER	N-CA-C	-10.20	93.43	109.23
1	C	62	ASP	CA-CB-CG	-10.19	102.41	112.60
1	D	218	ASP	N-CA-C	-10.19	100.71	113.55
2	6	129	GLY	N-CA-C	-10.16	97.57	111.09
3	L	221	ARG	CA-C-N	10.12	134.20	120.54
3	L	221	ARG	C-N-CA	10.12	134.20	120.54
2	k	104	PHE	CA-CB-CG	-10.11	103.69	113.80
3	H	143	ILE	N-CA-C	-10.11	103.26	113.47
1	E	22	PHE	CA-C-N	10.09	133.79	120.28
1	E	22	PHE	C-N-CA	10.09	133.79	120.28
2	6	156	THR	CA-C-O	-10.06	110.78	120.94
3	L	258	ASP	CA-CB-CG	-9.94	102.67	112.60
2	6	134	GLU	CA-C-N	9.91	133.33	120.44
2	6	134	GLU	C-N-CA	9.91	133.33	120.44
1	A	181	ASP	CA-CB-CG	-9.89	102.70	112.60
2	n	117	SER	CA-C-O	-9.88	109.95	120.42
1	a	138	ILE	N-CA-C	-9.81	92.90	107.51
2	2	202	GLU	CA-C-N	9.79	133.40	120.28
2	2	202	GLU	C-N-CA	9.79	133.40	120.28
1	f	18	ASP	CA-CB-CG	-9.78	102.82	112.60
2	4	156	THR	N-CA-C	-9.77	96.92	108.25
1	D	109	VAL	CA-C-N	9.76	133.13	120.44
1	D	109	VAL	C-N-CA	9.76	133.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	135	LYS	CA-C-N	9.73	132.00	119.84
3	H	135	LYS	C-N-CA	9.73	132.00	119.84
2	j	58	GLY	N-CA-C	-9.72	101.74	111.56
1	E	19	GLY	CA-C-O	9.71	129.79	119.01
1	B	64	ILE	CA-C-N	9.67	139.11	121.70
1	B	64	ILE	C-N-CA	9.67	139.11	121.70
1	e	71	ASP	CA-CB-CG	9.65	122.25	112.60
1	d	66	LYS	N-CA-C	-9.60	101.69	113.97
2	i	170	ARG	NE-CZ-NH2	9.58	127.82	119.20
1	D	73	HIS	CA-CB-CG	9.49	123.29	113.80
3	M	123	LYS	CA-C-O	9.49	123.44	117.94
1	f	228	GLU	N-CA-C	-9.46	101.86	113.97
2	5	170	ARG	NH1-CZ-NH2	9.45	131.58	119.30
1	g	145	PRO	N-CA-CB	9.44	111.77	103.27
3	I	302	ARG	N-CA-C	-9.41	90.76	110.80
1	g	43	LYS	N-CA-C	-9.40	100.19	112.41
1	B	103	TYR	N-CA-C	-9.38	103.93	114.62
1	E	130	ARG	CA-C-N	9.34	129.27	120.03
1	E	130	ARG	C-N-CA	9.34	129.27	120.03
3	H	276	ASP	N-CA-C	-9.33	98.26	110.39
3	K	280	ASP	CA-CB-CG	-9.32	103.28	112.60
2	l	83	ARG	NE-CZ-NH1	-9.32	112.18	121.50
1	e	91	ARG	NE-CZ-NH2	9.30	127.57	119.20
3	I	336	PHE	CA-CB-CG	-9.29	104.51	113.80
3	M	264	THR	O-C-N	-9.29	111.56	122.15
1	a	234	GLU	CA-C-N	9.27	132.49	120.44
1	a	234	GLU	C-N-CA	9.27	132.49	120.44
1	D	16	SER	CA-C-N	9.27	131.42	119.84
1	D	16	SER	C-N-CA	9.27	131.42	119.84
3	M	333	ASP	CA-C-N	9.25	132.89	120.50
3	M	333	ASP	C-N-CA	9.25	132.89	120.50
2	5	177	LYS	N-CA-C	-9.24	102.14	113.50
1	e	181	ASP	CA-CB-CG	-9.24	103.36	112.60
1	E	241	ARG	NE-CZ-NH2	9.23	127.50	119.20
1	g	29	GLU	O-C-N	9.21	131.89	122.12
1	G	129	VAL	O-C-N	-9.21	114.96	122.97
2	i	135	LYS	N-CA-C	-9.21	100.96	113.30
2	n	114	GLY	CA-C-O	9.18	127.24	120.91
3	H	50	ARG	CA-C-N	9.17	132.56	120.28
3	H	50	ARG	C-N-CA	9.17	132.56	120.28
3	K	397	PHE	CA-CB-CG	-9.14	104.66	113.80
1	b	169	ASN	CA-CB-CG	-9.11	103.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ARG	N-CA-C	-9.09	96.04	108.86
2	3	194	ASP	N-CA-CB	9.09	125.85	110.49
2	m	39	SER	CA-C-N	9.08	132.45	120.28
2	m	39	SER	C-N-CA	9.08	132.45	120.28
3	K	130	PHE	CA-CB-CG	-9.06	104.73	113.80
1	b	180	ARG	N-CA-CB	9.04	124.66	110.56
2	1	136	ASP	CA-CB-CG	9.03	121.63	112.60
2	l	147	ALA	CA-C-N	9.03	132.38	120.28
2	l	147	ALA	C-N-CA	9.03	132.38	120.28
1	G	184	SER	N-CA-C	-9.02	97.11	110.46
1	C	107	ILE	O-C-N	-9.01	113.08	122.63
1	F	57	LYS	N-CA-C	-9.01	101.81	113.17
2	5	32	THR	CA-C-O	9.01	130.10	120.46
3	M	289	ARG	CA-C-N	9.01	133.22	120.42
3	M	289	ARG	C-N-CA	9.01	133.22	120.42
3	K	120	PRO	CA-C-N	9.01	134.35	121.02
3	K	120	PRO	C-N-CA	9.01	134.35	121.02
2	5	183	GLY	N-CA-C	-8.98	103.30	114.16
3	K	324	HIS	ND1-CE1-NE2	8.96	117.36	108.40
3	L	55	VAL	CA-C-O	-8.95	111.64	120.95
3	H	62	PRO	CA-C-N	8.95	137.23	122.73
3	H	62	PRO	C-N-CA	8.95	137.23	122.73
1	C	105	GLU	CA-C-N	8.95	129.50	119.83
1	C	105	GLU	C-N-CA	8.95	129.50	119.83
3	I	121	THR	CA-C-N	8.94	137.79	121.70
3	I	121	THR	C-N-CA	8.94	137.79	121.70
1	c	33	ARG	CA-C-N	8.93	130.63	120.53
1	c	33	ARG	C-N-CA	8.93	130.63	120.53
1	A	230	LYS	CA-C-N	8.93	129.10	119.28
1	A	230	LYS	C-N-CA	8.93	129.10	119.28
1	d	144	VAL	CA-C-O	-8.92	113.39	119.19
1	D	65	GLU	N-CA-CB	8.92	125.66	110.50
3	H	100	LEU	CA-C-O	8.91	130.33	120.70
2	4	126	ASP	CA-CB-CG	-8.91	103.69	112.60
3	K	294	ASP	CA-C-N	8.91	129.47	119.32
3	K	294	ASP	C-N-CA	8.91	129.47	119.32
3	J	196	ALA	O-C-N	8.87	131.53	122.12
2	k	139	ALA	CA-C-N	8.87	137.66	121.70
2	k	139	ALA	C-N-CA	8.87	137.66	121.70
1	D	130	ARG	CA-C-O	-8.86	113.20	121.08
3	I	253	SER	O-C-N	8.86	133.28	123.10
2	2	116	ASP	CA-C-N	8.85	132.49	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	116	ASP	C-N-CA	8.85	132.49	120.54
2	k	191	ILE	N-CA-C	-8.85	94.67	107.77
1	F	186	ASP	CA-CB-CG	-8.85	103.75	112.60
3	J	36	PHE	CA-CB-CG	-8.82	104.98	113.80
2	5	128	ILE	N-CA-C	-8.81	104.01	112.29
1	c	151	ASP	N-CA-C	-8.78	98.91	110.40
1	D	114	LYS	CA-C-N	8.77	131.84	120.44
1	D	114	LYS	C-N-CA	8.77	131.84	120.44
1	b	53	ARG	CA-C-O	-8.74	112.28	121.55
3	M	220	ALA	N-CA-C	8.74	120.50	110.97
1	d	180	ARG	CA-C-N	8.73	132.85	120.28
1	d	180	ARG	C-N-CA	8.73	132.85	120.28
2	i	198	GLN	CA-C-N	8.73	131.98	120.28
2	i	198	GLN	C-N-CA	8.73	131.98	120.28
2	m	87	VAL	CA-C-N	8.73	131.97	120.28
2	m	87	VAL	C-N-CA	8.73	131.97	120.28
1	F	103	TYR	N-CA-C	-8.72	103.76	114.75
3	M	388	PRO	CA-C-N	8.71	130.43	122.85
3	M	388	PRO	C-N-CA	8.71	130.43	122.85
1	a	109	VAL	N-CA-C	-8.71	101.74	110.62
3	H	324	HIS	CE1-NE2-CD2	-8.71	100.29	109.00
1	G	26	TYR	N-CA-C	-8.70	102.80	113.41
3	M	311	LEU	CA-C-N	8.70	130.71	119.84
3	M	311	LEU	C-N-CA	8.70	130.71	119.84
2	1	21	ASP	CA-CB-CG	8.69	121.29	112.60
2	j	90	ILE	CA-C-O	-8.68	110.87	120.25
1	C	208	ASN	CA-CB-CG	8.68	121.28	112.60
1	d	177	LYS	CA-C-O	-8.66	109.48	120.31
1	g	154	GLY	O-C-N	-8.65	112.87	122.47
1	E	40	ILE	N-CA-C	-8.63	95.57	108.17
2	k	112	ILE	N-CA-C	-8.63	96.03	108.11
3	J	151	GLU	CA-C-N	8.63	131.84	120.28
3	J	151	GLU	C-N-CA	8.63	131.84	120.28
1	A	31	VAL	CA-C-N	8.62	133.41	120.31
1	A	31	VAL	C-N-CA	8.62	133.41	120.31
2	m	51	ARG	NE-CZ-NH2	8.62	126.95	119.20
3	K	279	GLY	N-CA-C	-8.60	100.45	111.72
3	H	259	ARG	CA-C-O	8.59	129.85	119.97
3	M	324	HIS	CA-C-N	8.59	131.79	120.28
3	M	324	HIS	C-N-CA	8.59	131.79	120.28
1	A	7	GLY	N-CA-C	-8.59	102.09	112.48
2	6	35	ASN	CA-CB-CG	-8.59	104.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	195	VAL	CA-C-N	8.57	132.62	120.28
3	H	195	VAL	C-N-CA	8.57	132.62	120.28
1	c	33	ARG	NE-CZ-NH2	8.57	126.91	119.20
1	d	200	ILE	N-CA-C	-8.56	104.35	112.83
1	c	241	ARG	NE-CZ-NH1	-8.56	112.94	121.50
2	m	156	THR	O-C-N	-8.55	116.24	121.71
3	L	294	ASP	N-CA-C	-8.55	97.02	110.10
1	b	106	PRO	CA-C-N	8.54	131.94	120.50
1	b	106	PRO	C-N-CA	8.54	131.94	120.50
2	h	140	THR	CA-CB-OG1	8.53	122.39	109.60
2	l	50	ASP	O-C-N	8.52	131.15	122.12
3	K	147	ASP	N-CA-C	8.52	120.18	111.07
1	c	57	LYS	N-CA-C	-8.51	102.45	112.92
3	I	12	LYS	N-CA-C	8.51	120.18	111.07
2	5	30	ARG	NE-CZ-NH2	8.51	126.86	119.20
2	i	102	ARG	N-CA-C	-8.50	102.92	113.38
1	F	108	THR	CA-C-O	8.50	131.73	121.87
1	D	21	LEU	N-CA-C	-8.49	90.62	107.69
3	H	391	ASP	CA-CB-CG	8.49	121.09	112.60
3	J	124	ASP	CA-C-N	8.49	129.32	119.47
3	J	124	ASP	C-N-CA	8.49	129.32	119.47
2	2	109	GLN	OE1-CD-NE2	8.48	131.08	122.60
2	3	62	ASP	CA-CB-CG	-8.48	104.12	112.60
3	L	244	ASP	CA-CB-CG	8.48	121.08	112.60
3	H	211	PHE	CA-CB-CG	-8.47	105.33	113.80
2	h	75	ASN	N-CA-C	-8.47	102.13	111.36
1	e	63	THR	N-CA-C	-8.46	103.55	114.04
2	j	156	THR	N-CA-C	-8.46	98.44	108.25
1	D	64	ILE	CA-C-N	8.44	136.89	121.70
1	D	64	ILE	C-N-CA	8.44	136.89	121.70
3	K	101	LYS	N-CA-C	-8.44	100.53	108.13
1	D	239	ARG	NE-CZ-NH2	-8.43	111.61	119.20
1	E	188	ALA	N-CA-C	8.43	120.55	111.36
2	3	21	ASP	CA-CB-CG	8.43	121.03	112.60
1	E	161	ALA	N-CA-C	-8.43	95.44	108.76
2	5	139	ALA	N-CA-C	-8.43	96.52	109.24
2	2	149	GLY	CA-C-N	8.42	132.00	120.46
2	2	149	GLY	C-N-CA	8.42	132.00	120.46
3	L	260	GLU	O-C-N	8.42	131.04	122.12
2	4	112	ILE	N-CA-C	-8.41	96.33	108.53
1	c	16	SER	CA-C-N	8.41	130.35	119.84
1	c	16	SER	C-N-CA	8.41	130.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	ALA	CA-C-N	8.41	134.14	120.94
1	D	50	ALA	C-N-CA	8.41	134.14	120.94
2	1	131	ALA	CB-CA-C	-8.40	96.21	110.16
2	n	116	ASP	N-CA-CB	8.40	124.52	111.24
2	2	91	ALA	N-CA-C	8.40	120.43	111.28
1	E	245	LYS	N-CA-C	-8.39	100.62	113.89
3	L	227	PHE	CA-CB-CG	-8.39	105.41	113.80
1	E	245	LYS	N-CA-CB	8.39	123.03	110.95
3	K	36	PHE	CA-C-N	8.39	131.95	120.46
3	K	36	PHE	C-N-CA	8.39	131.95	120.46
3	M	133	GLU	CA-C-N	8.39	133.04	121.05
3	M	133	GLU	C-N-CA	8.39	133.04	121.05
1	F	97	GLN	OE1-CD-NE2	8.38	130.98	122.60
1	B	214	VAL	N-CA-C	-8.37	95.38	107.77
2	j	129	GLY	CA-C-N	8.37	133.58	121.44
2	j	129	GLY	C-N-CA	8.37	133.58	121.44
1	F	12	ILE	CA-C-N	8.37	131.50	120.28
1	F	12	ILE	C-N-CA	8.37	131.50	120.28
1	g	56	SER	CA-C-N	8.36	131.48	120.28
1	g	56	SER	C-N-CA	8.36	131.48	120.28
2	k	65	PHE	CA-CB-CG	-8.36	105.44	113.80
2	l	15	VAL	CA-C-O	-8.34	112.91	121.67
1	D	95	GLU	CA-C-N	8.34	131.28	120.44
1	D	95	GLU	C-N-CA	8.34	131.28	120.44
1	c	144	VAL	CA-C-N	8.34	128.40	119.90
1	c	144	VAL	C-N-CA	8.34	128.40	119.90
3	H	331	ALA	CA-C-N	8.33	135.66	122.83
3	H	331	ALA	C-N-CA	8.33	135.66	122.83
3	K	168	ALA	CA-C-N	8.33	131.44	120.28
3	K	168	ALA	C-N-CA	8.33	131.44	120.28
1	E	10	ARG	N-CA-C	-8.31	103.16	113.38
1	G	72	GLU	N-CA-C	-8.30	103.25	112.72
3	J	228	GLN	CA-C-N	8.29	131.39	120.28
3	J	228	GLN	C-N-CA	8.29	131.39	120.28
1	a	46	VAL	CA-C-O	8.29	129.51	120.64
3	K	391	ASP	CA-CB-CG	8.27	120.87	112.60
2	l	203	GLU	N-CA-C	8.27	121.41	111.82
2	4	209	ALA	N-CA-C	-8.27	102.51	112.59
1	a	185	PHE	CA-CB-CG	-8.26	105.54	113.80
3	J	281	VAL	CA-C-N	8.26	136.56	121.70
3	J	281	VAL	C-N-CA	8.26	136.56	121.70
3	K	269	LEU	CA-C-N	8.25	131.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	269	LEU	C-N-CA	8.25	131.17	120.44
3	I	123	LYS	CA-C-N	8.25	136.55	121.70
3	I	123	LYS	C-N-CA	8.25	136.55	121.70
1	D	103	TYR	CB-CG-CD2	8.25	133.17	120.80
1	C	90	ASP	CA-C-N	8.24	131.15	120.44
1	C	90	ASP	C-N-CA	8.24	131.15	120.44
2	5	127	PRO	CA-C-N	8.24	133.98	122.28
2	5	127	PRO	C-N-CA	8.24	133.98	122.28
3	H	167	PHE	CA-CB-CG	-8.22	105.58	113.80
1	C	82	VAL	O-C-N	8.21	129.84	121.87
1	F	185	PHE	N-CA-C	8.22	119.86	111.07
3	L	24	ARG	CA-C-N	8.21	132.80	120.31
3	L	24	ARG	C-N-CA	8.21	132.80	120.31
3	L	10	LEU	O-C-N	8.20	130.81	122.12
1	a	29	GLU	CA-C-N	8.20	131.27	120.28
1	a	29	GLU	C-N-CA	8.20	131.27	120.28
2	n	55	THR	N-CA-C	-8.19	96.56	109.50
2	7	58	GLY	N-CA-C	-8.19	99.81	110.29
2	n	117	SER	CA-C-N	8.19	132.76	120.31
2	n	117	SER	C-N-CA	8.19	132.76	120.31
1	c	225	SER	CA-C-N	8.19	128.97	119.47
1	c	225	SER	C-N-CA	8.19	128.97	119.47
1	a	203	GLU	N-CA-C	-8.18	98.73	110.59
1	E	12	ILE	N-CA-C	-8.17	104.74	112.83
1	B	166	MET	CA-C-O	8.16	129.36	119.97
3	I	101	LYS	CA-C-N	8.16	128.66	119.93
3	I	101	LYS	C-N-CA	8.16	128.66	119.93
2	i	80	ARG	NE-CZ-NH2	8.16	126.54	119.20
2	i	131	ALA	CA-C-O	8.15	129.03	120.30
2	j	45	ILE	CB-CA-C	8.15	120.42	110.73
1	a	32	LYS	CA-C-N	8.14	131.85	120.29
1	a	32	LYS	C-N-CA	8.14	131.85	120.29
2	n	184	ASP	CA-CB-CG	8.13	120.73	112.60
2	2	124	SER	N-CA-C	-8.12	96.51	109.59
1	f	79	SER	N-CA-C	-8.12	96.24	108.99
2	6	194	ASP	N-CA-C	-8.11	102.63	114.39
3	K	210	GLU	N-CA-C	-8.11	103.18	113.72
2	j	195	GLU	CB-CG-CD	-8.10	98.83	112.60
1	d	197	GLY	O-C-N	8.10	129.96	122.19
2	h	212	ARG	N-CA-C	-8.09	103.35	113.55
3	K	142	ASP	N-CA-C	-8.09	102.97	112.92
3	K	314	PHE	O-C-N	8.09	130.41	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	105	ARG	N-CA-C	-8.09	98.31	110.28
2	1	134	GLU	CA-C-N	8.09	131.12	120.28
2	1	134	GLU	C-N-CA	8.09	131.12	120.28
1	C	225	SER	CA-C-O	-8.09	111.55	120.69
1	g	214	VAL	N-CA-CB	8.09	122.45	112.10
1	E	226	PRO	CA-C-N	8.08	131.11	120.28
1	E	226	PRO	C-N-CA	8.08	131.11	120.28
3	H	174	PRO	CA-C-N	8.08	129.94	119.84
3	H	174	PRO	C-N-CA	8.08	129.94	119.84
1	F	37	ALA	N-CA-CB	8.07	125.74	111.13
3	H	304	ASP	CA-CB-CG	8.07	120.67	112.60
1	b	212	GLY	O-C-N	8.06	130.30	123.29
2	h	85	PRO	N-CA-C	8.05	129.06	112.47
2	6	175	ALA	CA-C-N	8.05	131.07	120.28
2	6	175	ALA	C-N-CA	8.05	131.07	120.28
3	I	207	VAL	N-CA-C	-8.05	97.72	108.35
2	1	99	ASN	CA-CB-CG	-8.05	104.55	112.60
1	a	38	ILE	CA-C-N	8.04	127.12	121.65
1	a	38	ILE	C-N-CA	8.04	127.12	121.65
2	m	83	ARG	NE-CZ-NH2	8.04	126.44	119.20
2	j	27	THR	CA-C-O	-8.04	112.85	121.45
3	K	101	LYS	CA-C-O	-8.04	113.22	120.13
3	M	31	GLU	CA-C-N	8.04	131.05	120.28
3	M	31	GLU	C-N-CA	8.04	131.05	120.28
2	2	180	SER	N-CA-C	-8.04	103.50	113.38
3	M	370	VAL	N-CA-C	-8.03	96.88	108.53
3	H	275	PHE	CA-CB-CG	-8.03	105.77	113.80
1	e	198	LEU	CA-C-N	8.03	131.03	120.28
1	e	198	LEU	C-N-CA	8.03	131.03	120.28
2	7	126	ASP	CA-CB-CG	8.03	120.63	112.60
1	G	39	GLY	O-C-N	-8.02	116.42	123.80
3	J	46	ARG	NE-CZ-NH2	-8.02	111.98	119.20
1	f	169	ASN	CA-CB-CG	-8.01	104.59	112.60
2	3	154	ARG	O-C-N	-8.00	112.75	122.34
2	3	107	LEU	CA-C-N	7.99	132.41	120.75
2	3	107	LEU	C-N-CA	7.99	132.41	120.75
2	5	166	GLU	N-CA-C	-7.99	102.66	111.36
3	M	190	LEU	CA-C-N	7.99	130.98	120.28
3	M	190	LEU	C-N-CA	7.99	130.98	120.28
1	e	212	GLY	N-CA-C	-7.98	98.89	111.18
1	a	230	LYS	N-CA-C	7.98	123.62	113.25
2	7	148	TYR	CA-C-N	7.98	128.79	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	148	TYR	C-N-CA	7.98	128.79	119.94
3	I	255	THR	N-CA-C	-7.97	97.07	108.07
3	L	71	ILE	N-CA-C	-7.97	96.59	108.46
1	F	169	ASN	CA-CB-CG	-7.96	104.64	112.60
2	1	180	SER	N-CA-C	-7.96	102.61	112.88
1	g	131	PRO	CA-C-O	-7.96	111.89	122.08
2	n	30	ARG	NE-CZ-NH2	7.96	126.36	119.20
3	H	14	LYS	CA-C-N	7.96	130.79	120.44
3	H	14	LYS	C-N-CA	7.96	130.79	120.44
1	A	92	ALA	CA-C-N	7.96	130.94	120.28
1	A	92	ALA	C-N-CA	7.96	130.94	120.28
2	5	170	ARG	NE-CZ-NH1	7.96	129.46	121.50
2	n	202	GLU	N-CA-C	7.95	120.65	111.11
1	c	104	ASP	CA-CB-CG	-7.92	104.68	112.60
3	H	209	SER	N-CA-C	-7.92	102.44	114.16
2	m	45	ILE	CA-C-O	7.92	128.70	120.39
2	2	27	THR	N-CA-C	-7.92	97.29	109.24
3	I	337	LYS	CA-C-N	7.92	131.53	120.29
3	I	337	LYS	C-N-CA	7.92	131.53	120.29
2	h	104	PHE	CB-CA-C	7.91	119.04	109.31
2	6	139	ALA	CA-C-N	7.91	135.94	121.70
2	6	139	ALA	C-N-CA	7.91	135.94	121.70
1	E	235	ARG	CA-C-N	7.91	131.52	120.29
1	E	235	ARG	C-N-CA	7.91	131.52	120.29
1	d	102	THR	O-C-N	-7.90	112.46	122.34
1	c	239	ARG	CA-C-O	-7.90	112.05	120.42
2	7	194	ASP	N-CA-C	-7.90	104.80	114.75
3	J	57	ARG	N-CA-C	7.89	119.52	111.07
3	I	9	LEU	CA-C-N	7.89	130.85	120.28
3	I	9	LEU	C-N-CA	7.89	130.85	120.28
3	M	336	PHE	CA-CB-CG	-7.89	105.91	113.80
1	E	50	ALA	CA-C-N	7.88	132.69	121.02
1	E	50	ALA	C-N-CA	7.88	132.69	121.02
1	F	37	ALA	N-CA-C	-7.88	95.27	108.75
1	c	154	GLY	N-CA-C	-7.88	103.09	116.01
2	h	171	ALA	N-CA-C	7.87	119.49	111.07
2	j	148	TYR	CA-C-N	7.87	128.67	119.94
2	j	148	TYR	C-N-CA	7.87	128.67	119.94
3	M	374	ASP	CA-CB-CG	-7.87	104.73	112.60
1	c	191	LEU	N-CA-C	7.87	119.85	111.28
1	C	87	VAL	CA-C-O	7.86	129.12	120.95
2	4	184	ASP	CA-CB-CG	-7.86	104.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	64	GLN	N-CA-C	7.86	119.62	111.14
3	L	155	GLU	N-CA-C	7.85	120.74	111.71
2	i	91	ALA	CA-C-O	-7.84	112.58	120.82
2	4	46	TYR	N-CA-CB	7.84	123.55	110.77
2	m	170	ARG	NE-CZ-NH2	7.84	126.26	119.20
1	e	124	THR	CA-C-N	7.83	132.22	120.31
1	e	124	THR	C-N-CA	7.83	132.22	120.31
3	L	76	ARG	NE-CZ-NH2	-7.83	112.15	119.20
3	H	212	VAL	N-CA-CB	7.83	124.14	111.23
1	a	236	ALA	CA-C-O	-7.83	112.25	120.55
1	A	242	GLU	CA-C-N	7.82	130.76	120.28
1	A	242	GLU	C-N-CA	7.82	130.76	120.28
1	b	129	VAL	N-CA-C	-7.82	97.24	108.42
1	d	245	LYS	N-CA-C	-7.81	104.64	114.56
1	g	122	GLN	N-CA-CB	7.81	121.60	110.12
1	e	56	SER	N-CA-CB	7.81	122.16	110.29
3	L	28	ARG	N-CA-CB	7.81	121.59	110.12
2	j	168	ALA	CA-C-N	7.80	130.55	120.56
2	j	168	ALA	C-N-CA	7.80	130.55	120.56
3	I	105	ARG	O-C-N	-7.80	113.45	122.97
1	D	97	GLN	CA-C-N	7.80	131.50	120.42
1	D	97	GLN	C-N-CA	7.80	131.50	120.42
3	M	384	LYS	CA-C-N	7.80	130.73	120.28
3	M	384	LYS	C-N-CA	7.80	130.73	120.28
2	j	144	SER	N-CA-C	7.80	121.73	111.75
1	B	18	ASP	CA-CB-CG	-7.80	104.80	112.60
1	e	141	VAL	N-CA-C	-7.79	96.79	108.17
1	G	56	SER	N-CA-C	-7.79	101.27	108.75
1	e	25	GLU	O-C-N	7.79	131.03	122.15
3	M	197	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	243	LEU	N-CA-C	7.78	119.77	111.28
2	l	63	ALA	CA-C-O	7.78	128.67	120.42
1	B	186	ASP	CA-C-N	7.78	131.34	120.29
1	B	186	ASP	C-N-CA	7.78	131.34	120.29
1	d	16	SER	CB-CA-C	7.78	119.49	108.68
2	m	181	ALA	N-CA-C	-7.78	104.02	113.97
1	B	186	ASP	CA-CB-CG	-7.78	104.83	112.60
1	d	118	ASP	O-C-N	7.77	131.01	122.15
3	J	10	LEU	CA-C-N	7.77	130.70	120.28
3	J	10	LEU	C-N-CA	7.77	130.70	120.28
1	F	67	ILE	N-CA-CB	7.77	119.19	110.72
1	E	196	MET	N-CA-C	7.77	119.83	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	ALA	CA-C-N	7.76	131.74	120.71
1	E	35	ALA	C-N-CA	7.76	131.74	120.71
3	H	120	PRO	CA-C-N	7.76	130.68	120.28
3	H	120	PRO	C-N-CA	7.76	130.68	120.28
3	J	197	ASN	CA-CB-CG	7.76	120.36	112.60
1	b	98	ILE	CA-C-O	-7.75	112.64	120.85
1	D	67	ILE	CB-CA-C	-7.75	103.85	112.68
1	d	106	PRO	CA-C-N	7.75	131.12	120.35
1	d	106	PRO	C-N-CA	7.75	131.12	120.35
1	D	245	LYS	O-C-N	7.74	131.63	122.34
2	m	212	ARG	NE-CZ-NH1	7.74	129.24	121.50
2	j	109	GLN	N-CA-C	-7.73	96.62	109.07
1	b	230	LYS	O-C-N	-7.73	112.43	121.32
1	b	67	ILE	O-C-N	7.73	131.55	123.20
3	I	22	LYS	CA-C-N	7.73	131.41	120.28
3	I	22	LYS	C-N-CA	7.73	131.41	120.28
3	J	147	ASP	N-CA-C	7.73	120.68	111.33
1	a	105	GLU	CA-C-O	-7.73	112.44	119.86
1	D	143	GLU	N-CA-C	-7.72	102.73	114.16
3	H	229	LEU	CA-C-N	7.71	130.62	120.28
3	H	229	LEU	C-N-CA	7.71	130.62	120.28
1	F	194	VAL	CA-C-N	7.71	131.24	120.29
1	F	194	VAL	C-N-CA	7.71	131.24	120.29
3	H	69	SER	CA-C-N	7.71	134.51	121.87
3	H	69	SER	C-N-CA	7.71	134.51	121.87
3	J	125	PRO	CA-C-N	7.70	131.37	120.28
3	J	125	PRO	C-N-CA	7.70	131.37	120.28
2	5	134	GLU	CA-C-N	7.70	131.49	120.79
2	5	134	GLU	C-N-CA	7.70	131.49	120.79
1	C	23	GLN	OE1-CD-NE2	7.70	130.30	122.60
1	d	33	ARG	N-CA-C	-7.70	104.03	113.50
3	H	56	GLU	CA-C-N	7.69	130.59	120.28
3	H	56	GLU	C-N-CA	7.69	130.59	120.28
1	f	179	TYR	N-CA-C	-7.69	94.43	110.80
3	J	395	VAL	CA-C-N	7.69	130.58	120.28
3	J	395	VAL	C-N-CA	7.69	130.58	120.28
1	F	160	LYS	N-CA-C	-7.68	103.25	114.39
3	I	188	LYS	CA-C-N	7.68	130.43	120.44
3	I	188	LYS	C-N-CA	7.68	130.43	120.44
3	I	383	LEU	O-C-N	-7.66	114.00	122.12
1	B	61	ALA	CA-C-N	7.65	135.26	122.79
1	B	61	ALA	C-N-CA	7.65	135.26	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	64	LEU	O-C-N	-7.65	114.09	123.04
1	f	66	LYS	N-CA-C	-7.65	102.14	113.61
3	I	157	VAL	CB-CA-C	-7.65	103.44	110.63
2	n	17	LEU	O-C-N	-7.64	114.69	123.33
2	4	61	GLY	CA-C-N	7.64	130.37	120.44
2	4	61	GLY	C-N-CA	7.64	130.37	120.44
3	M	258	ASP	CA-CB-CG	-7.64	104.96	112.60
3	I	281	VAL	CA-C-N	7.63	135.44	121.70
3	I	281	VAL	C-N-CA	7.63	135.44	121.70
2	m	96	ASN	CA-C-N	7.63	131.12	120.29
2	m	96	ASN	C-N-CA	7.63	131.12	120.29
3	H	144	GLY	CA-C-N	7.63	131.50	122.19
3	H	144	GLY	C-N-CA	7.63	131.50	122.19
1	G	40	ILE	O-C-N	-7.62	115.25	123.18
1	B	225	SER	CA-C-O	-7.62	112.65	120.96
2	5	158	GLU	CA-C-N	7.61	131.33	120.98
2	5	158	GLU	C-N-CA	7.61	131.33	120.98
3	J	391	ASP	CA-CB-CG	-7.61	104.99	112.60
1	B	172	THR	N-CA-C	-7.61	102.93	111.14
1	g	64	ILE	CA-C-N	7.61	131.67	120.87
1	g	64	ILE	C-N-CA	7.61	131.67	120.87
2	k	50	ASP	CA-CB-CG	7.60	120.20	112.60
3	I	222	LEU	N-CA-C	7.60	119.57	111.28
3	I	97	GLU	N-CA-C	-7.59	103.61	113.17
2	m	87	VAL	CA-C-O	-7.59	112.27	120.47
1	D	173	GLU	CA-C-N	7.59	130.30	120.44
1	D	173	GLU	C-N-CA	7.59	130.30	120.44
2	i	200	SER	CA-C-N	7.59	129.32	119.84
2	i	200	SER	C-N-CA	7.59	129.32	119.84
2	1	55	THR	CA-CB-OG1	7.58	120.98	109.60
2	5	96	ASN	N-CA-CB	7.58	121.00	110.01
3	M	64	LEU	O-C-N	-7.58	114.58	123.22
2	i	211	PHE	N-CA-C	-7.58	102.97	112.90
1	d	155	ALA	CA-C-O	7.57	129.21	120.80
3	H	281	VAL	CA-C-N	7.57	135.33	121.70
3	H	281	VAL	C-N-CA	7.57	135.33	121.70
1	A	42	CYS	N-CA-C	-7.57	98.19	108.86
1	d	97	GLN	OE1-CD-NE2	7.57	130.17	122.60
1	G	20	ARG	N-CA-C	-7.57	101.12	110.65
3	M	382	VAL	CA-C-O	-7.56	112.83	120.85
3	H	108	LEU	CA-C-N	7.56	133.94	121.39
3	H	108	LEU	C-N-CA	7.56	133.94	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	322	LYS	N-CA-C	7.56	119.52	111.28
1	B	52	LYS	N-CA-C	-7.55	101.59	111.71
3	L	201	ALA	CA-C-N	7.55	135.97	121.54
3	L	201	ALA	C-N-CA	7.55	135.97	121.54
3	M	109	ASN	CA-CB-CG	-7.55	105.05	112.60
1	G	238	GLU	O-C-N	7.55	130.12	122.12
1	d	142	ASP	N-CA-C	-7.54	104.60	113.88
1	g	196	MET	CA-C-N	7.54	128.52	119.99
1	g	196	MET	C-N-CA	7.54	128.52	119.99
1	B	224	VAL	CA-C-O	-7.54	112.14	121.11
1	G	153	SER	CA-C-O	7.54	128.68	119.79
3	I	350	ASP	CA-CB-CG	-7.54	105.06	112.60
2	3	137	ILE	CA-C-O	-7.53	111.45	121.02
2	l	170	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	d	173	GLU	CA-C-N	7.53	130.68	120.44
1	d	173	GLU	C-N-CA	7.53	130.68	120.44
2	m	170	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	d	225	SER	CA-C-N	7.52	129.24	119.84
1	d	225	SER	C-N-CA	7.52	129.24	119.84
1	A	118	ASP	CA-CB-CG	-7.52	105.08	112.60
1	A	172	THR	CA-C-N	7.52	130.35	120.28
1	A	172	THR	C-N-CA	7.52	130.35	120.28
1	D	71	ASP	CA-CB-CG	7.52	120.12	112.60
2	7	155	PHE	CA-CB-CG	-7.52	106.28	113.80
2	k	198	GLN	CA-C-N	7.51	130.66	120.44
2	k	198	GLN	C-N-CA	7.51	130.66	120.44
3	J	102	PRO	N-CA-CB	7.51	111.14	103.25
1	c	91	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	c	100	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	C	68	TYR	N-CA-C	-7.50	95.92	108.75
1	f	197	GLY	CA-C-N	7.50	130.94	120.29
1	f	197	GLY	C-N-CA	7.50	130.94	120.29
3	L	166	LEU	CA-C-N	7.50	130.93	120.29
3	L	166	LEU	C-N-CA	7.50	130.93	120.29
3	H	40	GLU	CA-C-N	7.49	130.18	120.44
3	H	40	GLU	C-N-CA	7.49	130.18	120.44
1	a	60	GLU	N-CA-C	-7.49	98.30	108.86
3	I	351	ILE	CA-C-N	7.49	130.32	120.28
3	I	351	ILE	C-N-CA	7.49	130.32	120.28
2	k	140	THR	N-CA-CB	7.49	124.23	111.50
2	l	115	ILE	N-CA-C	-7.49	97.70	108.48
2	5	200	SER	CA-C-N	7.49	129.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	200	SER	C-N-CA	7.49	129.20	119.84
1	C	28	ARG	N-CA-C	-7.48	104.17	113.38
1	D	202	SER	CA-C-N	7.48	132.69	120.94
1	D	202	SER	C-N-CA	7.48	132.69	120.94
3	M	267	GLN	O-C-N	7.48	130.05	122.12
2	4	87	VAL	N-CA-CB	7.48	121.80	110.58
1	D	106	PRO	N-CA-CB	7.47	109.91	103.19
1	E	198	LEU	CA-C-N	7.47	130.90	120.29
1	E	198	LEU	C-N-CA	7.47	130.90	120.29
2	l	83	ARG	CA-C-O	7.47	129.22	121.23
1	C	194	VAL	N-CA-CB	7.46	119.27	110.55
2	1	82	GLU	N-CA-CB	7.46	123.80	112.47
3	H	98	GLU	N-CA-C	-7.45	104.19	113.28
3	M	378	ALA	O-C-N	7.45	130.01	122.12
1	b	52	LYS	CA-C-N	7.44	131.99	120.75
1	b	52	LYS	C-N-CA	7.44	131.99	120.75
2	5	123	TYR	CA-C-O	7.44	128.74	120.70
3	H	336	PHE	CA-C-N	7.44	130.85	120.29
3	H	336	PHE	C-N-CA	7.44	130.85	120.29
2	1	104	PHE	CA-C-O	-7.44	113.10	121.28
2	3	167	LEU	CA-C-N	7.44	130.24	120.28
2	3	167	LEU	C-N-CA	7.44	130.24	120.28
1	g	99	ASN	CA-CB-CG	7.43	120.03	112.60
2	j	112	ILE	CA-C-O	-7.43	112.59	120.39
2	4	116	ASP	N-CA-C	-7.43	98.48	108.74
2	m	148	TYR	CA-C-N	7.43	128.39	119.99
2	m	148	TYR	C-N-CA	7.43	128.39	119.99
3	I	79	VAL	CA-C-N	7.42	132.29	122.42
3	I	79	VAL	C-N-CA	7.42	132.29	122.42
3	M	39	SER	CA-C-N	7.42	130.83	120.29
3	M	39	SER	C-N-CA	7.42	130.83	120.29
1	e	174	PHE	CA-CB-CG	-7.42	106.38	113.80
1	C	104	ASP	CA-CB-CG	7.42	120.02	112.60
3	L	112	THR	N-CA-C	-7.42	104.08	113.43
1	a	62	ASP	CA-CB-CG	7.42	120.02	112.60
1	d	199	SER	N-CA-C	7.41	119.44	111.36
1	g	47	ILE	O-C-N	-7.41	115.25	123.03
3	M	38	GLU	CA-C-N	7.41	130.82	120.29
3	M	38	GLU	C-N-CA	7.41	130.82	120.29
3	L	242	GLU	N-CA-C	-7.41	95.01	110.80
2	h	33	MET	N-CA-C	-7.40	97.37	108.99
3	M	75	GLY	N-CA-C	-7.40	105.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	212	GLY	N-CA-C	-7.40	99.78	111.18
3	K	129	GLY	CA-C-N	7.40	132.33	121.31
3	K	129	GLY	C-N-CA	7.40	132.33	121.31
3	J	268	LEU	CA-C-N	7.40	130.19	120.28
3	J	268	LEU	C-N-CA	7.40	130.19	120.28
1	b	210	GLU	N-CA-C	-7.39	97.35	109.40
3	K	109	ASN	CA-CB-CG	7.39	119.99	112.60
1	C	212	GLY	N-CA-C	-7.39	99.33	111.38
1	B	170	ALA	CA-C-N	7.39	133.00	120.29
1	B	170	ALA	C-N-CA	7.39	133.00	120.29
3	L	387	THR	N-CA-CB	7.38	123.52	110.37
3	I	301	GLY	N-CA-C	-7.37	105.09	114.37
1	c	70	ILE	N-CA-C	-7.37	104.80	113.42
1	e	224	VAL	O-C-N	7.36	130.42	122.76
3	H	225	GLU	CA-C-N	7.36	130.09	120.60
3	H	225	GLU	C-N-CA	7.36	130.09	120.60
1	E	60	GLU	N-CA-C	7.36	120.07	110.43
3	M	150	ILE	CA-C-N	7.36	130.74	120.29
3	M	150	ILE	C-N-CA	7.36	130.74	120.29
1	C	58	LEU	N-CA-C	-7.36	104.45	113.50
2	5	207	ILE	N-CA-C	-7.35	103.29	110.72
2	2	151	LEU	CA-C-N	7.35	133.00	120.72
2	2	151	LEU	C-N-CA	7.35	133.00	120.72
2	2	102	ARG	N-CA-C	-7.35	103.91	113.17
3	J	18	GLU	CA-C-O	-7.35	112.76	120.55
3	K	82	SER	O-C-N	7.34	132.27	122.43
3	J	80	LYS	N-CA-CB	7.34	122.51	110.17
2	7	201	PRO	CA-C-N	7.34	129.98	120.44
2	7	201	PRO	C-N-CA	7.34	129.98	120.44
1	D	217	ASP	N-CA-CB	7.34	121.66	110.44
1	A	208	ASN	CA-CB-CG	-7.33	105.27	112.60
1	C	205	VAL	CA-C-O	-7.33	114.96	119.51
1	C	245	LYS	N-CA-C	-7.33	103.30	112.90
1	e	165	GLY	O-C-N	-7.33	116.60	122.90
3	H	119	LEU	N-CA-C	-7.33	99.92	110.40
1	d	135	SER	N-CA-C	-7.32	98.17	109.52
2	1	71	LYS	CA-C-N	7.32	130.49	120.46
2	1	71	LYS	C-N-CA	7.32	130.49	120.46
3	L	95	ILE	N-CA-CB	7.32	119.77	111.21
3	J	254	ASP	N-CA-C	-7.32	96.69	108.55
2	6	90	ILE	N-CA-C	-7.31	103.33	110.72
2	k	211	PHE	CA-CB-CG	-7.31	106.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	GLU	CA-C-O	7.31	128.30	120.55
2	j	148	TYR	CA-C-O	7.31	128.29	120.55
2	k	172	ILE	CA-C-O	7.31	128.42	119.58
3	I	223	VAL	CA-C-N	7.30	130.06	120.28
3	I	223	VAL	C-N-CA	7.30	130.06	120.28
3	K	331	ALA	O-C-N	-7.30	114.80	123.27
1	G	71	ASP	N-CA-C	-7.30	99.25	108.45
3	L	309	VAL	N-CA-C	-7.29	100.33	107.55
1	a	70	ILE	N-CA-C	-7.29	105.54	111.81
1	b	94	ILE	CA-C-O	7.29	128.58	120.85
1	G	193	LEU	N-CA-C	-7.29	102.72	111.69
2	h	136	ASP	CA-C-N	7.29	131.34	120.69
2	h	136	ASP	C-N-CA	7.29	131.34	120.69
1	A	189	MET	CG-SD-CE	-7.29	84.86	100.90
2	m	47	GLN	N-CA-CB	7.29	122.40	110.37
1	C	194	VAL	O-C-N	7.28	129.05	121.91
1	A	190	VAL	O-C-N	-7.28	114.33	121.83
1	c	20	ARG	CA-C-N	7.28	132.16	121.31
1	c	20	ARG	C-N-CA	7.28	132.16	121.31
2	j	47	GLN	OE1-CD-NE2	7.28	129.88	122.60
2	3	204	VAL	CA-C-O	-7.28	112.61	120.47
1	G	31	VAL	CA-C-N	7.27	130.03	120.28
1	G	31	VAL	C-N-CA	7.27	130.03	120.28
3	L	389	ILE	CA-C-O	-7.27	110.20	119.95
2	h	122	ILE	N-CA-C	-7.27	97.63	108.46
2	6	79	ILE	O-C-N	-7.26	114.35	121.90
1	B	104	ASP	N-CA-CB	7.26	122.94	111.91
3	M	125	PRO	CA-C-N	7.26	130.01	120.28
3	M	125	PRO	C-N-CA	7.26	130.01	120.28
1	D	79	SER	N-CA-C	-7.25	96.34	108.75
2	3	187	ASP	CA-CB-CG	7.25	119.86	112.60
1	b	90	ASP	CA-C-N	7.25	130.00	120.28
1	b	90	ASP	C-N-CA	7.25	130.00	120.28
3	M	109	ASN	OD1-CG-ND2	-7.25	115.35	122.60
2	h	37	ILE	O-C-N	-7.25	114.69	122.95
2	m	17	LEU	N-CA-CB	7.25	123.82	110.99
2	1	80	ARG	CD-NE-CZ	-7.24	114.26	124.40
3	K	211	PHE	CA-C-N	7.24	135.01	121.97
3	K	211	PHE	C-N-CA	7.24	135.01	121.97
2	n	17	LEU	CA-C-O	7.24	129.10	120.99
1	c	30	ALA	CB-CA-C	-7.24	99.00	110.94
2	h	30	ARG	NE-CZ-NH2	7.24	125.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	VAL	O-C-N	-7.23	116.68	122.97
1	b	88	LEU	N-CA-C	7.23	119.16	111.28
2	h	60	VAL	CB-CA-C	-7.23	102.55	112.02
2	h	170	ARG	NE-CZ-NH1	-7.23	114.27	121.50
3	J	363	ILE	O-C-N	7.23	128.88	121.87
2	m	29	LYS	N-CA-C	-7.23	101.63	110.88
2	7	132	ILE	CA-C-N	7.23	135.35	121.54
2	7	132	ILE	C-N-CA	7.23	135.35	121.54
3	K	294	ASP	CA-CB-CG	7.23	119.83	112.60
2	h	144	SER	N-CA-C	7.23	119.16	111.28
1	D	114	LYS	CA-C-O	7.22	128.41	120.82
1	G	68	TYR	CA-C-N	7.22	131.06	120.95
1	G	68	TYR	C-N-CA	7.22	131.06	120.95
2	1	149	GLY	CA-C-N	7.22	130.72	120.53
2	1	149	GLY	C-N-CA	7.22	130.72	120.53
3	K	95	ILE	O-C-N	-7.22	115.46	123.26
3	I	363	ILE	CA-C-N	7.22	129.95	120.28
3	I	363	ILE	C-N-CA	7.22	129.95	120.28
2	3	156	THR	N-CA-C	-7.21	99.84	108.14
1	C	146	LYS	N-CA-C	-7.21	98.05	109.23
2	h	88	ARG	NE-CZ-NH1	-7.21	114.29	121.50
3	L	82	SER	CA-C-N	7.21	129.81	120.44
3	L	82	SER	C-N-CA	7.21	129.81	120.44
3	M	223	VAL	CA-C-N	7.21	129.93	120.28
3	M	223	VAL	C-N-CA	7.21	129.93	120.28
3	J	149	GLN	OE1-CD-NE2	7.20	129.80	122.60
3	M	95	ILE	N-CA-C	-7.19	97.26	107.75
2	k	194	ASP	CB-CA-C	-7.19	96.12	110.42
1	G	135	SER	CA-C-O	-7.18	113.06	121.46
3	J	283	VAL	N-CA-CB	7.18	122.62	111.99
1	a	10	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	d	100	ARG	NE-CZ-NH1	-7.18	114.32	121.50
2	4	190	LYS	N-CA-C	-7.17	97.20	108.90
3	J	182	GLY	CA-C-N	7.17	127.77	120.38
3	J	182	GLY	C-N-CA	7.17	127.77	120.38
2	j	172	ILE	CA-C-N	7.17	130.60	120.28
2	j	172	ILE	C-N-CA	7.17	130.60	120.28
1	B	125	GLN	CA-C-N	7.17	130.93	120.82
1	B	125	GLN	C-N-CA	7.17	130.93	120.82
3	J	64	LEU	CA-C-O	7.17	128.86	120.69
1	D	165	GLY	CA-C-N	7.16	129.88	120.28
1	D	165	GLY	C-N-CA	7.16	129.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	48	ILE	CB-CA-C	-7.16	103.35	111.80
1	E	208	ASN	CA-CB-CG	7.16	119.76	112.60
2	6	32	THR	CA-C-O	7.16	129.08	120.28
3	J	291	ASP	N-CA-C	-7.15	104.68	113.41
2	1	146	THR	CA-C-N	7.15	129.86	120.28
2	1	146	THR	C-N-CA	7.15	129.86	120.28
3	M	266	MET	CA-C-N	7.15	129.86	120.28
3	M	266	MET	C-N-CA	7.15	129.86	120.28
1	G	120	LYS	O-C-N	7.15	129.69	122.12
1	g	180	ARG	CA-C-O	-7.15	113.32	121.40
2	1	57	ALA	N-CA-C	-7.15	98.56	109.85
3	H	375	PHE	CA-CB-CG	-7.15	106.65	113.80
2	4	164	ALA	CA-C-O	-7.14	112.85	120.42
3	H	75	GLY	N-CA-C	-7.14	105.93	115.21
1	b	33	ARG	NE-CZ-NH2	7.14	125.62	119.20
2	n	111	LEU	CA-C-O	-7.14	112.65	120.36
1	a	15	PHE	CA-CB-CG	7.13	120.94	113.80
1	C	22	PHE	CA-CB-CG	-7.13	106.67	113.80
2	4	131	ALA	CA-C-O	7.13	127.93	120.30
3	M	333	ASP	N-CA-C	-7.13	104.72	113.50
3	L	62	PRO	CB-CA-C	7.13	117.86	111.87
1	b	42	CYS	N-CA-C	-7.13	98.80	108.86
3	K	375	PHE	N-CA-CB	7.13	120.60	110.12
1	A	144	VAL	N-CA-C	-7.13	100.96	109.01
3	L	353	ALA	N-CA-CB	7.12	120.59	110.12
2	6	207	ILE	CA-C-O	-7.12	113.09	120.71
1	a	93	ARG	N-CA-CB	7.12	120.58	110.12
1	f	173	GLU	CA-C-N	7.12	129.82	120.28
1	f	173	GLU	C-N-CA	7.12	129.82	120.28
1	a	85	ALA	CA-C-N	7.11	129.81	120.28
1	a	85	ALA	C-N-CA	7.11	129.81	120.28
2	i	136	ASP	CA-CB-CG	7.11	119.71	112.60
1	E	219	ARG	N-CA-CB	7.11	122.71	111.91
1	G	198	LEU	N-CA-CB	7.10	120.56	110.12
2	6	211	PHE	CA-CB-CG	-7.10	106.70	113.80
1	A	193	LEU	N-CA-C	7.10	119.10	111.36
1	F	183	LEU	CB-CA-C	-7.10	96.91	109.62
1	F	105	GLU	CA-C-N	7.10	126.86	119.76
1	F	105	GLU	C-N-CA	7.10	126.86	119.76
1	f	185	PHE	CA-CB-CG	-7.09	106.71	113.80
1	f	70	ILE	N-CA-C	-7.09	105.71	111.81
2	3	126	ASP	CA-C-N	7.09	127.70	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	126	ASP	C-N-CA	7.09	127.70	120.04
2	3	96	ASN	CA-C-N	7.09	129.66	120.44
2	3	96	ASN	C-N-CA	7.09	129.66	120.44
1	D	207	GLU	CB-CA-C	-7.09	99.03	110.79
1	g	174	PHE	CA-CB-CG	-7.09	106.71	113.80
2	k	165	VAL	N-CA-CB	7.09	120.18	110.54
3	H	29	ARG	NE-CZ-NH1	-7.08	114.42	121.50
2	7	62	ASP	CA-CB-CG	7.07	119.67	112.60
2	7	169	VAL	CA-C-N	7.07	130.33	120.29
2	7	169	VAL	C-N-CA	7.07	130.33	120.29
2	2	63	ALA	CB-CA-C	-7.07	99.05	110.79
1	B	151	ASP	CA-C-N	7.07	128.68	119.84
1	B	151	ASP	C-N-CA	7.07	128.68	119.84
2	h	118	GLU	N-CA-CB	7.07	121.25	110.44
2	7	187	ASP	N-CA-C	-7.07	98.71	109.95
1	a	73	HIS	CA-CB-CG	7.06	120.86	113.80
3	I	47	GLU	CA-C-N	7.06	130.45	120.42
3	I	47	GLU	C-N-CA	7.06	130.45	120.42
3	I	248	ALA	N-CA-C	-7.06	96.68	108.75
3	M	158	GLU	O-C-N	-7.06	114.64	122.12
3	J	24	ARG	CA-C-N	7.06	129.74	120.28
3	J	24	ARG	C-N-CA	7.06	129.74	120.28
3	J	220	ALA	N-CA-CB	7.06	120.31	110.07
1	a	26	TYR	CA-C-O	-7.06	113.07	120.55
2	j	211	PHE	CA-CB-CG	7.05	120.85	113.80
2	5	55	THR	O-C-N	7.05	131.69	123.30
1	C	85	ALA	CA-C-N	7.05	130.06	120.54
1	C	85	ALA	C-N-CA	7.05	130.06	120.54
3	K	225	GLU	CA-C-O	-7.04	113.42	120.82
1	A	235	ARG	CB-CA-C	-7.04	96.02	110.38
3	J	221	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	d	38	ILE	CA-C-N	7.04	126.43	121.65
1	d	38	ILE	C-N-CA	7.04	126.43	121.65
1	B	204	LEU	CA-C-N	7.03	135.14	122.13
1	B	204	LEU	C-N-CA	7.03	135.14	122.13
1	E	119	PHE	CA-CB-CG	-7.03	106.77	113.80
1	E	93	ARG	NE-CZ-NH2	7.03	125.52	119.20
1	B	47	ILE	N-CA-C	-7.02	98.00	108.12
1	f	237	ASN	CA-C-N	7.02	132.36	121.19
1	f	237	ASN	C-N-CA	7.02	132.36	121.19
1	D	190	VAL	CA-C-N	7.02	130.26	120.29
1	D	190	VAL	C-N-CA	7.02	130.26	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	79	ILE	CA-C-O	-7.02	113.26	121.05
3	L	228	GLN	N-CA-C	-7.02	103.71	111.36
3	M	396	MET	N-CA-C	-7.01	104.60	113.72
2	l	166	GLU	CA-C-N	7.01	130.25	120.29
2	l	166	GLU	C-N-CA	7.01	130.25	120.29
1	g	70	ILE	N-CA-C	-7.01	105.95	112.96
1	d	99	ASN	CA-C-N	7.01	129.67	120.28
1	d	99	ASN	C-N-CA	7.01	129.67	120.28
1	f	180	ARG	N-CA-C	-7.01	98.78	109.85
3	M	311	LEU	CB-CA-C	-7.00	101.87	109.85
1	E	241	ARG	NE-CZ-NH1	-7.00	114.50	121.50
2	4	165	VAL	N-CA-CB	7.00	120.05	110.54
3	I	275	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	152	PRO	CA-C-N	7.00	129.95	120.44
1	A	152	PRO	C-N-CA	7.00	129.95	120.44
3	I	167	PHE	CA-C-N	6.99	129.53	120.44
3	I	167	PHE	C-N-CA	6.99	129.53	120.44
3	J	146	LEU	N-CA-C	-6.99	101.91	111.56
1	g	230	LYS	N-CA-C	6.99	122.99	113.77
2	k	146	THR	CA-C-O	6.99	127.82	120.42
3	H	186	THR	N-CA-C	-6.99	102.74	112.45
3	J	302	ARG	CA-C-N	6.99	131.11	121.33
3	J	302	ARG	C-N-CA	6.99	131.11	121.33
3	M	302	ARG	N-CA-C	-6.98	105.69	114.56
3	L	352	LYS	N-CA-C	6.98	118.89	111.28
3	J	57	ARG	CD-NE-CZ	-6.98	114.63	124.40
1	E	74	ILE	O-C-N	6.97	130.73	123.20
2	7	136	ASP	N-CA-CB	6.97	122.28	110.49
3	I	369	LYS	O-C-N	6.97	131.09	122.86
2	n	118	GLU	CA-C-O	6.97	127.99	119.97
1	C	222	LYS	N-CA-C	-6.97	98.05	108.99
2	j	63	ALA	CA-C-O	-6.97	113.52	120.70
3	K	324	HIS	CA-CB-CG	-6.97	106.83	113.80
1	A	196	MET	CA-C-N	6.97	127.66	120.00
1	A	196	MET	C-N-CA	6.97	127.66	120.00
1	E	69	LYS	N-CA-C	-6.97	98.33	109.76
3	H	15	LYS	CA-C-N	6.97	129.91	120.44
3	H	15	LYS	C-N-CA	6.97	129.91	120.44
3	H	336	PHE	CA-C-O	6.96	127.98	119.97
3	M	103	GLY	N-CA-C	-6.96	105.45	115.27
1	D	57	LYS	CB-CA-C	-6.96	98.40	110.17
1	g	147	LEU	N-CA-C	-6.96	98.44	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	145	LEU	CA-C-N	6.96	129.91	120.44
2	m	145	LEU	C-N-CA	6.96	129.91	120.44
3	I	221	ARG	NE-CZ-NH2	6.96	125.47	119.20
3	M	268	LEU	N-CA-C	6.96	118.95	111.36
2	m	83	ARG	N-CA-C	-6.96	96.38	108.69
1	F	33	ARG	O-C-N	-6.96	114.58	122.09
3	I	57	ARG	NE-CZ-NH2	6.96	125.46	119.20
2	4	202	GLU	CA-C-N	6.95	130.88	120.31
2	4	202	GLU	C-N-CA	6.95	130.88	120.31
2	n	83	ARG	NE-CZ-NH1	-6.95	114.55	121.50
1	F	19	GLY	N-CA-C	-6.95	105.23	115.72
2	i	172	ILE	CA-C-N	6.95	129.59	120.28
2	i	172	ILE	C-N-CA	6.95	129.59	120.28
1	A	116	ILE	CA-C-N	6.95	129.59	120.28
1	A	116	ILE	C-N-CA	6.95	129.59	120.28
3	J	363	ILE	CA-C-O	-6.94	113.73	120.95
2	7	44	LYS	N-CA-C	-6.94	104.09	114.64
3	K	218	GLU	N-CA-CB	6.94	121.04	110.28
3	J	95	ILE	N-CA-C	-6.94	98.12	108.12
1	A	169	ASN	CA-CB-CG	6.94	119.54	112.60
2	k	134	GLU	CA-C-N	6.94	132.01	120.70
2	k	134	GLU	C-N-CA	6.94	132.01	120.70
1	C	129	VAL	N-CA-C	-6.93	99.20	108.35
1	E	21	LEU	O-C-N	-6.93	115.32	123.22
1	d	229	LEU	N-CA-C	-6.93	103.50	112.23
1	E	98	ILE	N-CA-C	6.93	117.69	110.62
2	l	128	ILE	N-CA-C	-6.93	105.97	112.83
1	e	179	TYR	N-CA-C	-6.93	96.04	110.80
2	4	86	THR	N-CA-C	-6.92	100.27	110.52
1	C	111	GLU	N-CA-C	6.92	119.85	111.82
1	a	235	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	B	87	VAL	N-CA-CB	6.92	119.95	110.54
1	c	134	VAL	N-CA-C	6.92	118.31	108.42
1	f	181	ASP	N-CA-C	-6.92	104.15	112.59
1	b	172	THR	CA-C-N	6.91	130.11	120.29
1	b	172	THR	C-N-CA	6.91	130.11	120.29
2	i	176	MET	CA-C-N	6.91	129.43	120.44
2	i	176	MET	C-N-CA	6.91	129.43	120.44
3	I	294	ASP	CA-C-N	6.91	126.62	119.64
3	I	294	ASP	C-N-CA	6.91	126.62	119.64
3	I	292	ILE	CA-C-N	6.91	133.31	122.94
3	I	292	ILE	C-N-CA	6.91	133.31	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	154	GLY	CA-C-O	6.91	126.30	118.98
1	C	87	VAL	CB-CA-C	-6.91	102.81	112.14
2	i	181	ALA	O-C-N	6.91	129.18	122.07
1	g	98	ILE	CA-C-O	-6.91	113.53	120.85
2	2	162	ASP	O-C-N	6.91	130.60	122.24
1	E	142	ASP	CA-C-N	6.90	129.84	120.38
1	E	142	ASP	C-N-CA	6.90	129.84	120.38
3	L	351	ILE	N-CA-C	-6.90	103.58	110.62
2	l	159	ILE	CB-CA-C	6.90	119.47	110.91
2	l	181	ALA	N-CA-C	-6.90	101.88	112.99
2	6	60	VAL	CA-C-N	6.90	127.60	119.94
2	6	60	VAL	C-N-CA	6.90	127.60	119.94
3	H	257	GLY	CA-C-N	6.90	134.12	121.70
3	H	257	GLY	C-N-CA	6.90	134.12	121.70
1	F	187	ASP	CA-CB-CG	-6.90	105.70	112.60
3	L	115	ILE	N-CA-CB	6.90	118.68	110.95
1	A	150	THR	N-CA-C	-6.90	99.07	110.17
3	K	158	GLU	N-CA-C	6.90	119.43	111.02
2	5	196	PHE	N-CA-C	-6.89	93.10	107.37
1	c	172	THR	CA-C-N	6.89	129.51	120.28
1	c	172	THR	C-N-CA	6.89	129.51	120.28
2	n	60	VAL	CB-CA-C	-6.89	103.01	112.24
1	d	93	ARG	NE-CZ-NH2	-6.89	113.00	119.20
2	m	207	ILE	N-CA-C	-6.89	103.76	110.72
1	g	229	LEU	CA-C-O	-6.88	113.25	120.55
3	M	33	GLU	CA-C-O	-6.88	113.12	120.42
3	J	22	LYS	CA-C-O	-6.88	113.59	120.82
3	H	122	SER	CA-C-O	6.88	127.54	120.24
1	e	24	VAL	N-CA-CB	6.88	119.38	110.57
2	j	83	ARG	CA-C-N	6.88	129.96	120.39
2	j	83	ARG	C-N-CA	6.88	129.96	120.39
3	M	145	GLY	CA-C-N	6.88	134.69	121.54
3	M	145	GLY	C-N-CA	6.88	134.69	121.54
3	M	321	PHE	CA-CB-CG	-6.88	106.92	113.80
1	B	244	LEU	CA-C-O	6.88	126.62	119.05
2	3	147	ALA	CA-C-N	6.88	129.50	120.28
2	3	147	ALA	C-N-CA	6.88	129.50	120.28
3	K	335	ASP	N-CA-C	-6.88	97.06	108.34
1	c	182	ASP	CA-CB-CG	-6.88	105.72	112.60
1	C	200	ILE	CA-CB-CG2	-6.88	98.81	110.50
1	c	239	ARG	CA-C-N	6.87	129.88	120.46
1	c	239	ARG	C-N-CA	6.87	129.88	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	59	SER	CA-C-N	6.87	129.22	120.56
2	2	59	SER	C-N-CA	6.87	129.22	120.56
2	4	104	PHE	CA-CB-CG	-6.87	106.93	113.80
1	G	109	VAL	CA-C-N	6.87	129.49	120.28
1	G	109	VAL	C-N-CA	6.87	129.49	120.28
1	g	134	VAL	N-CA-C	-6.87	97.79	108.44
1	A	184	SER	CA-C-N	6.87	129.81	120.54
1	A	184	SER	C-N-CA	6.87	129.81	120.54
1	c	14	VAL	CA-C-O	-6.87	114.91	121.64
2	4	164	ALA	N-CA-CB	6.87	120.32	110.16
3	M	387	THR	O-C-N	-6.87	113.42	121.32
2	l	59	SER	CA-C-N	6.86	129.34	120.56
2	l	59	SER	C-N-CA	6.86	129.34	120.56
3	H	150	ILE	CA-C-O	-6.86	113.81	120.95
3	L	188	LYS	N-CA-C	-6.86	104.79	113.43
2	k	135	LYS	CA-C-O	6.86	126.06	118.52
1	C	160	LYS	N-CA-C	-6.86	104.45	114.39
2	h	140	THR	N-CA-CB	6.86	122.08	110.49
2	4	142	SER	CA-C-O	6.86	126.36	118.55
2	7	116	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	170	ALA	CB-CA-C	-6.85	99.43	110.79
1	F	19	GLY	CA-C-O	6.85	126.67	118.86
1	f	99	ASN	CA-C-O	6.84	128.01	120.82
3	M	167	PHE	CA-C-N	6.84	129.34	120.44
3	M	167	PHE	C-N-CA	6.84	129.34	120.44
1	c	187	ASP	CA-CB-CG	-6.84	105.76	112.60
2	h	46	TYR	CA-CB-CG	-6.84	101.59	113.90
2	3	59	SER	CA-C-N	6.84	130.13	120.42
2	3	59	SER	C-N-CA	6.84	130.13	120.42
2	n	18	VAL	N-CA-CB	6.84	119.63	110.26
1	f	67	ILE	N-CA-CB	6.83	120.84	111.41
2	k	99	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	A	160	LYS	N-CA-CB	6.83	119.99	110.98
1	E	169	ASN	N-CA-C	6.83	118.72	111.28
2	3	70	ILE	CA-C-N	6.83	130.28	120.79
2	3	70	ILE	C-N-CA	6.83	130.28	120.79
2	k	93	LEU	N-CA-C	-6.83	103.84	111.28
3	J	41	ARG	CA-C-O	-6.83	113.19	120.42
1	b	174	PHE	CA-CB-CG	6.82	120.62	113.80
1	F	173	GLU	CA-C-N	6.82	129.42	120.28
1	F	173	GLU	C-N-CA	6.82	129.42	120.28
1	E	110	LYS	N-CA-CB	6.82	119.90	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	141	GLU	CA-C-O	6.82	127.68	119.43
3	J	195	VAL	N-CA-CB	6.82	119.81	110.54
1	G	151	ASP	CA-C-N	6.82	126.96	119.87
1	G	151	ASP	C-N-CA	6.82	126.96	119.87
2	I	73	GLU	N-CA-CB	6.82	120.14	110.12
3	M	365	GLU	CA-C-O	-6.82	111.18	119.43
1	a	235	ARG	NE-CZ-NH1	-6.81	114.69	121.50
2	m	77	TYR	CA-C-N	6.81	129.30	120.44
2	m	77	TYR	C-N-CA	6.81	129.30	120.44
3	K	157	VAL	CB-CA-C	-6.81	104.99	111.05
1	C	94	ILE	N-CA-C	-6.81	103.84	110.72
1	c	42	CYS	O-C-N	-6.81	113.34	122.74
3	I	111	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	E	94	ILE	N-CA-C	6.81	117.56	110.62
2	n	212	ARG	N-CA-C	-6.81	98.63	109.59
2	4	211	PHE	N-CA-C	-6.80	103.35	112.94
1	B	208	ASN	N-CA-C	-6.80	104.29	112.59
1	b	212	GLY	N-CA-C	-6.80	99.73	111.57
1	d	180	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	C	91	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	G	227	GLU	CA-C-O	6.80	127.27	119.18
1	B	63	THR	CA-C-N	6.80	134.20	121.97
1	B	63	THR	C-N-CA	6.80	134.20	121.97
1	C	196	MET	O-C-N	-6.80	114.40	122.15
2	j	179	ASP	CA-CB-CG	-6.80	105.80	112.60
3	I	96	ASN	CA-CB-CG	-6.80	105.80	112.60
1	E	136	LEU	N-CA-C	-6.79	98.76	109.50
3	I	243	LEU	CA-C-O	6.79	127.66	119.78
3	I	391	ASP	CA-C-N	6.79	132.01	122.36
3	I	391	ASP	C-N-CA	6.79	132.01	122.36
1	D	81	LEU	N-CA-CB	6.79	120.08	109.83
2	4	170	ARG	NE-CZ-NH1	-6.79	114.71	121.50
2	m	126	ASP	CA-CB-CG	-6.79	105.81	112.60
3	H	311	LEU	N-CA-C	6.79	117.41	109.60
1	B	143	GLU	O-C-N	6.79	131.62	122.59
1	G	137	LEU	N-CA-C	-6.79	97.84	108.90
2	4	205	GLU	CA-C-O	6.79	127.80	120.20
2	m	58	GLY	N-CA-C	-6.79	104.15	111.21
3	H	122	SER	O-C-N	-6.79	115.33	123.27
3	K	35	LYS	CA-C-N	6.79	129.37	120.28
3	K	35	LYS	C-N-CA	6.79	129.37	120.28
1	D	108	THR	N-CA-CB	6.78	120.76	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	60	GLU	CA-C-N	6.78	129.70	120.54
1	E	60	GLU	C-N-CA	6.78	129.70	120.54
3	K	268	LEU	CA-C-N	6.78	129.37	120.28
3	K	268	LEU	C-N-CA	6.78	129.37	120.28
1	b	209	ILE	O-C-N	-6.78	115.23	123.09
1	f	200	ILE	CA-C-N	6.78	131.74	122.19
1	f	200	ILE	C-N-CA	6.78	131.74	122.19
1	d	236	ALA	CA-C-O	-6.77	113.37	120.55
1	F	163	ALA	CA-C-N	6.77	132.30	122.69
1	F	163	ALA	C-N-CA	6.77	132.30	122.69
1	a	113	ALA	N-CA-C	6.77	118.31	111.07
2	k	148	TYR	N-CA-CB	6.77	120.07	110.12
3	H	280	ASP	N-CA-C	-6.77	96.39	110.80
3	K	316	GLY	CA-C-N	6.76	129.35	120.28
3	K	316	GLY	C-N-CA	6.76	129.35	120.28
2	5	211	PHE	N-CA-C	-6.76	104.60	112.92
2	l	109	GLN	N-CA-C	-6.76	98.18	109.07
3	K	263	ARG	CA-C-N	6.76	129.64	120.44
3	K	263	ARG	C-N-CA	6.76	129.64	120.44
3	L	397	PHE	CA-CB-CG	-6.76	107.04	113.80
2	7	172	ILE	CA-C-N	6.76	129.33	120.28
2	7	172	ILE	C-N-CA	6.76	129.33	120.28
2	5	194	ASP	CA-CB-CG	-6.75	105.84	112.60
2	7	212	ARG	N-CA-C	-6.75	102.44	111.96
1	F	91	ARG	NE-CZ-NH1	-6.75	114.75	121.50
2	7	174	SER	CA-C-N	6.75	129.33	120.28
2	7	174	SER	C-N-CA	6.75	129.33	120.28
1	B	135	SER	N-CA-C	-6.75	97.90	108.90
2	i	183	GLY	CA-C-N	6.75	134.43	121.54
2	i	183	GLY	C-N-CA	6.75	134.43	121.54
3	J	163	LYS	CA-C-N	6.75	126.54	119.05
3	J	163	LYS	C-N-CA	6.75	126.54	119.05
2	l	66	LEU	CA-C-N	6.74	129.32	120.28
2	l	66	LEU	C-N-CA	6.74	129.32	120.28
1	C	226	PRO	O-C-N	6.74	131.74	122.64
1	A	179	TYR	O-C-N	-6.74	114.67	122.89
1	d	128	GLY	CA-C-N	6.74	129.66	122.11
1	d	128	GLY	C-N-CA	6.74	129.66	122.11
2	4	87	VAL	N-CA-C	-6.74	103.92	110.72
2	7	91	ALA	CA-C-N	6.74	129.86	120.29
2	7	91	ALA	C-N-CA	6.74	129.86	120.29
2	n	94	THR	CA-C-N	6.74	129.86	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	94	THR	C-N-CA	6.74	129.86	120.29
1	d	117	CYS	CA-C-N	6.74	129.86	120.29
1	d	117	CYS	C-N-CA	6.74	129.86	120.29
1	d	185	PHE	CA-C-N	6.74	129.86	120.29
1	d	185	PHE	C-N-CA	6.74	129.86	120.29
2	7	71	LYS	CB-CA-C	-6.74	99.61	110.79
2	7	29	LYS	CA-C-N	6.73	130.27	120.71
2	7	29	LYS	C-N-CA	6.73	130.27	120.71
3	I	372	MET	CA-C-N	6.73	129.85	120.29
3	I	372	MET	C-N-CA	6.73	129.85	120.29
3	L	288	ASN	N-CA-C	-6.73	103.72	112.68
2	5	149	GLY	CA-C-N	6.73	129.68	120.46
2	5	149	GLY	C-N-CA	6.73	129.68	120.46
3	I	10	LEU	CB-CA-C	-6.73	99.62	110.79
1	b	36	THR	CA-CB-OG1	6.72	119.69	109.60
1	c	197	GLY	CA-C-N	6.72	130.53	120.31
1	c	197	GLY	C-N-CA	6.72	130.53	120.31
1	B	234	GLU	N-CA-C	-6.72	103.88	111.07
2	2	65	PHE	N-CA-CB	6.72	120.22	110.20
2	7	100	SER	CA-C-O	-6.72	113.43	120.55
2	7	112	ILE	N-CA-C	-6.72	97.94	107.75
2	6	49	ALA	N-CA-C	-6.72	99.98	108.45
3	H	10	LEU	CA-C-N	6.72	129.18	120.44
3	H	10	LEU	C-N-CA	6.72	129.18	120.44
1	c	218	ASP	CA-CB-CG	-6.72	105.88	112.60
1	a	188	ALA	O-C-N	6.72	129.24	122.12
2	3	59	SER	CA-C-O	-6.71	113.36	121.28
3	I	202	THR	O-C-N	-6.71	113.87	123.07
2	h	157	PRO	O-C-N	6.71	131.57	122.37
3	L	48	VAL	CB-CA-C	6.71	120.56	111.97
2	n	96	ASN	CA-C-N	6.71	129.16	120.44
2	n	96	ASN	C-N-CA	6.71	129.16	120.44
1	C	118	ASP	N-CA-C	-6.70	104.05	111.36
1	c	45	GLY	O-C-N	-6.70	115.91	124.15
1	E	90	ASP	CA-C-N	6.70	129.26	120.28
1	E	90	ASP	C-N-CA	6.70	129.26	120.28
1	b	167	GLY	CA-C-N	6.70	129.26	120.28
1	b	167	GLY	C-N-CA	6.70	129.26	120.28
2	2	158	GLU	N-CA-C	-6.70	103.71	112.41
3	K	16	LEU	O-C-N	6.70	129.22	122.12
2	3	15	VAL	N-CA-C	-6.69	99.03	108.80
3	I	176	LYS	N-CA-C	-6.69	104.25	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	299	ARG	NE-CZ-NH2	6.69	125.22	119.20
3	K	351	ILE	CA-C-N	6.69	129.13	120.44
3	K	351	ILE	C-N-CA	6.69	129.13	120.44
1	c	35	ALA	CA-C-N	6.69	130.65	120.82
1	c	35	ALA	C-N-CA	6.69	130.65	120.82
2	4	78	GLU	CA-C-O	6.69	127.51	120.42
1	E	98	ILE	CA-CB-CG2	6.68	121.86	110.50
1	C	103	TYR	N-CA-C	-6.68	106.33	114.75
1	F	129	VAL	N-CA-C	-6.68	99.51	108.06
2	1	131	ALA	N-CA-CB	6.68	121.07	110.65
1	A	130	ARG	CA-C-O	-6.68	113.42	120.70
2	i	120	LYS	N-CA-C	-6.68	97.71	109.06
3	J	109	ASN	N-CA-C	-6.68	97.85	108.73
1	G	217	ASP	N-CA-C	-6.67	104.71	112.92
2	j	159	ILE	N-CA-CB	6.67	118.52	110.31
2	4	71	LYS	CA-C-N	6.67	129.60	120.46
2	4	71	LYS	C-N-CA	6.67	129.60	120.46
1	G	97	GLN	CA-C-N	6.67	129.90	120.42
1	G	97	GLN	C-N-CA	6.67	129.90	120.42
3	I	276	ASP	N-CA-C	-6.67	98.90	109.04
1	e	73	HIS	CE1-NE2-CD2	-6.67	102.33	109.00
2	l	161	VAL	CA-C-N	6.67	129.88	120.28
2	l	161	VAL	C-N-CA	6.67	129.88	120.28
3	J	141	GLU	N-CA-C	-6.66	104.77	113.17
1	e	28	ARG	NE-CZ-NH1	6.66	128.16	121.50
1	f	61	ALA	N-CA-C	-6.66	103.24	112.30
1	a	109	VAL	CA-C-O	-6.66	114.02	120.95
1	a	187	ASP	CB-CA-C	-6.66	99.73	110.79
1	c	31	VAL	N-CA-C	-6.66	105.14	112.80
1	c	200	ILE	O-C-N	6.66	128.86	122.20
2	6	125	ILE	N-CA-C	-6.66	98.85	108.17
1	C	193	LEU	CA-C-N	6.66	128.95	120.56
1	C	193	LEU	C-N-CA	6.66	128.95	120.56
1	D	134	VAL	O-C-N	-6.66	115.65	123.04
1	D	167	GLY	CA-C-N	6.66	129.09	120.44
1	D	167	GLY	C-N-CA	6.66	129.09	120.44
1	G	235	ARG	NE-CZ-NH1	-6.66	114.84	121.50
2	k	33	MET	N-CA-C	-6.66	99.51	109.83
1	D	82	VAL	CA-C-N	6.66	129.09	120.44
1	D	82	VAL	C-N-CA	6.66	129.09	120.44
2	7	84	LYS	CA-C-N	6.65	126.69	119.90
2	7	84	LYS	C-N-CA	6.65	126.69	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	235	PRO	N-CD-CG	6.65	111.78	103.80
3	I	362	ALA	CA-C-N	6.65	129.07	120.56
3	I	362	ALA	C-N-CA	6.65	129.07	120.56
1	b	84	ASP	CA-C-N	6.65	129.19	120.28
1	b	84	ASP	C-N-CA	6.65	129.19	120.28
1	A	171	VAL	CA-C-N	6.65	129.08	120.44
1	A	171	VAL	C-N-CA	6.65	129.08	120.44
3	L	283	VAL	N-CA-C	-6.65	98.86	108.17
1	a	165	GLY	CA-C-N	6.65	130.41	120.31
1	a	165	GLY	C-N-CA	6.65	130.41	120.31
2	m	130	GLY	O-C-N	-6.64	114.06	122.70
3	I	315	GLU	N-CA-C	-6.64	104.12	111.36
3	M	228	GLN	CA-C-N	6.64	129.18	120.28
3	M	228	GLN	C-N-CA	6.64	129.18	120.28
1	d	86	ARG	CA-C-O	-6.64	113.84	120.82
1	f	151	ASP	CA-C-O	-6.64	113.72	120.96
3	H	241	ASP	O-C-N	6.64	131.11	122.68
2	k	85	PRO	CA-C-O	-6.64	114.13	121.23
1	G	153	SER	N-CA-C	-6.63	103.87	112.23
2	2	200	SER	CA-C-N	6.63	126.88	119.32
2	2	200	SER	C-N-CA	6.63	126.88	119.32
2	6	163	GLU	CB-CA-C	-6.63	96.98	109.72
3	L	152	GLU	N-CA-CB	6.63	119.97	110.16
2	l	177	LYS	CA-C-O	6.63	127.59	119.97
1	f	79	SER	O-C-N	-6.62	115.85	123.33
2	l	212	ARG	NE-CZ-NH1	6.62	128.12	121.50
3	M	203	PHE	CA-C-N	6.62	130.65	122.37
3	M	203	PHE	C-N-CA	6.62	130.65	122.37
1	C	216	VAL	CB-CA-C	-6.62	103.35	112.02
2	j	146	THR	CA-C-N	6.62	129.69	120.29
2	j	146	THR	C-N-CA	6.62	129.69	120.29
3	J	251	THR	CA-C-N	6.62	130.11	120.71
3	J	251	THR	C-N-CA	6.62	130.11	120.71
3	L	234	ALA	CA-C-O	-6.62	113.21	120.69
1	A	98	ILE	O-C-N	-6.61	115.45	121.87
1	D	159	TYR	N-CA-C	-6.61	99.36	109.41
2	i	13	THR	N-CA-C	-6.61	99.05	109.50
3	K	115	ILE	O-C-N	-6.61	115.47	122.68
1	g	205	VAL	N-CA-CB	6.61	120.46	111.21
2	2	23	VAL	N-CA-C	-6.61	98.97	108.42
1	A	197	GLY	CA-C-N	6.60	129.13	120.28
1	A	197	GLY	C-N-CA	6.60	129.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ALA	O-C-N	6.60	129.68	122.15
1	a	96	ALA	O-C-N	-6.60	115.12	122.12
2	k	33	MET	CG-SD-CE	-6.60	86.38	100.90
3	J	326	ARG	NE-CZ-NH1	-6.60	114.90	121.50
2	n	203	GLU	CA-C-N	6.60	129.79	120.42
2	n	203	GLU	C-N-CA	6.60	129.79	120.42
3	K	14	LYS	CA-C-O	6.59	127.41	120.42
3	L	186	THR	N-CA-C	-6.59	104.17	111.36
1	G	130	ARG	CA-C-O	-6.59	114.05	120.97
2	m	135	LYS	N-CA-C	-6.59	104.55	112.59
1	a	41	LYS	N-CA-C	-6.59	98.66	109.40
1	G	149	GLU	N-CA-C	-6.59	98.66	109.40
1	E	62	ASP	CB-CA-C	6.59	121.10	110.16
2	h	139	ALA	N-CA-C	-6.59	96.77	110.80
3	H	220	ALA	CA-C-N	6.59	129.65	120.29
3	H	220	ALA	C-N-CA	6.59	129.65	120.29
1	a	88	LEU	N-CA-CB	6.59	119.80	110.12
2	6	201	PRO	N-CA-CB	6.58	110.16	103.25
1	G	67	ILE	CB-CA-C	6.58	118.40	111.09
1	E	99	ASN	CA-CB-CG	6.58	119.18	112.60
2	3	62	ASP	CB-CA-C	-6.58	99.66	110.85
1	F	125	GLN	N-CA-CB	6.58	119.55	110.01
2	6	101	TYR	CA-C-O	6.58	128.23	120.66
1	A	151	ASP	CA-C-O	-6.58	113.89	120.66
1	E	220	THR	N-CA-C	-6.58	96.79	110.80
1	c	177	LYS	N-CA-CB	6.57	120.69	110.44
2	n	45	ILE	O-C-N	-6.57	116.34	123.18
3	I	213	GLN	CA-C-N	6.57	129.09	120.28
3	I	213	GLN	C-N-CA	6.57	129.09	120.28
3	L	353	ALA	CA-C-N	6.57	129.46	120.46
3	L	353	ALA	C-N-CA	6.57	129.46	120.46
1	C	174	PHE	CA-CB-CG	-6.57	107.23	113.80
3	I	76	ARG	CA-C-O	6.57	129.13	121.44
3	L	73	GLU	N-CA-C	-6.57	103.78	112.72
2	2	117	SER	N-CA-C	-6.57	103.23	111.11
2	3	88	ARG	CA-C-N	6.57	129.37	120.44
2	3	88	ARG	C-N-CA	6.57	129.37	120.44
2	l	93	LEU	CA-C-O	-6.57	113.59	120.55
3	L	223	VAL	CA-C-O	-6.57	114.12	120.95
3	M	54	GLU	N-CA-C	6.57	119.44	111.82
1	C	23	GLN	CA-C-O	6.56	127.38	120.42
2	l	74	ALA	CA-C-N	6.56	129.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	74	ALA	C-N-CA	6.56	129.07	120.28
3	I	172	ILE	N-CA-C	-6.56	99.04	108.42
1	E	169	ASN	CA-C-N	6.56	129.60	120.29
1	E	169	ASN	C-N-CA	6.56	129.60	120.29
2	h	143	GLY	CA-C-N	6.55	129.06	120.28
2	h	143	GLY	C-N-CA	6.55	129.06	120.28
1	D	31	VAL	CA-C-N	6.55	129.06	120.28
1	D	31	VAL	C-N-CA	6.55	129.06	120.28
1	e	106	PRO	CA-C-O	-6.55	113.45	121.31
1	F	165	GLY	CA-C-N	6.55	129.60	120.29
1	F	165	GLY	C-N-CA	6.55	129.60	120.29
1	e	211	VAL	N-CA-CB	6.55	120.73	111.82
3	J	183	PRO	CA-C-N	6.55	128.03	119.84
3	J	183	PRO	C-N-CA	6.55	128.03	119.84
2	h	135	LYS	CA-C-O	6.55	127.21	119.48
1	F	59	LEU	N-CA-C	-6.55	98.96	109.96
1	F	230	LYS	O-C-N	-6.55	114.33	120.55
2	6	51	ARG	N-CA-C	-6.55	100.70	110.06
3	H	13	LEU	CA-C-O	6.55	127.49	120.55
3	L	254	ASP	N-CA-C	-6.54	104.92	113.17
2	i	89	ALA	CB-CA-C	-6.54	100.61	110.88
1	d	109	VAL	N-CA-C	-6.54	104.11	110.72
2	4	18	VAL	N-CA-C	-6.54	98.32	107.80
1	E	57	LYS	N-CA-C	-6.54	105.17	113.02
2	2	91	ALA	CA-C-N	6.54	129.57	120.29
2	2	91	ALA	C-N-CA	6.54	129.57	120.29
2	i	81	ARG	CA-C-N	6.54	131.64	122.36
2	i	81	ARG	C-N-CA	6.54	131.64	122.36
2	3	60	VAL	CA-C-N	6.54	127.06	119.94
2	3	60	VAL	C-N-CA	6.54	127.06	119.94
3	J	215	TYR	CA-CB-CG	-6.54	102.14	113.90
1	G	169	ASN	CA-CB-CG	-6.53	106.07	112.60
2	5	159	ILE	CA-C-O	-6.53	113.59	121.04
3	H	208	GLY	CA-C-O	-6.53	110.87	119.10
2	n	116	ASP	CA-C-N	6.53	129.57	120.29
2	n	116	ASP	C-N-CA	6.53	129.57	120.29
1	E	183	LEU	CA-C-O	6.53	127.55	120.43
2	l	164	ALA	N-CA-C	6.53	118.47	111.36
3	M	192	ALA	N-CA-C	6.53	119.22	111.71
1	f	58	LEU	CA-C-N	6.53	130.75	121.42
1	f	58	LEU	C-N-CA	6.53	130.75	121.42
3	I	91	THR	CA-C-O	-6.53	114.01	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	153	ILE	N-CA-C	-6.53	104.13	110.72
1	G	202	SER	CA-C-O	-6.52	114.30	121.28
2	n	191	ILE	N-CA-C	-6.52	96.91	107.28
2	l	174	SER	CA-C-N	6.52	129.02	120.28
2	l	174	SER	C-N-CA	6.52	129.02	120.28
3	K	233	LYS	CA-C-N	6.52	130.57	120.60
3	K	233	LYS	C-N-CA	6.52	130.57	120.60
2	1	167	LEU	CA-C-N	6.51	129.01	120.28
2	1	167	LEU	C-N-CA	6.51	129.01	120.28
1	A	108	THR	CA-C-N	6.51	129.71	120.53
1	A	108	THR	C-N-CA	6.51	129.71	120.53
2	n	30	ARG	N-CA-CB	6.51	121.50	110.49
1	g	33	ARG	O-C-N	-6.51	114.26	122.27
2	l	134	GLU	N-CA-C	-6.51	98.79	109.40
2	j	161	VAL	CA-C-N	6.51	130.21	120.31
2	j	161	VAL	C-N-CA	6.51	130.21	120.31
3	L	46	ARG	CA-C-N	6.51	129.00	120.28
3	L	46	ARG	C-N-CA	6.51	129.00	120.28
1	b	232	TYR	CB-CA-C	-6.51	99.78	110.85
1	G	13	THR	N-CA-C	-6.51	104.97	113.17
3	K	324	HIS	CE1-NE2-CD2	-6.51	102.49	109.00
1	a	46	VAL	N-CA-C	-6.51	99.36	108.27
1	F	180	ARG	CA-C-O	6.51	128.75	121.40
3	M	393	LYS	N-CA-C	-6.51	105.64	112.93
3	J	124	ASP	CA-C-O	-6.51	111.25	120.16
1	g	99	ASN	CA-C-N	6.50	129.00	120.28
1	g	99	ASN	C-N-CA	6.50	129.00	120.28
2	k	36	PHE	CA-CB-CG	6.50	120.31	113.80
2	l	14	THR	N-CA-C	-6.50	99.44	109.52
2	1	204	VAL	O-C-N	6.50	128.17	121.87
2	3	140	THR	N-CA-CB	6.50	122.55	111.50
2	3	169	VAL	CA-C-N	6.50	128.99	120.28
2	3	169	VAL	C-N-CA	6.50	128.99	120.28
3	H	44	TYR	N-CA-CB	6.50	120.35	110.28
3	L	177	GLY	N-CA-C	-6.50	99.78	110.56
2	n	68	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	C	190	VAL	CA-C-N	6.49	128.98	120.28
1	C	190	VAL	C-N-CA	6.49	128.98	120.28
1	f	120	LYS	CA-C-N	6.49	129.63	120.28
1	f	120	LYS	C-N-CA	6.49	129.63	120.28
3	L	382	VAL	CA-C-N	6.49	128.98	120.28
3	L	382	VAL	C-N-CA	6.49	128.98	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	317	ARG	NE-CZ-NH2	-6.49	113.36	119.20
2	2	17	LEU	CA-C-N	6.49	131.11	122.93
2	2	17	LEU	C-N-CA	6.49	131.11	122.93
3	K	76	ARG	CD-NE-CZ	-6.49	115.31	124.40
3	K	99	GLU	N-CA-C	-6.49	105.40	113.38
3	J	198	GLN	O-C-N	6.49	129.55	122.15
2	h	61	GLY	CA-C-O	-6.49	114.07	120.75
2	m	195	GLU	N-CA-C	-6.49	99.21	109.07
3	H	135	LYS	N-CA-CB	-6.49	102.16	109.49
1	a	118	ASP	CA-CB-CG	-6.49	106.11	112.60
2	1	96	ASN	N-CA-C	-6.49	104.29	111.36
2	h	80	ARG	N-CA-C	6.49	118.14	111.14
2	2	142	SER	N-CA-C	-6.49	105.50	113.41
2	j	157	PRO	N-CA-CB	6.48	109.49	103.46
2	7	28	GLU	CA-C-N	6.48	128.97	120.28
2	7	28	GLU	C-N-CA	6.48	128.97	120.28
1	b	81	LEU	CA-C-N	6.48	131.40	120.64
1	b	81	LEU	C-N-CA	6.48	131.40	120.64
3	M	24	ARG	CA-C-N	6.48	128.97	120.28
3	M	24	ARG	C-N-CA	6.48	128.97	120.28
2	h	63	ALA	O-C-N	6.48	129.54	122.15
3	K	135	LYS	CA-C-N	6.48	126.50	119.89
3	K	135	LYS	C-N-CA	6.48	126.50	119.89
3	L	379	ILE	O-C-N	6.48	128.50	121.83
3	J	151	GLU	O-C-N	-6.48	115.25	122.12
1	e	37	ALA	N-CA-C	-6.48	98.82	108.99
1	f	16	SER	O-C-N	-6.48	113.73	121.31
2	j	30	ARG	N-CA-CB	6.48	121.56	110.68
3	L	88	VAL	CA-C-O	-6.48	113.64	120.57
3	M	94	TYR	N-CA-C	-6.47	105.01	113.17
1	g	37	ALA	CA-C-O	6.47	128.95	120.21
3	H	379	ILE	CA-C-N	6.47	128.95	120.28
3	H	379	ILE	C-N-CA	6.47	128.95	120.28
3	K	61	PRO	N-CA-C	6.47	118.59	110.70
1	d	213	TYR	CA-CB-CG	6.47	125.55	113.90
3	K	115	ILE	CA-C-N	6.47	129.55	121.85
3	K	115	ILE	C-N-CA	6.47	129.55	121.85
1	F	236	ALA	N-CA-C	6.47	118.13	111.14
3	I	175	PRO	CA-C-O	-6.47	113.80	122.08
2	j	156	THR	CA-C-O	-6.47	114.39	120.34
3	L	212	VAL	CB-CA-C	6.47	119.46	111.25
1	a	171	VAL	N-CA-C	6.46	117.25	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	ILE	O-C-N	-6.46	116.18	123.10
2	1	126	ASP	CA-C-N	6.46	126.15	119.82
2	1	126	ASP	C-N-CA	6.46	126.15	119.82
2	n	68	ARG	N-CA-CB	6.46	119.62	110.12
3	K	239	PHE	N-CA-CB	6.46	119.97	109.95
1	f	237	ASN	O-C-N	-6.46	114.66	122.22
1	E	143	GLU	CA-C-O	-6.46	113.66	120.63
2	2	24	VAL	N-CA-C	-6.46	98.90	108.45
1	b	33	ARG	CD-NE-CZ	-6.45	115.37	124.40
3	L	321	PHE	CA-C-N	6.45	128.83	120.44
3	L	321	PHE	C-N-CA	6.45	128.83	120.44
1	f	104	ASP	N-CA-C	-6.45	103.03	111.74
2	n	90	ILE	N-CA-C	-6.45	104.20	110.72
1	A	113	ALA	CA-C-N	6.45	128.92	120.28
1	A	113	ALA	C-N-CA	6.45	128.92	120.28
1	f	124	THR	CA-C-N	6.45	129.45	120.29
1	f	124	THR	C-N-CA	6.45	129.45	120.29
3	H	52	ARG	CA-C-N	6.45	128.92	120.28
3	H	52	ARG	C-N-CA	6.45	128.92	120.28
3	I	288	ASN	N-CA-C	-6.44	102.76	112.04
3	J	76	ARG	N-CA-C	-6.44	100.15	110.14
2	7	203	GLU	CB-CA-C	-6.44	100.10	110.79
1	G	170	ALA	N-CA-C	6.44	117.96	111.07
2	3	186	ILE	CA-C-O	6.44	127.08	120.39
2	6	51	ARG	NE-CZ-NH2	6.44	124.99	119.20
3	J	234	ALA	CA-C-O	-6.44	113.30	120.25
3	J	339	LEU	CA-C-N	6.43	129.54	120.28
3	J	339	LEU	C-N-CA	6.43	129.54	120.28
1	G	64	ILE	N-CA-C	-6.43	99.16	108.17
2	4	168	ALA	CA-C-N	6.43	128.67	120.56
2	4	168	ALA	C-N-CA	6.43	128.67	120.56
2	7	170	ARG	NE-CZ-NH2	6.43	124.99	119.20
3	M	249	ARG	NE-CZ-NH1	-6.43	115.07	121.50
2	7	202	GLU	O-C-N	-6.43	115.45	122.07
1	B	143	GLU	CA-C-O	-6.43	111.32	120.51
2	1	27	THR	N-CA-C	-6.43	99.54	109.24
1	e	152	PRO	N-CA-C	-6.42	105.68	114.80
3	K	276	ASP	N-CA-CB	6.42	121.80	110.37
1	f	171	VAL	CA-C-N	6.42	129.17	120.44
1	f	171	VAL	C-N-CA	6.42	129.17	120.44
1	b	101	LEU	CA-C-O	-6.42	113.68	120.55
2	h	97	LEU	O-C-N	-6.42	115.32	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	203	GLU	CA-C-N	6.42	129.53	120.42
2	m	203	GLU	C-N-CA	6.42	129.53	120.42
3	L	47	GLU	CA-C-N	6.42	128.65	120.56
3	L	47	GLU	C-N-CA	6.42	128.65	120.56
3	L	92	SER	N-CA-C	-6.42	99.64	109.65
1	B	229	LEU	N-CA-CB	6.42	119.66	110.16
2	2	96	ASN	CA-CB-CG	-6.42	106.18	112.60
1	a	96	ALA	CA-C-O	6.41	127.35	120.55
1	c	109	VAL	CA-C-N	6.41	128.87	120.28
1	c	109	VAL	C-N-CA	6.41	128.87	120.28
1	d	231	PRO	CA-C-O	-6.41	109.91	119.34
1	g	85	ALA	CA-C-N	6.41	128.87	120.28
1	g	85	ALA	C-N-CA	6.41	128.87	120.28
1	C	81	LEU	N-CA-CB	6.41	119.39	109.97
1	e	131	PRO	N-CA-C	-6.41	101.58	111.13
2	5	152	GLU	CB-CG-CD	-6.41	101.70	112.60
3	I	227	PHE	CA-CB-CG	-6.41	107.39	113.80
3	K	88	VAL	N-CA-C	-6.41	98.64	107.99
1	B	91	ARG	CA-C-N	6.41	128.77	120.44
1	B	91	ARG	C-N-CA	6.41	128.77	120.44
2	3	133	GLU	CA-C-N	6.41	130.95	122.30
2	3	133	GLU	C-N-CA	6.41	130.95	122.30
3	K	119	LEU	CA-C-N	6.40	126.32	119.85
3	K	119	LEU	C-N-CA	6.40	126.32	119.85
1	f	196	MET	CA-C-N	6.40	127.20	120.03
1	f	196	MET	C-N-CA	6.40	127.20	120.03
2	n	31	ALA	N-CA-CB	6.40	121.44	110.68
2	3	154	ARG	N-CA-C	-6.40	105.05	112.92
3	I	65	VAL	N-CA-CB	6.40	118.12	110.95
3	L	156	ALA	CA-C-O	-6.40	113.64	120.42
3	L	201	ALA	O-C-N	6.40	129.83	122.99
1	b	168	ARG	CA-C-N	6.39	128.85	120.28
1	b	168	ARG	C-N-CA	6.39	128.85	120.28
1	f	50	ALA	CA-C-O	6.39	128.01	120.66
1	g	100	ARG	NE-CZ-NH1	-6.39	115.11	121.50
2	4	104	PHE	CA-C-O	-6.39	113.35	120.25
2	n	15	VAL	CB-CA-C	6.39	120.66	110.82
3	K	284	ILE	CA-C-N	6.39	130.50	121.30
3	K	284	ILE	C-N-CA	6.39	130.50	121.30
1	C	91	ARG	O-C-N	6.39	128.65	122.07
3	K	60	SER	CA-C-N	6.39	126.96	120.38
3	K	60	SER	C-N-CA	6.39	126.96	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	TYR	CA-C-N	6.39	131.43	122.36
1	E	103	TYR	C-N-CA	6.39	131.43	122.36
2	j	93	LEU	N-CA-C	6.39	118.32	111.36
3	I	291	ASP	CA-CB-CG	-6.39	106.21	112.60
3	J	137	GLU	CA-C-N	6.39	129.23	120.35
3	J	137	GLU	C-N-CA	6.39	129.23	120.35
1	F	38	ILE	CA-C-O	6.38	127.78	120.76
2	i	24	VAL	N-CA-C	-6.38	99.29	108.48
2	4	199	TYR	CB-CG-CD1	6.38	130.38	120.80
3	K	251	THR	N-CA-C	-6.38	100.83	110.28
3	M	234	ALA	N-CA-C	6.38	117.75	109.64
3	J	283	VAL	CA-C-N	6.38	133.19	121.70
3	J	283	VAL	C-N-CA	6.38	133.19	121.70
1	E	128	GLY	CA-C-N	-6.38	115.28	123.19
1	E	128	GLY	C-N-CA	-6.38	115.28	123.19
2	2	166	GLU	CA-C-N	6.38	128.83	120.28
2	2	166	GLU	C-N-CA	6.38	128.83	120.28
3	M	288	ASN	CB-CA-C	-6.38	100.82	110.90
2	h	40	LYS	N-CA-C	-6.38	106.46	114.56
2	k	156	THR	N-CA-C	-6.38	101.51	110.31
3	L	179	LEU	CA-C-N	6.38	131.80	123.00
3	L	179	LEU	C-N-CA	6.38	131.80	123.00
1	G	240	ILE	CA-C-N	6.38	128.82	120.28
1	G	240	ILE	C-N-CA	6.38	128.82	120.28
3	J	360	MET	CG-SD-CE	6.38	114.92	100.90
1	f	178	GLU	N-CA-CB	6.37	121.16	110.77
2	h	109	GLN	CA-C-N	6.37	132.15	122.65
2	h	109	GLN	C-N-CA	6.37	132.15	122.65
2	7	173	TYR	CA-C-N	6.37	128.82	120.28
2	7	173	TYR	C-N-CA	6.37	128.82	120.28
1	D	53	ARG	N-CA-CB	6.37	119.36	109.48
2	m	114	GLY	N-CA-C	-6.37	101.98	110.58
2	7	151	LEU	CA-C-N	6.37	129.34	120.29
2	7	151	LEU	C-N-CA	6.37	129.34	120.29
3	L	10	LEU	CA-C-O	-6.37	113.80	120.55
1	b	86	ARG	O-C-N	6.37	128.63	122.07
1	b	120	LYS	CA-C-N	6.37	128.82	120.28
1	b	120	LYS	C-N-CA	6.37	128.82	120.28
1	F	205	VAL	CA-C-O	-6.37	111.42	119.95
2	h	99	ASN	OD1-CG-ND2	6.37	128.97	122.60
2	2	156	THR	O-C-N	6.37	127.50	121.71
3	I	57	ARG	N-CA-C	-6.37	104.20	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	110	LYS	CA-C-N	6.37	128.71	120.44
1	d	110	LYS	C-N-CA	6.37	128.71	120.44
3	L	28	ARG	CA-CB-CG	6.36	126.83	114.10
1	D	124	THR	CA-C-O	6.36	127.16	120.42
2	n	84	LYS	CA-C-O	-6.36	113.77	119.75
3	K	95	ILE	CA-C-N	6.36	130.35	120.75
3	K	95	ILE	C-N-CA	6.36	130.35	120.75
1	b	51	ASP	CA-CB-CG	-6.36	106.24	112.60
1	B	99	ASN	CA-C-N	6.36	129.32	120.29
1	B	99	ASN	C-N-CA	6.36	129.32	120.29
2	7	30	ARG	NE-CZ-NH1	-6.36	115.14	121.50
2	5	150	VAL	O-C-N	-6.35	115.71	121.87
2	n	171	ALA	CB-CA-C	-6.35	100.24	110.79
3	L	325	THR	CA-C-O	-6.35	111.57	119.38
3	J	113	LEU	N-CA-C	6.35	118.34	110.91
1	E	91	ARG	N-CA-C	6.35	118.20	111.28
2	i	170	ARG	NE-CZ-NH1	-6.35	115.15	121.50
2	l	165	VAL	N-CA-CB	6.35	119.17	110.54
3	M	216	ILE	N-CA-C	-6.35	98.59	107.80
1	C	87	VAL	N-CA-C	6.35	117.09	110.62
1	g	111	GLU	CA-C-N	6.35	129.30	120.29
1	g	111	GLU	C-N-CA	6.35	129.30	120.29
1	F	84	ASP	CB-CA-C	-6.34	100.26	110.79
2	h	163	GLU	CB-CG-CD	-6.34	101.81	112.60
3	K	13	LEU	N-CA-CB	6.34	119.45	110.12
1	C	139	ALA	CA-C-O	6.34	126.96	120.24
3	K	280	ASP	N-CA-CB	6.34	121.15	110.69
3	J	19	ASP	CA-C-N	6.34	129.29	120.29
3	J	19	ASP	C-N-CA	6.34	129.29	120.29
1	g	174	PHE	N-CA-C	-6.34	104.37	111.28
2	6	62	ASP	CA-C-N	6.34	129.06	120.44
2	6	62	ASP	C-N-CA	6.34	129.06	120.44
1	B	131	PRO	N-CA-C	-6.33	101.19	111.77
1	F	82	VAL	CA-C-N	6.33	128.67	120.44
1	F	82	VAL	C-N-CA	6.33	128.67	120.44
2	i	78	GLU	O-C-N	6.33	128.83	122.12
2	k	25	MET	N-CA-C	-6.33	99.68	109.24
3	J	55	VAL	CA-C-O	-6.33	114.46	121.17
3	I	329	LYS	CA-C-O	-6.33	113.53	120.36
1	B	167	GLY	CA-C-N	6.33	128.66	120.44
1	B	167	GLY	C-N-CA	6.33	128.66	120.44
1	d	137	LEU	N-CA-CB	6.33	120.70	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	49	ILE	N-CA-C	-6.32	99.37	108.48
2	h	25	MET	CG-SD-CE	-6.32	86.99	100.90
2	k	166	GLU	O-C-N	6.32	128.92	122.09
2	m	200	SER	CA-C-N	6.32	127.74	119.84
2	m	200	SER	C-N-CA	6.32	127.74	119.84
1	e	58	LEU	N-CA-C	-6.32	103.92	111.69
2	n	173	TYR	CA-C-N	6.32	128.66	120.44
2	n	173	TYR	C-N-CA	6.32	128.66	120.44
1	e	123	TYR	N-CA-C	-6.32	105.51	113.72
1	b	214	VAL	N-CA-C	-6.32	95.36	106.61
3	H	13	LEU	O-C-N	-6.32	115.42	122.12
2	k	189	VAL	N-CA-C	-6.32	98.64	107.80
1	c	214	VAL	N-CA-C	-6.31	99.03	108.12
2	6	156	THR	O-C-N	6.31	126.69	121.32
1	g	89	ILE	CA-C-N	6.31	129.25	120.29
1	g	89	ILE	C-N-CA	6.31	129.25	120.29
2	3	150	VAL	CA-C-N	6.31	128.74	120.28
2	3	150	VAL	C-N-CA	6.31	128.74	120.28
3	J	162	LEU	CA-C-N	6.31	129.84	122.52
3	J	162	LEU	C-N-CA	6.31	129.84	122.52
1	A	82	VAL	CA-C-O	-6.31	114.39	120.95
1	C	149	GLU	CA-C-O	-6.31	113.32	120.32
1	a	233	VAL	O-C-N	6.30	128.32	121.83
2	3	41	ALA	N-CA-C	-6.30	104.21	112.41
2	k	206	GLN	OE1-CD-NE2	6.30	128.91	122.60
3	H	250	ARG	NE-CZ-NH2	6.30	124.87	119.20
3	K	12	LYS	N-CA-CB	6.30	119.15	110.01
3	H	34	LYS	N-CA-C	-6.30	105.59	113.28
1	C	107	ILE	CA-C-O	6.30	128.29	121.36
1	g	164	ILE	CA-C-O	-6.30	115.05	121.67
1	g	240	ILE	O-C-N	6.30	128.09	121.91
1	A	15	PHE	CA-C-N	6.30	131.11	121.03
1	A	15	PHE	C-N-CA	6.30	131.11	121.03
2	3	102	ARG	CA-C-N	6.30	129.23	120.29
2	3	102	ARG	C-N-CA	6.30	129.23	120.29
2	7	19	CYS	N-CA-C	-6.30	100.88	109.95
3	I	113	LEU	CA-C-N	6.30	130.43	121.42
3	I	113	LEU	C-N-CA	6.30	130.43	121.42
3	M	282	LYS	N-CA-CB	6.30	121.21	110.50
1	D	27	ALA	N-CA-C	-6.30	105.56	113.18
1	E	154	GLY	N-CA-C	-6.30	106.21	115.72
1	g	16	SER	CA-C-N	6.30	126.42	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	16	SER	C-N-CA	6.30	126.42	119.87
2	7	146	THR	CA-C-N	6.30	128.62	120.44
2	7	146	THR	C-N-CA	6.30	128.62	120.44
3	L	363	ILE	CA-C-O	-6.29	114.40	120.95
3	M	199	THR	N-CA-CB	6.29	119.14	110.01
1	C	180	ARG	N-CA-C	-6.29	99.84	109.41
1	F	177	LYS	O-C-N	6.29	129.79	122.17
1	G	226	PRO	N-CD-CG	6.29	112.64	103.20
3	K	128	TYR	N-CA-C	-6.29	99.89	108.38
1	D	172	THR	O-C-N	6.29	128.55	122.07
2	2	125	ILE	CA-C-N	6.29	130.93	120.86
2	2	125	ILE	C-N-CA	6.29	130.93	120.86
3	K	387	THR	CA-C-O	-6.29	114.16	120.64
3	K	12	LYS	CA-C-N	6.29	128.71	120.28
3	K	12	LYS	C-N-CA	6.29	128.71	120.28
1	G	98	ILE	CA-C-N	6.29	128.70	120.28
1	G	98	ILE	C-N-CA	6.29	128.70	120.28
2	l	194	ASP	N-CA-CB	-6.29	99.87	110.49
2	3	109	GLN	N-CA-C	-6.28	98.14	108.76
2	k	104	PHE	O-C-N	-6.28	115.70	121.42
2	j	63	ALA	N-CA-C	6.28	117.92	111.14
2	4	92	THR	N-CA-C	-6.28	104.32	112.23
3	L	93	GLN	N-CA-C	-6.28	104.09	112.94
3	L	224	ARG	CA-C-N	6.28	128.60	120.44
3	L	224	ARG	C-N-CA	6.28	128.60	120.44
3	J	115	ILE	N-CA-CB	6.28	117.79	110.82
2	n	50	ASP	CA-C-O	6.28	127.31	119.59
1	F	61	ALA	CA-C-N	6.28	128.60	120.44
1	F	61	ALA	C-N-CA	6.28	128.60	120.44
1	B	90	ASP	CA-C-O	-6.28	113.77	120.42
1	g	84	ASP	CA-C-O	6.28	127.07	120.42
2	5	102	ARG	N-CA-C	-6.28	105.78	113.50
2	m	84	LYS	CA-C-O	-6.28	113.97	120.87
3	H	324	HIS	N-CA-CB	6.27	119.17	110.07
2	2	72	ILE	CA-CB-CG2	6.27	121.16	110.50
2	l	105	PRO	N-CA-C	6.27	121.18	111.21
3	K	16	LEU	CA-C-N	6.27	128.69	120.28
3	K	16	LEU	C-N-CA	6.27	128.69	120.28
2	6	21	ASP	CA-CB-CG	6.27	118.87	112.60
3	M	375	PHE	CA-CB-CG	-6.27	107.53	113.80
1	d	191	LEU	CA-C-N	6.27	126.90	120.00
1	d	191	LEU	C-N-CA	6.27	126.90	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	50	ALA	CA-C-N	6.27	129.73	120.95
1	F	50	ALA	C-N-CA	6.27	129.73	120.95
3	H	112	THR	N-CA-C	-6.27	105.79	113.50
3	H	249	ARG	CD-NE-CZ	6.27	133.18	124.40
3	M	217	GLY	N-CA-C	-6.27	106.46	113.79
2	k	121	SER	O-C-N	6.27	129.69	122.99
3	L	314	PHE	CA-CB-CG	-6.27	107.53	113.80
1	f	118	ASP	CA-C-N	6.26	128.68	120.28
1	f	118	ASP	C-N-CA	6.26	128.68	120.28
2	6	43	LYS	N-CA-C	6.26	118.64	110.43
2	m	163	GLU	N-CA-C	-6.26	104.69	112.90
2	m	189	VAL	CA-C-N	6.26	131.82	123.05
2	m	189	VAL	C-N-CA	6.26	131.82	123.05
3	H	31	GLU	CA-C-N	6.26	129.19	120.29
3	H	31	GLU	C-N-CA	6.26	129.19	120.29
3	K	36	PHE	N-CA-CB	6.26	119.33	110.12
2	7	196	PHE	CA-CB-CG	6.26	120.06	113.80
1	B	196	MET	CA-C-N	6.26	127.97	120.14
1	B	196	MET	C-N-CA	6.26	127.97	120.14
1	b	144	VAL	CA-CB-CG2	6.26	121.04	110.40
2	1	101	TYR	CB-CG-CD2	-6.26	111.41	120.80
3	M	320	ILE	N-CA-C	6.26	117.00	110.62
1	b	12	ILE	N-CA-C	-6.26	105.25	111.88
2	3	109	GLN	CA-C-O	-6.26	113.37	120.32
2	5	75	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	a	38	ILE	N-CA-C	-6.25	98.67	108.86
1	B	52	LYS	CA-C-N	6.25	131.27	120.58
1	B	52	LYS	C-N-CA	6.25	131.27	120.58
1	g	62	ASP	CA-CB-CG	6.25	118.85	112.60
3	L	55	VAL	N-CA-CB	6.25	119.05	110.54
3	I	269	LEU	N-CA-C	6.25	124.12	110.80
3	L	298	LEU	N-CA-C	-6.25	105.52	113.02
3	I	315	GLU	CA-C-N	6.25	127.03	120.03
3	I	315	GLU	C-N-CA	6.25	127.03	120.03
2	5	90	ILE	CA-C-N	6.25	128.65	120.28
2	5	90	ILE	C-N-CA	6.25	128.65	120.28
2	j	77	TYR	CA-C-N	6.25	129.16	120.29
2	j	77	TYR	C-N-CA	6.25	129.16	120.29
1	e	24	VAL	CA-C-N	6.24	129.16	120.29
1	e	24	VAL	C-N-CA	6.24	129.16	120.29
3	H	123	LYS	CA-C-O	-6.24	114.31	121.68
2	h	172	ILE	CA-C-N	6.24	128.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	172	ILE	C-N-CA	6.24	128.64	120.28
2	4	197	TYR	CB-CG-CD2	6.24	130.16	120.80
3	L	29	ARG	N-CA-C	6.24	118.08	111.28
1	c	93	ARG	CB-CA-C	-6.24	101.09	110.88
3	I	162	LEU	N-CA-C	-6.24	105.99	113.97
2	6	95	SER	N-CA-CB	6.24	119.05	110.01
1	d	144	VAL	O-C-N	6.24	127.28	121.61
1	F	105	GLU	CB-CG-CD	-6.24	102.00	112.60
2	h	207	ILE	N-CA-C	-6.24	104.20	111.00
2	4	60	VAL	CB-CA-C	-6.24	103.87	112.04
3	K	342	ILE	CA-C-O	6.24	127.44	120.95
3	H	322	LYS	CA-C-N	6.23	128.41	120.56
3	H	322	LYS	C-N-CA	6.23	128.41	120.56
1	d	180	ARG	NE-CZ-NH1	-6.23	115.27	121.50
2	1	59	SER	N-CA-C	6.23	118.59	110.43
3	H	33	GLU	CA-C-O	-6.23	113.81	120.42
3	K	333	ASP	N-CA-C	-6.23	103.82	112.30
2	n	92	THR	O-C-N	6.23	128.49	122.07
3	J	87	PHE	CB-CG-CD1	-6.23	110.11	120.70
3	J	306	ILE	O-C-N	6.23	129.81	122.83
3	H	324	HIS	ND1-CE1-NE2	6.23	114.63	108.40
2	k	44	LYS	CB-CA-C	-6.23	100.78	110.37
1	A	196	MET	N-CA-CB	6.22	119.27	110.12
1	E	25	GLU	N-CA-C	6.22	118.87	111.71
3	M	325	THR	CA-C-N	6.22	128.91	120.38
3	M	325	THR	C-N-CA	6.22	128.91	120.38
3	J	211	PHE	CB-CG-CD2	-6.22	110.12	120.70
1	g	85	ALA	N-CA-CB	6.22	119.03	110.01
2	3	200	SER	N-CA-C	-6.22	101.03	108.25
2	k	213	LYS	N-CA-CB	6.22	121.08	110.50
2	6	40	LYS	N-CA-CB	6.22	121.00	110.49
1	B	35	ALA	CA-C-N	6.22	133.42	121.54
1	B	35	ALA	C-N-CA	6.22	133.42	121.54
1	A	177	LYS	CA-C-O	-6.22	112.54	120.31
1	f	27	ALA	CA-C-N	6.22	128.61	120.28
1	f	27	ALA	C-N-CA	6.22	128.61	120.28
1	f	59	LEU	CA-C-O	-6.22	113.96	121.05
1	b	169	ASN	CA-C-N	6.21	128.89	120.44
1	b	169	ASN	C-N-CA	6.21	128.89	120.44
1	c	151	ASP	CA-C-N	6.21	125.90	119.56
1	c	151	ASP	C-N-CA	6.21	125.90	119.56
1	D	119	PHE	CA-C-N	6.21	128.52	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	PHE	C-N-CA	6.21	128.52	120.44
3	M	180	LEU	N-CA-CB	6.21	120.33	110.57
3	K	320	ILE	CA-C-O	-6.21	114.27	120.85
2	i	157	PRO	CA-C-N	6.21	132.59	122.65
2	i	157	PRO	C-N-CA	6.21	132.59	122.65
2	j	104	PHE	CA-CB-CG	6.21	120.01	113.80
1	B	100	ARG	N-CA-CB	6.21	119.35	110.16
1	F	222	LYS	N-CA-C	-6.21	99.89	109.14
1	g	234	GLU	CA-C-N	6.21	128.60	120.28
1	g	234	GLU	C-N-CA	6.21	128.60	120.28
2	3	70	ILE	CA-C-O	-6.21	114.27	120.85
2	j	44	LYS	CA-C-N	6.21	131.68	123.11
2	j	44	LYS	C-N-CA	6.21	131.68	123.11
1	a	169	ASN	CA-CB-CG	-6.21	106.39	112.60
2	j	155	PHE	O-C-N	-6.21	115.99	122.94
1	E	25	GLU	CA-C-O	6.20	127.11	120.10
1	g	49	ILE	CB-CA-C	6.20	119.86	110.62
1	g	63	THR	N-CA-CB	6.20	120.21	111.15
2	2	28	GLU	N-CA-CB	6.20	120.39	110.46
3	I	251	THR	O-C-N	-6.20	115.24	122.87
1	d	149	GLU	N-CA-C	-6.20	99.29	109.40
1	b	147	LEU	N-CA-C	-6.20	97.32	108.48
2	n	156	THR	O-C-N	-6.20	116.71	121.55
3	I	378	ALA	CA-C-N	6.20	128.96	120.46
3	I	378	ALA	C-N-CA	6.20	128.96	120.46
3	M	45	GLU	CA-C-O	6.20	127.12	120.55
1	b	188	ALA	N-CA-C	6.20	118.03	111.28
2	5	87	VAL	CA-C-N	6.20	128.59	120.28
2	5	87	VAL	C-N-CA	6.20	128.59	120.28
3	L	173	GLU	CB-CA-C	-6.20	102.16	109.47
2	2	171	ALA	N-CA-C	-6.20	104.61	111.36
3	J	311	LEU	O-C-N	-6.20	113.28	121.34
1	C	100	ARG	CD-NE-CZ	-6.19	115.73	124.40
2	n	73	GLU	N-CA-C	-6.19	105.21	112.89
3	L	324	HIS	ND1-CE1-NE2	6.19	114.59	108.40
2	m	22	GLY	CA-C-N	6.19	131.97	122.25
2	m	22	GLY	C-N-CA	6.19	131.97	122.25
2	1	67	ALA	CA-C-N	6.19	128.57	120.28
2	1	67	ALA	C-N-CA	6.19	128.57	120.28
2	j	148	TYR	O-C-N	-6.19	115.56	122.12
1	C	148	TYR	N-CA-C	-6.19	100.35	109.81
1	F	154	GLY	N-CA-C	-6.19	106.23	114.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	88	LEU	N-CA-C	6.18	118.02	111.28
3	I	329	LYS	N-CA-C	-6.18	98.82	108.90
1	D	63	THR	CA-CB-OG1	6.18	118.87	109.60
3	K	119	LEU	O-C-N	-6.18	115.12	120.99
1	C	125	GLN	CB-CG-CD	-6.18	102.10	112.60
1	c	56	SER	CB-CA-C	-6.18	99.60	109.80
2	3	81	ARG	O-C-N	6.18	131.13	122.36
3	I	10	LEU	O-C-N	6.18	128.67	122.12
2	h	211	PHE	N-CA-C	-6.18	105.74	113.28
2	4	104	PHE	CA-C-N	6.18	126.09	119.85
2	4	104	PHE	C-N-CA	6.18	126.09	119.85
1	c	186	ASP	CA-C-N	6.18	129.06	120.29
1	c	186	ASP	C-N-CA	6.18	129.06	120.29
1	B	51	ASP	CA-C-O	-6.17	115.00	121.55
1	C	138	ILE	N-CA-CB	6.17	119.13	111.41
2	3	198	GLN	CA-C-N	6.17	133.52	121.66
2	3	198	GLN	C-N-CA	6.17	133.52	121.66
3	L	86	LYS	N-CA-C	-6.17	99.34	109.40
3	M	224	ARG	NE-CZ-NH1	-6.17	115.33	121.50
3	K	156	ALA	N-CA-C	6.17	117.81	111.14
1	F	16	SER	N-CA-C	-6.17	101.12	110.50
3	M	365	GLU	O-C-N	6.17	130.35	122.39
3	L	394	GLY	O-C-N	-6.17	116.32	122.86
1	A	77	ALA	CA-C-O	-6.17	114.14	121.66
1	E	232	TYR	CA-C-N	6.17	128.33	120.56
1	E	232	TYR	C-N-CA	6.17	128.33	120.56
2	j	78	GLU	CA-C-O	-6.17	113.88	120.42
2	1	209	ALA	N-CA-C	-6.17	105.52	113.16
2	i	173	TYR	O-C-N	6.17	128.66	122.12
2	4	43	LYS	N-CA-C	6.16	118.92	110.24
1	F	103	TYR	N-CA-CB	6.16	120.14	111.15
1	g	72	GLU	CB-CG-CD	-6.16	102.13	112.60
2	j	126	ASP	CA-CB-CG	-6.16	106.44	112.60
2	l	129	GLY	CA-C-O	-6.16	117.30	122.29
1	f	237	ASN	CA-C-O	6.16	127.06	120.10
1	g	70	ILE	CB-CA-C	-6.16	105.64	111.06
3	I	163	LYS	CA-C-O	-6.16	111.72	120.16
1	E	91	ARG	NE-CZ-NH1	-6.16	115.34	121.50
2	1	91	ALA	N-CA-CB	6.16	119.27	110.16
2	k	202	GLU	O-C-N	6.16	128.49	122.09
1	c	239	ARG	CD-NE-CZ	-6.15	115.78	124.40
3	H	65	VAL	CA-CB-CG1	6.15	120.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	TYR	CB-CG-CD2	6.15	130.03	120.80
1	G	221	PHE	CA-CB-CG	-6.15	107.65	113.80
2	n	62	ASP	CA-C-N	6.15	128.52	120.28
2	n	62	ASP	C-N-CA	6.15	128.52	120.28
3	J	170	VAL	N-CA-C	-6.15	105.66	113.22
3	H	20	TYR	CB-CG-CD2	-6.15	111.58	120.80
2	6	13	THR	CA-CB-OG1	6.14	118.81	109.60
3	I	74	ASP	CA-C-N	6.14	130.86	120.91
3	I	74	ASP	C-N-CA	6.14	130.86	120.91
3	L	9	LEU	CA-C-N	6.14	128.51	120.28
3	L	9	LEU	C-N-CA	6.14	128.51	120.28
1	A	85	ALA	CA-C-N	6.14	128.51	120.28
1	A	85	ALA	C-N-CA	6.14	128.51	120.28
2	l	80	ARG	NE-CZ-NH1	-6.14	115.36	121.50
3	I	168	ALA	CA-C-O	6.14	127.27	120.82
1	D	14	VAL	N-CA-C	6.14	117.66	109.37
1	F	144	VAL	N-CA-CB	6.14	119.80	111.21
1	f	42	CYS	N-CA-C	-6.14	100.08	109.41
2	4	146	THR	N-CA-CB	6.14	119.25	110.16
3	J	141	GLU	CA-C-N	6.14	131.87	122.29
3	J	141	GLU	C-N-CA	6.14	131.87	122.29
3	I	78	VAL	N-CA-CB	6.13	118.39	111.21
3	K	303	PHE	N-CA-C	-6.13	97.58	108.13
1	B	163	ALA	N-CA-C	-6.13	99.75	109.07
1	e	53	ARG	NE-CZ-NH2	6.13	124.72	119.20
3	I	265	MET	CB-CA-C	-6.13	101.25	110.88
1	C	98	ILE	CA-CB-CG1	-6.13	99.98	110.40
3	H	49	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	A	160	LYS	CB-CA-C	-6.12	99.23	109.27
2	i	17	LEU	CA-C-N	6.12	130.27	122.37
2	i	17	LEU	C-N-CA	6.12	130.27	122.37
2	6	93	LEU	CA-C-N	6.12	128.99	120.29
2	6	93	LEU	C-N-CA	6.12	128.99	120.29
1	b	32	LYS	CA-C-N	6.12	128.40	120.44
1	b	32	LYS	C-N-CA	6.12	128.40	120.44
1	D	241	ARG	N-CA-C	6.12	117.95	111.28
1	d	52	LYS	N-CA-C	-6.12	104.16	111.69
3	I	86	LYS	N-CA-C	-6.12	100.59	110.32
1	g	19	GLY	O-C-N	-6.12	114.76	122.41
2	h	115	ILE	CA-C-N	6.12	131.84	122.11
2	h	115	ILE	C-N-CA	6.12	131.84	122.11
1	A	39	GLY	CA-C-O	-6.12	114.76	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	192	THR	CA-C-O	6.12	126.51	119.35
3	I	386	THR	O-C-N	-6.12	114.45	122.59
3	K	108	LEU	CB-CA-C	-6.12	98.37	109.38
1	f	118	ASP	CA-CB-CG	6.12	118.72	112.60
1	c	31	VAL	CA-CB-CG1	-6.12	100.00	110.40
1	e	223	GLU	N-CA-C	-6.12	99.43	109.40
2	4	64	GLN	CB-CG-CD	-6.11	102.21	112.60
1	g	191	LEU	CA-C-O	-6.11	113.94	120.42
1	a	191	LEU	O-C-N	6.11	128.59	122.12
3	L	123	LYS	CA-C-N	6.11	132.69	121.70
3	L	123	LYS	C-N-CA	6.11	132.69	121.70
3	L	190	LEU	N-CA-C	-6.11	104.70	111.36
1	A	163	ALA	N-CA-C	-6.11	100.04	109.14
1	a	207	GLU	N-CA-C	-6.11	105.78	113.72
1	a	216	VAL	CA-C-O	6.11	124.76	118.96
1	g	160	LYS	N-CA-C	-6.11	105.66	113.23
3	K	198	GLN	N-CA-CB	6.10	119.19	110.16
2	3	60	VAL	N-CA-C	6.10	116.88	110.72
1	b	58	LEU	CA-C-O	6.10	126.11	119.15
2	n	49	ALA	CA-C-O	-6.10	114.68	121.51
1	g	63	THR	N-CA-C	-6.10	107.06	114.75
1	d	152	PRO	N-CA-CB	6.10	109.14	103.41
1	g	169	ASN	CA-CB-CG	-6.10	106.50	112.60
1	g	218	ASP	CA-C-N	6.10	133.18	121.54
1	g	218	ASP	C-N-CA	6.10	133.18	121.54
3	I	90	ASN	CA-CB-CG	-6.09	106.51	112.60
3	I	190	LEU	CA-C-N	6.09	128.45	120.28
3	I	190	LEU	C-N-CA	6.09	128.45	120.28
1	B	128	GLY	N-CA-C	-6.09	105.16	115.34
3	M	218	GLU	CB-CG-CD	-6.09	102.24	112.60
3	J	239	PHE	N-CA-C	-6.09	97.21	107.99
1	C	242	GLU	N-CA-C	6.09	117.92	111.28
1	b	103	TYR	CB-CA-C	-6.09	99.16	109.38
3	L	127	VAL	CA-C-O	-6.09	114.71	119.46
3	M	352	LYS	N-CA-C	-6.09	104.72	111.36
1	A	222	LYS	N-CA-C	-6.08	100.08	109.14
3	M	228	GLN	OE1-CD-NE2	6.08	128.68	122.60
2	k	191	ILE	CA-CB-CG1	-6.08	100.06	110.40
1	D	28	ARG	N-CA-C	-6.08	105.69	113.23
1	f	52	LYS	CA-C-O	-6.08	113.36	120.53
2	j	103	TYR	CA-C-O	-6.08	114.44	120.82
2	l	169	VAL	O-C-N	-6.08	115.97	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	67	VAL	N-CA-CB	6.08	123.29	111.92
3	M	183	PRO	O-C-N	-6.08	114.29	121.46
3	J	99	GLU	CA-C-O	6.08	126.76	119.59
3	K	52	ARG	CA-C-N	6.07	128.42	120.28
3	K	52	ARG	C-N-CA	6.07	128.42	120.28
1	F	24	VAL	N-CA-C	-6.07	104.38	111.00
2	5	202	GLU	N-CA-CB	6.07	118.98	109.94
2	n	15	VAL	O-C-N	-6.07	116.66	123.03
1	a	62	ASP	N-CA-C	-6.07	104.38	112.94
1	D	103	TYR	CB-CG-CD1	-6.07	111.70	120.80
2	6	29	LYS	CA-C-O	-6.07	114.45	120.70
1	b	89	ILE	CA-C-N	6.07	128.90	120.29
1	b	89	ILE	C-N-CA	6.07	128.90	120.29
1	G	200	ILE	O-C-N	6.07	128.42	122.05
1	a	245	LYS	N-CA-C	-6.06	104.31	113.89
1	c	181	ASP	N-CA-CB	6.06	119.83	110.80
1	E	159	TYR	N-CA-C	-6.06	100.08	109.24
3	M	123	LYS	CB-CA-C	-6.06	108.34	117.07
1	a	66	LYS	N-CA-C	-6.06	103.32	111.87
1	G	240	ILE	CA-C-O	-6.06	114.42	120.85
2	h	175	ALA	N-CA-C	-6.06	104.23	111.69
2	h	198	GLN	CA-C-N	6.06	128.40	120.28
2	h	198	GLN	C-N-CA	6.06	128.40	120.28
1	a	143	GLU	CA-C-N	6.06	133.34	122.13
1	a	143	GLU	C-N-CA	6.06	133.34	122.13
1	d	104	ASP	CA-CB-CG	-6.06	106.54	112.60
3	J	96	ASN	N-CA-C	-6.06	100.32	108.86
1	C	173	GLU	CA-C-N	6.06	128.87	120.63
1	C	173	GLU	C-N-CA	6.06	128.87	120.63
3	M	381	LYS	CA-C-O	6.06	126.97	120.55
2	h	68	ARG	CA-CB-CG	-6.05	101.99	114.10
3	K	397	PHE	N-CA-CB	6.05	120.01	110.87
3	L	379	ILE	CA-C-N	6.05	128.39	120.28
3	L	379	ILE	C-N-CA	6.05	128.39	120.28
1	e	182	ASP	N-CA-C	-6.05	104.07	112.30
3	I	233	LYS	CA-C-N	6.05	129.86	120.60
3	I	233	LYS	C-N-CA	6.05	129.86	120.60
1	f	230	LYS	CA-C-N	6.05	125.53	119.24
1	f	230	LYS	C-N-CA	6.05	125.53	119.24
3	H	326	ARG	N-CA-C	6.05	117.87	111.28
1	A	40	ILE	CA-CB-CG1	6.05	120.68	110.40
2	l	108	VAL	N-CA-C	-6.05	99.77	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	GLY	N-CA-C	-6.04	105.49	112.50
1	C	21	LEU	N-CA-C	-6.04	99.36	108.96
1	d	95	GLU	CA-C-O	6.04	126.95	120.55
3	L	218	GLU	CA-C-N	6.04	132.57	121.70
3	L	218	GLU	C-N-CA	6.04	132.57	121.70
3	J	19	ASP	CA-CB-CG	-6.04	106.56	112.60
1	b	228	GLU	N-CA-C	-6.04	106.24	113.97
1	d	177	LYS	O-C-N	6.04	130.45	122.30
2	m	211	PHE	CA-CB-CG	-6.04	107.76	113.80
2	6	146	THR	CA-C-N	6.04	128.37	120.28
2	6	146	THR	C-N-CA	6.04	128.37	120.28
3	H	21	TYR	CA-C-N	6.04	128.86	120.29
3	H	21	TYR	C-N-CA	6.04	128.86	120.29
3	I	356	THR	O-C-N	6.04	128.29	122.07
1	b	242	GLU	N-CA-CB	6.04	118.76	110.01
1	G	113	ALA	N-CA-C	6.04	117.86	111.28
1	g	148	TYR	CA-C-O	6.04	127.75	120.99
2	i	99	ASN	CA-CB-CG	-6.04	106.56	112.60
2	4	21	ASP	CA-CB-CG	6.04	118.64	112.60
2	k	86	THR	CA-C-O	-6.04	114.30	121.66
3	L	220	ALA	CA-C-N	6.04	128.37	120.28
3	L	220	ALA	C-N-CA	6.04	128.37	120.28
1	D	157	LEU	N-CA-C	-6.03	98.01	108.69
2	i	193	GLU	CA-CB-CG	6.03	126.17	114.10
2	n	38	ALA	N-CA-C	-6.03	104.27	111.69
1	B	188	ALA	N-CA-CB	6.03	118.99	110.12
2	1	37	ILE	N-CA-C	-6.03	98.84	107.77
3	I	235	PRO	N-CA-CB	6.03	109.23	102.60
2	j	95	SER	O-C-N	6.03	128.51	122.12
3	L	168	ALA	CA-C-N	6.03	128.36	120.28
3	L	168	ALA	C-N-CA	6.03	128.36	120.28
1	A	15	PHE	N-CA-C	-6.03	100.73	110.32
2	i	162	ASP	CA-CB-CG	-6.03	106.57	112.60
2	k	77	TYR	CA-C-N	6.03	128.84	120.29
2	k	77	TYR	C-N-CA	6.03	128.84	120.29
2	7	180	SER	N-CA-C	-6.02	105.97	113.38
2	n	162	ASP	CA-C-N	6.02	128.84	120.29
2	n	162	ASP	C-N-CA	6.02	128.84	120.29
2	n	43	LYS	N-CA-CB	6.02	119.79	110.21
2	n	69	ILE	O-C-N	6.02	127.81	121.91
3	H	191	LEU	CA-C-N	6.02	128.27	120.44
3	H	191	LEU	C-N-CA	6.02	128.27	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	101	LYS	O-C-N	-6.02	117.64	121.85
1	e	109	VAL	N-CA-C	-6.02	104.48	110.62
3	H	361	PHE	CA-CB-CG	-6.02	107.78	113.80
3	L	66	GLY	CA-C-N	6.02	131.49	122.58
3	L	66	GLY	C-N-CA	6.02	131.49	122.58
2	5	90	ILE	N-CA-C	-6.02	104.48	110.62
3	H	388	PRO	CA-C-N	6.02	133.26	122.13
3	H	388	PRO	C-N-CA	6.02	133.26	122.13
3	J	299	ARG	CA-C-O	-6.02	114.25	120.87
3	H	47	GLU	N-CA-C	6.02	118.63	111.71
3	J	145	GLY	N-CA-C	-6.01	107.02	115.32
1	F	230	LYS	CA-C-O	-6.01	113.10	118.63
3	I	387	THR	N-CA-CB	6.01	121.72	111.50
3	K	274	GLY	N-CA-C	6.01	121.11	113.24
3	H	305	ARG	CD-NE-CZ	-6.01	115.99	124.40
2	m	42	ALA	N-CA-CB	6.01	120.73	111.24
3	L	167	PHE	O-C-N	-6.01	115.30	122.15
2	m	138	VAL	O-C-N	-6.00	117.75	122.97
1	D	232	TYR	CA-C-N	6.00	128.68	120.46
1	D	232	TYR	C-N-CA	6.00	128.68	120.46
2	3	112	ILE	O-C-N	-6.00	116.84	123.20
3	L	149	GLN	CA-C-N	6.00	128.68	120.46
3	L	149	GLN	C-N-CA	6.00	128.68	120.46
2	7	101	TYR	N-CA-CB	6.00	119.67	110.79
1	f	183	LEU	O-C-N	6.00	129.77	122.75
1	g	22	PHE	CA-CB-CG	-6.00	107.80	113.80
2	3	152	GLU	CA-C-N	6.00	128.60	120.44
2	3	152	GLU	C-N-CA	6.00	128.60	120.44
3	I	190	LEU	N-CA-C	6.00	117.82	111.28
1	c	101	LEU	CA-C-O	6.00	126.90	120.24
1	b	46	VAL	O-C-N	-5.99	116.14	123.03
3	L	325	THR	CA-CB-OG1	5.99	118.59	109.60
1	A	233	VAL	CA-CB-CG2	-5.99	100.21	110.40
2	k	75	ASN	N-CA-CB	5.99	119.03	110.16
2	l	83	ARG	N-CA-CB	5.99	120.85	111.56
3	M	11	GLU	O-C-N	5.99	128.24	122.07
1	E	87	VAL	CA-CB-CG1	5.99	120.58	110.40
1	E	187	ASP	CA-CB-CG	-5.99	106.61	112.60
3	J	27	TYR	CB-CG-CD2	5.99	129.78	120.80
1	a	209	ILE	CA-C-O	-5.99	115.38	121.67
1	e	240	ILE	CA-C-N	5.99	128.59	120.38
1	e	240	ILE	C-N-CA	5.99	128.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	111	LEU	CB-CA-C	-5.99	98.75	109.71
2	j	204	VAL	N-CA-CB	5.99	119.56	110.58
2	5	93	LEU	N-CA-C	-5.99	104.75	111.28
1	A	77	ALA	CB-CA-C	-5.99	99.92	109.80
1	D	90	ASP	CA-C-N	5.99	128.30	120.28
1	D	90	ASP	C-N-CA	5.99	128.30	120.28
1	d	160	LYS	CA-C-O	5.99	126.24	119.18
2	4	196	PHE	CA-CB-CG	5.99	119.78	113.80
2	l	18	VAL	N-CA-CB	5.99	117.05	110.53
1	C	218	ASP	N-CA-C	-5.98	106.52	113.88
1	c	183	LEU	O-C-N	5.98	130.19	122.89
1	D	107	ILE	CA-C-N	5.98	133.89	121.32
1	D	107	ILE	C-N-CA	5.98	133.89	121.32
1	F	182	ASP	N-CA-C	-5.98	105.80	114.12
2	2	60	VAL	CB-CA-C	-5.98	104.31	111.97
2	1	161	VAL	CA-C-N	5.98	128.30	120.28
2	1	161	VAL	C-N-CA	5.98	128.30	120.28
2	3	168	ALA	N-CA-CB	5.98	118.92	110.12
3	J	331	ALA	CA-C-N	5.98	128.58	120.44
3	J	331	ALA	C-N-CA	5.98	128.58	120.44
2	3	72	ILE	N-CA-CB	-5.98	102.41	110.54
3	I	152	GLU	CB-CA-C	-5.98	100.69	110.85
3	M	392	LEU	N-CA-C	-5.98	105.97	113.20
2	n	159	ILE	CA-C-N	5.98	128.88	121.83
2	n	159	ILE	C-N-CA	5.98	128.88	121.83
2	6	186	ILE	CA-C-N	5.98	132.41	122.73
2	6	186	ILE	C-N-CA	5.98	132.41	122.73
3	J	225	GLU	N-CA-C	5.98	117.87	111.36
3	H	174	PRO	N-CA-C	5.97	117.99	110.70
3	K	144	GLY	N-CA-C	-5.97	101.76	110.90
1	B	84	ASP	O-C-N	5.97	129.62	122.27
1	B	125	GLN	CB-CG-CD	-5.97	102.45	112.60
1	E	36	THR	CA-CB-OG1	5.97	118.56	109.60
3	K	128	TYR	N-CA-CB	5.97	120.68	111.24
2	1	40	LYS	N-CA-C	-5.97	104.40	111.03
2	2	108	VAL	CA-C-O	-5.97	114.51	120.90
2	2	189	VAL	N-CA-CB	5.97	121.24	111.45
3	K	298	LEU	CA-C-N	5.97	128.77	120.65
3	K	298	LEU	C-N-CA	5.97	128.77	120.65
3	M	227	PHE	N-CA-C	-5.97	104.35	111.69
1	a	80	GLY	N-CA-C	-5.97	105.00	111.21
1	D	59	LEU	N-CA-CB	5.97	118.84	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	239	ARG	CA-C-N	5.97	128.08	120.56
1	g	239	ARG	C-N-CA	5.97	128.08	120.56
3	J	377	LYS	CA-C-N	5.97	128.28	120.28
3	J	377	LYS	C-N-CA	5.97	128.28	120.28
1	F	180	ARG	N-CA-C	-5.97	100.23	109.24
3	J	67	VAL	N-CA-C	-5.97	99.53	108.12
3	J	390	PRO	N-CA-CB	-5.97	96.98	103.25
1	F	157	LEU	N-CA-CB	5.96	121.12	110.80
1	f	128	GLY	CA-C-N	5.96	130.53	122.90
1	f	128	GLY	C-N-CA	5.96	130.53	122.90
3	I	17	GLU	CA-C-N	5.96	128.19	120.44
3	I	17	GLU	C-N-CA	5.96	128.19	120.44
1	A	230	LYS	N-CA-CB	5.96	120.98	110.37
1	c	175	PHE	CA-C-O	5.96	126.74	119.11
3	K	397	PHE	N-CA-C	-5.96	101.10	109.69
1	a	188	ALA	N-CA-C	5.96	117.78	111.28
1	d	120	LYS	N-CA-CB	5.96	118.98	110.16
2	m	132	ILE	CA-CB-CG2	-5.96	100.36	110.50
1	c	185	PHE	CA-C-N	5.96	128.75	120.29
1	c	185	PHE	C-N-CA	5.96	128.75	120.29
3	H	39	SER	CB-CA-C	-5.96	101.52	110.88
1	d	21	LEU	N-CA-CB	5.96	118.73	109.97
1	G	180	ARG	NE-CZ-NH2	5.96	124.56	119.20
2	6	68	ARG	NE-CZ-NH2	5.96	124.56	119.20
3	M	203	PHE	CB-CG-CD1	-5.96	110.57	120.70
3	M	337	LYS	N-CA-C	5.96	117.85	111.36
3	I	302	ARG	N-CA-CB	5.96	120.56	110.49
3	I	360	MET	CA-C-N	5.96	128.75	120.29
3	I	360	MET	C-N-CA	5.96	128.75	120.29
1	B	240	ILE	CA-C-N	5.95	128.74	120.29
1	B	240	ILE	C-N-CA	5.95	128.74	120.29
1	F	38	ILE	CA-C-N	5.95	126.19	121.61
1	F	38	ILE	C-N-CA	5.95	126.19	121.61
3	I	361	PHE	N-CA-C	-5.95	104.87	111.36
1	f	93	ARG	N-CA-C	-5.95	104.37	111.69
2	1	45	ILE	O-C-N	-5.95	116.77	123.20
1	a	109	VAL	CB-CA-C	-5.95	104.11	112.14
2	3	51	ARG	CB-CA-C	-5.95	100.13	111.97
2	5	173	TYR	CA-C-N	5.95	128.25	120.28
2	5	173	TYR	C-N-CA	5.95	128.25	120.28
2	6	132	ILE	N-CA-C	-5.95	100.11	108.80
3	L	59	ARG	N-CA-C	-5.95	105.85	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	CYS	O-C-N	-5.95	114.79	122.94
3	L	394	GLY	CA-C-N	5.95	132.40	121.70
3	L	394	GLY	C-N-CA	5.95	132.40	121.70
1	e	188	ALA	CA-C-O	-5.95	113.38	120.10
2	4	101	TYR	CB-CG-CD2	5.95	129.72	120.80
3	J	371	THR	CA-C-N	5.95	128.53	120.38
3	J	371	THR	C-N-CA	5.95	128.53	120.38
1	g	141	VAL	N-CA-C	-5.94	98.97	107.77
1	a	93	ARG	NE-CZ-NH2	5.94	124.55	119.20
2	i	201	PRO	CA-C-N	5.94	128.56	120.54
2	i	201	PRO	C-N-CA	5.94	128.56	120.54
2	6	154	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	a	225	SER	CA-C-O	-5.94	113.84	120.25
1	B	185	PHE	CA-C-O	5.94	127.05	120.82
1	f	103	TYR	N-CA-C	-5.94	107.85	114.62
3	K	60	SER	CA-C-O	-5.94	114.23	120.70
1	a	117	CYS	CA-C-N	5.94	128.24	120.28
1	a	117	CYS	C-N-CA	5.94	128.24	120.28
1	D	142	ASP	N-CA-C	-5.94	104.44	111.03
2	2	169	VAL	CA-C-N	5.94	128.16	120.44
2	2	169	VAL	C-N-CA	5.94	128.16	120.44
3	K	278	ARG	CB-CA-C	-5.93	101.21	111.30
3	L	48	VAL	N-CA-CB	5.93	117.49	110.55
3	J	158	GLU	CB-CG-CD	-5.93	102.51	112.60
3	J	385	LYS	CA-C-N	5.93	132.88	121.54
3	J	385	LYS	C-N-CA	5.93	132.88	121.54
2	5	21	ASP	N-CA-C	-5.93	103.41	110.41
1	A	59	LEU	CA-C-N	5.93	130.89	120.87
1	A	59	LEU	C-N-CA	5.93	130.89	120.87
1	g	195	ALA	N-CA-CB	5.93	118.94	110.16
2	m	68	ARG	NH1-CZ-NH2	-5.93	111.59	119.30
3	I	358	ALA	N-CA-C	5.93	117.74	111.28
1	b	73	HIS	ND1-CE1-NE2	5.93	114.33	108.40
1	f	202	SER	CB-CA-C	-5.93	97.64	111.09
2	j	117	SER	N-CA-C	-5.93	104.90	111.36
3	I	154	ARG	N-CA-CB	5.93	118.83	109.82
1	c	238	GLU	CB-CA-C	-5.92	101.58	110.88
1	D	196	MET	O-C-N	-5.92	115.29	122.22
2	l	104	PHE	O-C-N	-5.92	116.43	121.23
2	n	201	PRO	CA-C-N	5.92	128.54	120.54
2	n	201	PRO	C-N-CA	5.92	128.54	120.54
3	J	154	ARG	CB-CA-C	-5.92	100.96	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	131	PRO	CA-C-N	5.92	129.69	120.75
1	e	131	PRO	C-N-CA	5.92	129.69	120.75
2	1	171	ALA	CA-C-O	5.92	126.70	120.42
2	h	56	THR	CA-C-N	5.92	132.11	122.81
2	h	56	THR	C-N-CA	5.92	132.11	122.81
2	3	212	ARG	N-CA-C	-5.92	99.00	109.06
2	l	157	PRO	N-CA-C	-5.92	106.34	114.98
1	E	230	LYS	O-C-N	-5.92	115.01	120.51
1	G	64	ILE	CA-C-N	5.92	132.35	121.70
1	G	64	ILE	C-N-CA	5.92	132.35	121.70
2	3	55	THR	N-CA-C	-5.92	100.54	109.95
2	n	13	THR	O-C-N	-5.92	116.85	123.48
1	F	174	PHE	CA-C-O	-5.92	114.28	120.55
2	l	121	SER	N-CA-C	-5.92	99.15	108.14
2	n	120	LYS	CA-C-O	-5.92	114.31	120.70
3	I	254	ASP	CA-CB-CG	5.92	118.52	112.60
3	L	195	VAL	CA-C-N	5.92	128.21	120.28
3	L	195	VAL	C-N-CA	5.92	128.21	120.28
1	B	76	ALA	CA-C-N	5.92	132.90	122.67
1	B	76	ALA	C-N-CA	5.92	132.90	122.67
2	n	106	TYR	N-CA-C	-5.92	99.00	109.06
3	M	91	THR	O-C-N	-5.92	114.72	122.59
1	a	189	MET	O-C-N	-5.91	115.41	122.15
1	G	235	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	7	121	SER	CA-C-O	-5.91	114.90	121.23
1	D	139	ALA	N-CA-C	-5.91	99.26	108.90
3	M	161	LEU	O-C-N	5.91	128.47	122.09
1	d	203	GLU	CB-CA-C	-5.91	99.40	109.51
2	7	32	THR	CA-CB-OG1	5.91	118.47	109.60
3	I	69	SER	N-CA-C	-5.91	104.23	112.45
3	M	281	VAL	O-C-N	-5.91	116.94	123.03
1	a	172	THR	CA-C-O	5.91	126.68	120.42
2	5	73	GLU	CA-C-O	-5.91	111.98	119.31
2	6	59	SER	CA-C-N	5.91	128.55	120.46
2	6	59	SER	C-N-CA	5.91	128.55	120.46
3	L	392	LEU	CA-C-O	5.91	130.84	120.80
3	H	51	LEU	CA-C-N	5.91	128.19	120.28
3	H	51	LEU	C-N-CA	5.91	128.19	120.28
1	a	120	LYS	CA-C-N	5.90	128.78	120.28
1	a	120	LYS	C-N-CA	5.90	128.78	120.28
2	j	147	ALA	CA-C-N	5.90	128.19	120.28
2	j	147	ALA	C-N-CA	5.90	128.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	207	ILE	N-CA-C	-5.90	104.98	110.53
1	a	18	ASP	N-CA-C	-5.90	106.04	113.18
3	I	267	GLN	N-CA-CB	5.90	118.90	110.16
3	J	281	VAL	CA-C-O	-5.90	114.31	120.27
2	h	192	THR	CA-C-N	5.90	132.81	121.54
2	h	192	THR	C-N-CA	5.90	132.81	121.54
3	M	265	MET	CA-C-N	5.90	128.67	120.29
3	M	265	MET	C-N-CA	5.90	128.67	120.29
1	e	47	ILE	N-CA-C	-5.90	99.85	108.11
2	l	74	ALA	CA-C-O	5.90	126.67	120.42
3	K	237	ILE	CA-C-O	5.90	126.09	120.31
3	J	47	GLU	CA-C-N	5.90	127.99	120.56
3	J	47	GLU	C-N-CA	5.90	127.99	120.56
1	c	22	PHE	N-CA-C	5.89	117.71	111.28
1	D	20	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	d	12	ILE	CA-C-O	5.89	125.45	119.20
3	K	41	ARG	CA-C-N	5.89	128.54	120.46
3	K	41	ARG	C-N-CA	5.89	128.54	120.46
1	D	77	ALA	N-CA-C	-5.89	101.01	110.14
3	J	382	VAL	CA-C-N	5.89	130.03	120.60
3	J	382	VAL	C-N-CA	5.89	130.03	120.60
1	e	33	ARG	NE-CZ-NH1	-5.89	115.61	121.50
3	J	351	ILE	CA-C-N	5.89	128.17	120.28
3	J	351	ILE	C-N-CA	5.89	128.17	120.28
2	3	37	ILE	N-CA-C	-5.89	99.64	108.12
2	j	71	LYS	CA-C-N	5.89	127.98	120.56
2	j	71	LYS	C-N-CA	5.89	127.98	120.56
2	m	55	THR	N-CA-C	-5.89	100.19	109.50
3	L	110	GLN	N-CA-C	-5.89	106.33	112.93
1	b	46	VAL	CA-C-O	5.89	126.94	120.64
1	a	168	ARG	CA-C-N	5.88	129.65	120.82
1	a	168	ARG	C-N-CA	5.88	129.65	120.82
1	c	50	ALA	CA-C-O	5.88	127.66	120.60
2	k	178	ARG	NE-CZ-NH1	-5.88	115.62	121.50
3	M	50	ARG	N-CA-C	-5.88	104.78	111.14
3	I	102	PRO	CA-C-O	-5.88	114.91	121.32
2	j	91	ALA	CA-C-N	5.88	128.16	120.28
2	j	91	ALA	C-N-CA	5.88	128.16	120.28
2	k	189	VAL	CA-C-O	5.88	126.82	120.53
1	f	71	ASP	CA-C-N	5.88	129.25	120.31
1	f	71	ASP	C-N-CA	5.88	129.25	120.31
2	n	23	VAL	CA-C-O	-5.88	115.05	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	346	ALA	O-C-N	5.88	130.09	123.27
3	K	286	ALA	N-CA-CB	5.88	121.68	111.39
3	J	221	ARG	CB-CG-CD	5.88	124.82	111.30
1	a	91	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	F	237	ASN	CA-C-N	5.88	128.15	120.28
1	F	237	ASN	C-N-CA	5.88	128.15	120.28
2	6	148	TYR	CA-CB-CG	5.88	124.48	113.90
3	M	183	PRO	N-CA-C	-5.88	103.53	110.70
3	J	77	VAL	CA-C-O	-5.88	114.02	120.43
3	L	271	GLU	N-CA-C	5.88	117.36	111.07
1	A	84	ASP	N-CA-C	5.87	118.63	111.82
1	B	26	TYR	N-CA-C	-5.87	106.16	113.38
1	F	172	THR	CA-C-N	5.87	128.63	120.29
1	F	172	THR	C-N-CA	5.87	128.63	120.29
2	j	140	THR	O-C-N	-5.87	117.06	123.52
2	5	62	ASP	CA-C-N	5.87	128.63	120.29
2	5	62	ASP	C-N-CA	5.87	128.63	120.29
1	A	164	ILE	CA-CB-CG1	5.87	120.38	110.40
1	G	37	ALA	N-CA-C	-5.87	99.04	108.55
3	I	147	ASP	CA-C-N	5.87	127.96	120.56
3	I	147	ASP	C-N-CA	5.87	127.96	120.56
3	M	379	ILE	N-CA-C	5.87	116.61	110.62
1	B	55	GLY	N-CA-C	-5.87	102.78	110.29
1	e	87	VAL	N-CA-CB	5.87	119.38	110.58
1	e	114	LYS	N-CA-C	5.87	117.68	111.28
1	g	149	GLU	N-CA-C	-5.87	99.62	109.07
2	4	172	ILE	CA-C-N	5.87	128.62	120.29
2	4	172	ILE	C-N-CA	5.87	128.62	120.29
3	H	208	GLY	O-C-N	5.87	128.96	122.27
2	h	200	SER	CA-C-N	5.87	127.17	119.84
2	h	200	SER	C-N-CA	5.87	127.17	119.84
1	b	137	LEU	CA-C-O	5.87	126.56	120.40
3	H	106	VAL	CB-CA-C	-5.87	101.64	110.55
3	L	356	THR	CA-C-N	5.87	130.65	120.68
3	L	356	THR	C-N-CA	5.87	130.65	120.68
1	A	160	LYS	N-CA-C	-5.86	105.89	114.39
1	F	73	HIS	CG-CD2-NE2	5.86	113.06	107.20
1	E	238	GLU	CA-C-O	5.86	126.97	120.82
2	n	143	GLY	CA-C-N	5.86	128.41	120.38
2	n	143	GLY	C-N-CA	5.86	128.41	120.38
2	n	162	ASP	N-CA-C	5.86	117.75	111.36
3	M	381	LYS	CA-C-N	5.86	128.74	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	381	LYS	C-N-CA	5.86	128.74	120.42
1	c	182	ASP	CA-C-O	-5.86	112.34	119.43
1	F	132	PHE	O-C-N	-5.86	116.34	122.96
1	g	77	ALA	CA-C-O	-5.86	114.58	121.44
1	c	80	GLY	CA-C-N	5.86	129.03	120.71
1	c	80	GLY	C-N-CA	5.86	129.03	120.71
2	m	173	TYR	CA-C-O	-5.86	114.21	120.42
1	d	194	VAL	CA-C-N	5.86	128.05	120.44
1	d	194	VAL	C-N-CA	5.86	128.05	120.44
2	2	191	ILE	N-CA-C	-5.86	97.16	109.34
3	M	193	LYS	CA-C-O	-5.86	112.88	119.79
1	F	139	ALA	O-C-N	5.85	130.16	123.31
1	C	45	GLY	CA-C-O	5.85	124.95	120.91
3	H	303	PHE	O-C-N	5.85	130.37	122.59
3	M	94	TYR	CB-CG-CD1	5.85	129.58	120.80
1	b	44	GLU	N-CA-C	-5.85	104.83	113.61
2	h	59	SER	N-CA-CB	5.85	118.57	109.97
2	6	88	ARG	CA-C-N	5.85	128.05	120.44
2	6	88	ARG	C-N-CA	5.85	128.05	120.44
1	B	116	ILE	O-C-N	5.85	127.85	121.83
1	g	137	LEU	N-CA-C	-5.85	99.20	108.73
3	K	244	ASP	CA-CB-CG	5.85	118.45	112.60
2	l	13	THR	O-C-N	-5.85	116.72	123.33
3	K	262	GLN	O-C-N	-5.85	115.08	122.27
1	B	138	ILE	N-CA-C	5.84	117.17	108.23
2	j	55	THR	N-CA-C	-5.84	99.87	109.40
3	I	387	THR	N-CA-C	-5.84	94.64	111.00
3	M	288	ASN	N-CA-C	5.84	117.45	111.14
2	j	23	VAL	N-CA-CB	5.84	120.87	111.23
3	L	393	LYS	N-CA-C	-5.84	98.35	108.69
3	L	93	GLN	OE1-CD-NE2	5.84	128.44	122.60
3	J	193	LYS	CA-C-N	5.84	128.03	120.44
3	J	193	LYS	C-N-CA	5.84	128.03	120.44
1	F	150	THR	N-CA-C	-5.84	100.18	109.76
3	M	82	SER	CA-C-N	5.84	128.03	120.44
3	M	82	SER	C-N-CA	5.84	128.03	120.44
2	h	123	TYR	CA-C-O	-5.84	114.39	120.70
2	4	39	SER	N-CA-C	-5.84	100.08	108.60
1	c	50	ALA	N-CA-CB	5.84	121.58	111.13
3	L	193	LYS	CA-C-N	5.84	128.10	120.28
3	L	193	LYS	C-N-CA	5.84	128.10	120.28
2	j	60	VAL	CA-CB-CG1	5.83	120.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLU	N-CA-CB	5.83	119.20	110.22
2	j	51	ARG	NE-CZ-NH1	-5.83	115.67	121.50
2	5	169	VAL	CA-C-O	-5.83	114.99	121.17
1	e	73	HIS	CG-CD2-NE2	5.83	113.03	107.20
2	m	136	ASP	CA-CB-CG	5.83	118.43	112.60
1	d	40	ILE	O-C-N	5.83	129.24	123.00
2	6	143	GLY	N-CA-C	-5.83	105.66	115.80
2	m	196	PHE	CA-CB-CG	-5.83	107.97	113.80
3	J	53	SER	CA-C-N	5.83	128.09	120.28
3	J	53	SER	C-N-CA	5.83	128.09	120.28
3	J	336	PHE	CB-CG-CD2	5.83	130.61	120.70
3	H	354	ILE	CA-C-N	5.83	128.09	120.28
3	H	354	ILE	C-N-CA	5.83	128.09	120.28
1	a	43	LYS	N-CA-C	-5.83	106.03	113.02
2	k	99	ASN	CA-CB-CG	-5.83	106.78	112.60
2	2	181	ALA	N-CA-C	-5.82	98.40	110.80
3	L	350	ASP	CA-C-N	5.82	128.44	120.46
3	L	350	ASP	C-N-CA	5.82	128.44	120.46
1	B	168	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	b	237	ASN	CA-C-N	5.82	128.08	120.28
1	b	237	ASN	C-N-CA	5.82	128.08	120.28
1	g	30	ALA	N-CA-C	5.82	117.63	111.28
3	K	311	LEU	N-CA-C	-5.82	100.19	109.04
3	L	19	ASP	CA-C-O	5.82	126.59	120.42
1	g	72	GLU	N-CA-C	-5.82	104.58	112.26
3	L	236	SER	CA-C-O	-5.82	115.05	121.28
1	D	118	ASP	CA-CB-CG	5.82	118.42	112.60
1	F	86	ARG	O-C-N	-5.82	115.11	122.27
2	5	159	ILE	O-C-N	5.82	129.01	122.67
2	7	47	GLN	CA-C-N	5.82	129.84	120.82
2	7	47	GLN	C-N-CA	5.82	129.84	120.82
1	E	51	ASP	CA-C-O	-5.82	114.01	120.70
1	g	152	PRO	CB-CA-C	-5.82	103.14	112.21
2	i	189	VAL	CA-C-O	5.82	126.64	120.48
2	5	178	ARG	N-CA-C	-5.82	106.03	114.12
2	n	171	ALA	N-CA-CB	5.82	118.67	110.12
1	C	63	THR	CA-CB-CG2	5.81	120.38	110.50
1	c	240	ILE	CA-C-N	5.81	128.54	120.29
1	c	240	ILE	C-N-CA	5.81	128.54	120.29
2	1	102	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	A	172	THR	N-CA-C	-5.81	104.85	111.07
1	c	150	THR	N-CA-C	-5.81	99.93	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	96	ASN	N-CA-C	-5.81	104.85	111.07
1	a	114	LYS	CB-CA-C	-5.81	101.15	110.79
1	B	188	ALA	CB-CA-C	-5.81	101.15	110.79
1	E	230	LYS	CA-C-O	5.81	123.90	118.44
1	F	73	HIS	CE1-NE2-CD2	-5.81	103.19	109.00
1	a	90	ASP	CA-C-N	5.81	128.06	120.28
1	a	90	ASP	C-N-CA	5.81	128.06	120.28
1	a	117	CYS	N-CA-CB	5.81	118.43	110.01
1	d	145	PRO	N-CA-C	5.81	120.34	111.11
2	n	140	THR	N-CA-CB	5.81	120.31	110.49
3	K	136	PRO	CA-C-O	-5.81	114.92	121.43
1	E	204	LEU	CA-C-N	5.81	131.34	121.88
1	E	204	LEU	C-N-CA	5.81	131.34	121.88
3	K	365	GLU	N-CA-C	-5.81	106.05	113.02
2	k	123	TYR	CA-CB-CG	-5.80	103.45	113.90
2	k	188	VAL	CA-CB-CG1	5.80	120.27	110.40
3	H	255	THR	N-CA-C	-5.80	100.49	109.14
3	K	54	GLU	CB-CG-CD	-5.80	102.73	112.60
3	L	252	ASN	CA-CB-CG	-5.80	106.80	112.60
1	D	18	ASP	CA-CB-CG	-5.80	106.80	112.60
2	m	199	TYR	CB-CA-C	-5.80	100.99	110.85
3	L	393	LYS	CB-CG-CD	5.80	124.64	111.30
1	C	92	ALA	N-CA-C	5.80	117.60	111.28
2	2	98	LEU	CA-C-O	-5.80	114.40	120.55
1	B	13	THR	CA-C-N	5.80	130.14	122.95
1	B	13	THR	C-N-CA	5.80	130.14	122.95
2	l	150	VAL	CA-C-N	5.80	128.52	120.29
2	l	150	VAL	C-N-CA	5.80	128.52	120.29
3	J	174	PRO	CA-C-O	-5.80	116.73	120.90
2	n	182	SER	N-CA-C	-5.79	104.73	113.89
3	H	17	GLU	N-CA-C	5.79	117.60	111.28
3	K	388	PRO	N-CA-CB	5.79	108.33	103.17
1	a	26	TYR	N-CA-CB	5.79	118.64	110.12
1	D	35	ALA	N-CA-CB	5.79	119.09	110.40
3	H	67	VAL	N-CA-C	-5.79	99.71	108.17
3	K	314	PHE	CA-C-O	-5.79	114.74	120.82
3	L	159	LEU	CA-C-O	-5.79	113.23	118.79
3	M	85	PRO	N-CA-CB	5.79	109.33	103.25
3	J	76	ARG	N-CA-CB	5.79	119.77	110.85
1	D	6	MET	N-CA-CB	5.79	120.28	110.49
1	g	45	GLY	N-CA-C	-5.79	102.97	110.38
2	l	44	LYS	N-CA-C	-5.79	104.74	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	74	ASP	CA-CB-CG	-5.79	106.81	112.60
1	G	233	VAL	CA-C-N	5.79	128.04	120.28
1	G	233	VAL	C-N-CA	5.79	128.04	120.28
2	4	199	TYR	CB-CG-CD2	-5.79	112.12	120.80
2	7	22	GLY	CA-C-O	5.79	128.13	121.47
3	L	139	SER	N-CA-C	-5.79	101.43	110.17
1	c	137	LEU	N-CA-C	-5.79	98.85	108.34
1	A	232	TYR	CA-C-N	5.79	129.79	120.30
1	A	232	TYR	C-N-CA	5.79	129.79	120.30
3	M	78	VAL	N-CA-CB	5.79	117.60	111.00
1	e	144	VAL	CA-C-N	5.78	125.54	119.76
1	e	144	VAL	C-N-CA	5.78	125.54	119.76
1	G	94	ILE	CA-C-N	5.78	128.03	120.28
1	G	94	ILE	C-N-CA	5.78	128.03	120.28
2	2	98	LEU	CA-C-N	5.78	128.03	120.28
2	2	98	LEU	C-N-CA	5.78	128.03	120.28
1	e	213	TYR	O-C-N	5.78	129.84	123.25
2	n	150	VAL	CA-C-N	5.78	127.96	120.44
2	n	150	VAL	C-N-CA	5.78	127.96	120.44
3	H	157	VAL	CA-CB-CG2	5.78	120.23	110.40
2	i	78	GLU	N-CA-CB	5.78	118.62	110.12
2	3	83	ARG	CA-C-N	5.78	128.89	120.51
2	3	83	ARG	C-N-CA	5.78	128.89	120.51
2	7	121	SER	O-C-N	5.78	129.60	123.42
3	K	95	ILE	N-CA-C	-5.78	100.02	108.11
1	b	33	ARG	N-CA-C	-5.78	104.89	111.07
2	1	65	PHE	CA-CB-CG	5.78	119.58	113.80
2	m	123	TYR	N-CA-C	-5.78	99.48	108.90
1	A	191	LEU	CA-C-O	5.78	126.61	119.97
1	A	207	GLU	N-CA-C	-5.78	106.09	113.02
1	b	91	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	C	115	LYS	CA-C-N	5.78	128.62	120.42
1	C	115	LYS	C-N-CA	5.78	128.62	120.42
1	C	166	MET	O-C-N	-5.78	115.46	122.22
1	f	86	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	f	194	VAL	CB-CA-C	-5.77	104.34	112.14
1	D	71	ASP	N-CA-C	-5.77	101.18	108.45
1	F	213	TYR	N-CA-CB	5.77	120.35	111.46
3	H	248	ALA	CA-C-N	5.77	130.62	120.87
3	H	248	ALA	C-N-CA	5.77	130.62	120.87
3	L	287	THR	N-CA-C	-5.77	99.93	108.99
3	M	38	GLU	N-CA-C	5.77	117.57	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	126	TYR	N-CA-CB	5.77	118.77	110.06
3	L	96	ASN	CB-CG-ND2	-5.77	107.74	116.40
3	H	71	ILE	N-CA-C	-5.77	100.17	108.42
1	B	192	GLY	CA-C-N	5.77	128.48	120.29
1	B	192	GLY	C-N-CA	5.77	128.48	120.29
1	g	30	ALA	CA-C-N	5.77	128.61	120.42
1	g	30	ALA	C-N-CA	5.77	128.61	120.42
3	K	11	GLU	CA-CB-CG	5.77	125.64	114.10
1	d	105	GLU	CA-C-N	5.77	125.67	119.85
1	d	105	GLU	C-N-CA	5.77	125.67	119.85
3	L	42	ILE	N-CA-C	-5.77	104.74	110.62
3	L	323	ILE	CA-C-N	5.77	128.01	120.28
3	L	323	ILE	C-N-CA	5.77	128.01	120.28
3	J	134	GLU	N-CA-C	5.77	118.84	110.42
3	L	146	LEU	O-C-N	-5.76	114.92	122.59
2	m	77	TYR	N-CA-C	5.76	117.56	111.28
3	H	359	GLY	CA-C-O	5.76	126.77	120.66
2	5	179	ASP	N-CA-C	-5.76	99.51	108.90
2	6	14	THR	N-CA-C	-5.76	100.40	109.50
2	6	121	SER	N-CA-C	-5.76	100.31	109.07
3	H	163	LYS	CA-C-N	5.76	125.29	119.19
3	H	163	LYS	C-N-CA	5.76	125.29	119.19
1	A	53	ARG	CA-CB-CG	5.76	125.61	114.10
1	A	11	ALA	N-CA-C	-5.75	99.95	108.99
1	b	168	ARG	NE-CZ-NH2	-5.75	114.02	119.20
3	H	236	SER	N-CA-C	-5.75	99.95	108.99
1	G	54	VAL	N-CA-C	5.75	121.31	109.34
2	j	79	ILE	N-CA-C	5.75	115.94	110.42
2	j	93	LEU	CA-C-O	5.75	126.52	120.42
1	A	236	ALA	O-C-N	5.75	128.71	122.15
1	E	7	GLY	CA-C-O	5.75	125.50	119.06
2	4	70	ILE	N-CA-C	-5.75	104.91	110.72
1	E	20	ARG	CA-C-N	5.75	130.42	122.77
1	E	20	ARG	C-N-CA	5.75	130.42	122.77
2	l	103	TYR	CA-C-N	5.75	128.15	122.28
2	l	103	TYR	C-N-CA	5.75	128.15	122.28
3	J	350	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	186	ASP	CA-C-O	-5.75	114.33	120.42
2	k	136	ASP	CA-CB-CG	5.75	118.35	112.60
3	K	23	LEU	CA-C-O	-5.75	114.33	120.42
1	a	75	CYS	N-CA-C	-5.75	100.58	109.14
1	B	220	THR	N-CA-C	-5.75	98.52	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	91	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	f	142	ASP	N-CA-CB	5.75	118.64	110.13
3	M	240	ILE	CA-C-N	5.75	128.45	120.29
3	M	240	ILE	C-N-CA	5.75	128.45	120.29
1	B	112	LEU	N-CA-C	-5.75	105.10	111.36
1	c	107	ILE	CB-CA-C	5.74	119.20	111.28
1	G	40	ILE	CA-C-O	5.74	126.07	120.27
2	5	95	SER	O-C-N	-5.74	116.03	122.12
2	7	212	ARG	NE-CZ-NH1	-5.74	115.76	121.50
3	K	301	GLY	CA-C-O	5.74	125.49	119.06
3	L	247	ALA	CA-C-N	5.74	132.51	121.54
3	L	247	ALA	C-N-CA	5.74	132.51	121.54
3	J	303	PHE	N-CA-CB	5.74	119.70	110.86
1	b	199	SER	CB-CA-C	-5.74	101.09	110.85
2	m	68	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	F	233	VAL	N-CA-C	5.74	116.52	110.72
1	A	81	LEU	CA-C-N	5.74	128.32	120.46
1	A	81	LEU	C-N-CA	5.74	128.32	120.46
2	5	191	ILE	N-CA-C	-5.74	97.41	109.34
2	3	60	VAL	CA-CB-CG2	5.74	120.15	110.40
2	k	156	THR	CA-C-N	5.74	125.35	119.56
2	k	156	THR	C-N-CA	5.74	125.35	119.56
2	m	143	GLY	N-CA-C	-5.74	106.11	115.46
1	A	132	PHE	CB-CG-CD2	-5.73	110.95	120.70
1	b	241	ARG	CA-C-O	-5.73	114.47	120.55
1	E	23	GLN	N-CA-C	-5.73	105.03	111.28
1	F	113	ALA	CA-C-O	-5.73	114.34	120.42
2	j	84	LYS	CA-C-N	5.73	126.02	119.83
2	j	84	LYS	C-N-CA	5.73	126.02	119.83
3	K	170	VAL	N-CA-C	-5.73	106.88	111.81
1	c	132	PHE	CA-CB-CG	-5.73	108.07	113.80
2	6	196	PHE	CA-CB-CG	5.73	119.53	113.80
3	L	78	VAL	CA-C-O	5.73	126.83	120.59
1	f	156	LEU	CA-C-N	5.73	131.95	122.33
1	f	156	LEU	C-N-CA	5.73	131.95	122.33
1	G	229	LEU	CA-C-N	5.73	127.25	120.09
1	G	229	LEU	C-N-CA	5.73	127.25	120.09
3	K	133	GLU	CB-CA-C	-5.73	103.07	111.77
1	c	106	PRO	N-CA-CB	5.72	108.42	103.27
3	I	101	LYS	N-CA-C	-5.72	101.61	108.25
2	j	146	THR	N-CA-CB	5.72	118.53	110.12
1	c	129	VAL	N-CA-CB	-5.72	105.74	112.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	261	VAL	N-CA-CB	5.72	121.12	110.77
3	J	80	LYS	N-CA-C	-5.72	99.86	108.96
1	D	121	GLN	N-CA-C	5.72	117.51	111.28
1	F	240	ILE	CB-CA-C	-5.72	104.33	112.22
1	f	220	THR	N-CA-C	-5.72	99.69	109.24
1	B	124	THR	N-CA-CB	5.72	119.05	110.19
1	G	152	PRO	CA-C-N	5.72	130.40	120.68
1	G	152	PRO	C-N-CA	5.72	130.40	120.68
3	H	365	GLU	CB-CA-C	-5.72	100.54	110.09
3	L	58	LEU	CB-CA-C	-5.72	99.69	110.67
1	G	18	ASP	CA-CB-CG	-5.72	106.88	112.60
2	j	87	VAL	CB-CA-C	-5.72	103.30	112.16
2	l	28	GLU	O-C-N	5.72	129.34	122.94
2	6	99	ASN	CA-C-N	5.72	127.87	120.44
2	6	99	ASN	C-N-CA	5.72	127.87	120.44
3	M	276	ASP	O-C-N	-5.72	116.30	121.39
2	k	63	ALA	CB-CA-C	-5.71	101.13	110.85
1	d	200	ILE	CA-C-N	5.71	130.28	122.34
1	d	200	ILE	C-N-CA	5.71	130.28	122.34
2	h	146	THR	CA-C-N	5.71	127.87	120.44
2	h	146	THR	C-N-CA	5.71	127.87	120.44
2	4	50	ASP	CA-CB-CG	-5.71	106.89	112.60
3	I	147	ASP	N-CA-C	5.71	117.31	111.14
1	a	59	LEU	N-CA-CB	5.71	119.94	110.63
1	D	185	PHE	CA-CB-CG	-5.71	108.09	113.80
1	f	53	ARG	CD-NE-CZ	5.71	132.40	124.40
1	E	234	GLU	O-C-N	5.71	127.95	122.07
1	f	121	GLN	CA-C-N	5.71	128.50	120.28
1	f	121	GLN	C-N-CA	5.71	128.50	120.28
1	g	240	ILE	CA-C-N	5.71	128.40	120.29
1	g	240	ILE	C-N-CA	5.71	128.40	120.29
2	6	138	VAL	CA-CB-CG1	5.71	120.10	110.40
2	2	78	GLU	CA-C-O	5.71	126.47	120.42
3	H	189	THR	CA-C-N	5.71	132.44	121.54
3	H	189	THR	C-N-CA	5.71	132.44	121.54
3	H	397	PHE	CA-CB-CG	-5.71	108.09	113.80
3	K	157	VAL	N-CA-CB	5.71	116.32	111.64
3	L	109	ASN	CA-CB-CG	-5.71	106.89	112.60
3	H	149	GLN	CA-C-N	5.71	128.28	120.46
3	H	149	GLN	C-N-CA	5.71	128.28	120.46
3	K	391	ASP	N-CA-C	-5.71	105.22	113.21
1	g	220	THR	N-CA-C	-5.70	96.22	107.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	19	GLY	CA-C-N	5.70	130.56	122.24
1	G	19	GLY	C-N-CA	5.70	130.56	122.24
2	k	41	ALA	CA-C-N	5.70	130.23	122.19
2	k	41	ALA	C-N-CA	5.70	130.23	122.19
3	H	36	PHE	CA-CB-CG	-5.70	108.10	113.80
3	H	123	LYS	N-CA-CB	-5.70	102.50	111.05
3	I	248	ALA	O-C-N	5.70	130.08	123.41
1	D	89	ILE	N-CA-CB	5.70	121.09	110.77
1	F	101	LEU	CB-CA-C	-5.70	101.33	110.79
1	G	21	LEU	N-CA-CB	5.70	117.97	109.19
2	4	177	LYS	N-CA-C	-5.70	105.99	113.17
3	M	56	GLU	CA-C-N	5.70	127.92	120.28
3	M	56	GLU	C-N-CA	5.70	127.92	120.28
3	H	173	GLU	CA-C-N	5.70	126.25	120.38
3	H	173	GLU	C-N-CA	5.70	126.25	120.38
3	H	326	ARG	NE-CZ-NH1	5.70	127.20	121.50
2	l	60	VAL	CB-CA-C	-5.70	104.56	112.02
1	c	104	ASP	CA-C-O	-5.70	114.98	121.65
1	g	105	GLU	CA-C-N	5.70	126.03	119.93
1	g	105	GLU	C-N-CA	5.70	126.03	119.93
2	m	183	GLY	N-CA-C	-5.70	103.87	112.41
3	K	346	ALA	O-C-N	-5.70	116.89	123.33
1	B	11	ALA	N-CA-C	-5.69	100.42	109.07
2	j	164	ALA	N-CA-CB	5.69	119.06	110.30
3	K	348	GLY	N-CA-C	5.69	120.70	113.24
2	5	196	PHE	CA-CB-CG	5.69	119.49	113.80
3	K	32	ASP	N-CA-CB	5.69	118.48	110.12
1	C	151	ASP	CA-C-O	-5.69	113.64	120.41
3	M	114	ALA	CA-C-N	5.69	132.21	121.97
3	M	114	ALA	C-N-CA	5.69	132.21	121.97
3	J	337	LYS	CA-C-N	5.69	127.84	120.44
3	J	337	LYS	C-N-CA	5.69	127.84	120.44
1	b	117	CYS	CA-C-O	-5.69	113.43	119.97
2	l	134	GLU	N-CA-C	-5.69	99.74	109.24
2	m	143	GLY	CA-C-N	5.69	127.90	120.28
2	m	143	GLY	C-N-CA	5.69	127.90	120.28
2	n	38	ALA	CB-CA-C	-5.69	100.29	110.70
3	H	34	LYS	CA-C-N	5.69	128.37	120.29
3	H	34	LYS	C-N-CA	5.69	128.37	120.29
3	M	296	ALA	CA-C-N	5.69	128.50	120.42
3	M	296	ALA	C-N-CA	5.69	128.50	120.42
1	D	47	ILE	N-CA-C	-5.69	99.99	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	MET	CA-C-N	5.69	128.25	120.46
1	E	189	MET	C-N-CA	5.69	128.25	120.46
3	K	36	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	191	LEU	N-CA-C	5.68	118.41	111.82
1	a	93	ARG	CB-CA-C	-5.68	101.35	110.79
1	B	233	VAL	CA-C-O	-5.68	115.04	120.95
1	F	194	VAL	CA-C-O	-5.68	114.33	120.47
1	G	152	PRO	N-CA-C	-5.68	107.04	114.03
2	2	81	ARG	NE-CZ-NH2	-5.68	114.08	119.20
2	4	161	VAL	CA-C-N	5.68	127.89	120.28
2	4	161	VAL	C-N-CA	5.68	127.89	120.28
1	a	74	ILE	N-CA-C	-5.68	100.04	108.45
1	F	119	PHE	CA-CB-CG	-5.68	108.12	113.80
3	I	87	PHE	CA-C-O	-5.68	114.63	120.99
3	K	171	GLY	CA-C-O	5.68	125.34	118.86
1	D	152	PRO	CA-C-N	5.68	128.35	120.29
1	D	152	PRO	C-N-CA	5.68	128.35	120.29
2	1	96	ASN	CA-CB-CG	-5.68	106.92	112.60
2	1	104	PHE	N-CA-C	-5.68	99.10	108.75
3	J	335	ASP	N-CA-C	-5.68	98.70	110.80
1	A	102	THR	CA-CB-OG1	5.68	118.12	109.60
2	h	99	ASN	N-CA-C	-5.68	105.23	111.82
3	I	314	PHE	CA-C-N	5.68	128.35	120.29
3	I	314	PHE	C-N-CA	5.68	128.35	120.29
1	B	131	PRO	N-CA-CB	5.68	109.26	102.85
1	c	71	ASP	N-CA-C	5.68	116.77	108.14
1	B	57	LYS	CA-C-N	5.67	128.20	120.54
1	B	57	LYS	C-N-CA	5.67	128.20	120.54
1	d	73	HIS	CA-CB-CG	5.67	119.47	113.80
1	e	237	ASN	N-CA-CB	5.67	118.96	110.22
1	g	100	ARG	CD-NE-CZ	-5.67	116.46	124.40
3	H	90	ASN	CA-CB-CG	-5.67	106.93	112.60
1	c	161	ALA	N-CA-C	-5.67	98.27	108.48
1	e	177	LYS	N-CA-C	-5.67	103.87	112.04
1	F	160	LYS	N-CA-CB	-5.67	103.49	110.98
3	J	242	GLU	CB-CG-CD	-5.67	102.96	112.60
1	c	176	GLU	N-CA-CB	5.67	118.71	110.26
1	b	196	MET	N-CA-C	5.67	117.46	111.28
1	C	131	PRO	CA-C-O	-5.67	114.98	121.56
1	F	204	LEU	N-CA-C	5.67	118.45	110.23
3	H	31	GLU	CB-CA-C	-5.67	101.38	110.79
3	I	74	ASP	N-CA-C	-5.67	106.40	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	376	THR	CA-C-N	5.67	128.34	120.29
3	K	376	THR	C-N-CA	5.67	128.34	120.29
3	M	241	ASP	CB-CA-C	-5.67	101.21	110.85
2	1	203	GLU	CA-C-N	5.67	128.22	120.46
2	1	203	GLU	C-N-CA	5.67	128.22	120.46
3	H	106	VAL	N-CA-CB	5.67	121.96	112.44
1	A	35	ALA	N-CA-CB	5.67	118.33	110.17
2	3	60	VAL	CB-CA-C	-5.67	104.40	112.22
2	n	117	SER	O-C-N	5.67	128.61	122.15
3	J	147	ASP	CA-CB-CG	-5.67	106.94	112.60
1	D	207	GLU	N-CA-CB	5.66	118.44	110.12
1	e	44	GLU	N-CA-C	-5.66	106.03	113.17
3	H	43	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	F	26	TYR	N-CA-C	-5.66	105.19	111.36
1	g	151	ASP	CA-C-O	-5.66	115.38	121.27
1	f	187	ASP	CA-CB-CG	-5.66	106.94	112.60
1	g	15	PHE	CA-CB-CG	-5.66	108.14	113.80
2	m	171	ALA	N-CA-C	5.66	117.45	111.28
2	n	79	ILE	N-CA-C	-5.66	105.21	110.53
2	m	212	ARG	NH1-CZ-NH2	-5.66	111.95	119.30
1	D	99	ASN	CA-C-N	5.66	128.91	120.31
1	D	99	ASN	C-N-CA	5.66	128.91	120.31
2	i	77	TYR	N-CA-C	-5.66	105.11	111.28
3	J	35	LYS	CB-CG-CD	5.66	124.31	111.30
2	6	68	ARG	CB-CG-CD	5.65	124.30	111.30
1	g	199	SER	CA-C-O	-5.65	114.43	120.42
2	m	66	LEU	CA-C-N	5.65	128.12	120.38
2	m	66	LEU	C-N-CA	5.65	128.12	120.38
3	H	93	GLN	N-CA-C	-5.65	106.05	113.17
1	C	56	SER	N-CA-C	5.65	116.01	108.38
1	c	226	PRO	N-CA-C	5.65	122.00	113.81
1	d	187	ASP	CA-CB-CG	-5.65	106.95	112.60
3	K	358	ALA	N-CA-C	-5.65	105.27	111.82
2	5	181	ALA	CA-C-N	5.65	131.60	121.15
2	5	181	ALA	C-N-CA	5.65	131.60	121.15
2	n	198	GLN	CA-C-N	5.65	127.85	120.28
2	n	198	GLN	C-N-CA	5.65	127.85	120.28
1	B	210	GLU	N-CA-C	-5.65	100.19	109.40
3	J	355	CYS	N-CA-C	5.65	117.44	111.28
3	H	159	LEU	N-CA-C	5.65	120.43	112.75
1	a	63	THR	N-CA-C	-5.64	105.74	113.30
1	C	171	VAL	N-CA-CB	-5.64	100.56	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	CYS	CB-CA-C	-5.64	101.25	110.85
1	G	209	ILE	CA-C-N	5.64	130.79	123.00
1	G	209	ILE	C-N-CA	5.64	130.79	123.00
2	m	51	ARG	NH1-CZ-NH2	-5.64	111.96	119.30
3	L	213	GLN	N-CA-C	-5.64	100.73	109.14
3	M	264	THR	CA-C-N	5.64	128.41	120.28
3	M	264	THR	C-N-CA	5.64	128.41	120.28
3	M	370	VAL	CB-CA-C	5.64	119.39	110.81
1	C	18	ASP	CA-C-N	5.64	130.70	123.08
1	C	18	ASP	C-N-CA	5.64	130.70	123.08
2	3	59	SER	N-CA-CB	5.64	119.83	110.63
2	j	203	GLU	CG-CD-OE1	5.64	131.38	118.40
2	5	95	SER	CA-C-N	5.64	127.77	120.44
2	5	95	SER	C-N-CA	5.64	127.77	120.44
2	l	44	LYS	CA-C-O	5.64	125.41	119.03
3	H	269	LEU	CB-CA-C	-5.64	102.02	110.88
1	f	232	TYR	CA-C-N	5.64	128.19	120.46
1	f	232	TYR	C-N-CA	5.64	128.19	120.46
2	m	30	ARG	N-CA-C	-5.64	100.13	108.99
1	f	183	LEU	CA-C-O	-5.64	115.67	121.87
1	G	112	LEU	N-CA-C	-5.64	105.21	111.36
2	i	168	ALA	CA-C-N	5.64	127.67	120.56
2	i	168	ALA	C-N-CA	5.64	127.67	120.56
3	M	354	ILE	CA-C-N	5.64	127.83	120.28
3	M	354	ILE	C-N-CA	5.64	127.83	120.28
1	a	100	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	C	212	GLY	O-C-N	-5.64	118.41	123.37
1	f	41	LYS	CA-C-O	-5.64	114.44	120.92
1	G	161	ALA	O-C-N	-5.64	116.96	123.33
3	K	277	PRO	CA-C-N	5.64	130.69	122.41
3	K	277	PRO	C-N-CA	5.64	130.69	122.41
3	M	322	LYS	CA-C-N	5.64	128.42	120.42
3	M	322	LYS	C-N-CA	5.64	128.42	120.42
1	b	114	LYS	CA-CB-CG	5.63	125.37	114.10
1	g	169	ASN	O-C-N	5.63	128.18	122.09
2	j	79	ILE	O-C-N	-5.63	116.39	121.91
2	l	184	ASP	CA-CB-CG	5.63	118.23	112.60
2	m	168	ALA	O-C-N	5.63	128.57	122.15
2	m	189	VAL	CA-CB-CG1	5.63	119.98	110.40
1	E	179	TYR	CB-CA-C	5.63	119.91	109.54
1	g	122	GLN	OE1-CD-NE2	-5.63	116.97	122.60
2	k	162	ASP	N-CA-C	5.63	118.36	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	69	SER	N-CA-C	-5.63	105.19	112.68
3	J	104	ALA	CA-C-N	5.63	128.87	120.87
3	J	104	ALA	C-N-CA	5.63	128.87	120.87
3	J	382	VAL	N-CA-C	5.63	117.14	111.00
3	K	391	ASP	CA-C-N	5.63	130.96	122.68
3	K	391	ASP	C-N-CA	5.63	130.96	122.68
3	M	87	PHE	N-CA-CB	5.63	121.20	111.13
3	J	302	ARG	N-CA-C	-5.63	107.66	114.75
1	F	93	ARG	O-C-N	5.63	127.86	122.07
1	G	100	ARG	NE-CZ-NH2	5.63	124.26	119.20
2	7	49	ALA	N-CA-C	-5.63	100.78	108.38
3	H	53	SER	N-CA-C	5.63	117.41	111.28
3	H	54	GLU	N-CA-CB	5.63	119.00	110.28
3	J	77	VAL	CA-C-N	5.63	129.63	122.37
3	J	77	VAL	C-N-CA	5.63	129.63	122.37
1	b	11	ALA	CA-C-N	5.62	133.38	122.69
1	b	11	ALA	C-N-CA	5.62	133.38	122.69
3	M	337	LYS	O-C-N	5.62	128.56	122.15
2	3	86	THR	CA-C-N	5.62	128.16	120.46
2	3	86	THR	C-N-CA	5.62	128.16	120.46
2	7	204	VAL	CA-C-N	5.62	128.38	120.28
2	7	204	VAL	C-N-CA	5.62	128.38	120.28
3	H	203	PHE	CA-C-O	5.62	126.39	120.54
1	a	100	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	B	121	GLN	CB-CG-CD	-5.62	103.04	112.60
1	b	144	VAL	N-CA-C	-5.62	102.66	109.01
1	D	142	ASP	CA-C-N	5.62	129.87	120.70
1	D	142	ASP	C-N-CA	5.62	129.87	120.70
2	k	135	LYS	N-CA-CB	5.62	121.45	110.88
3	K	289	ARG	CA-C-O	-5.62	115.30	121.31
3	J	40	GLU	N-CA-CB	5.62	118.48	110.16
1	A	57	LYS	N-CA-C	-5.62	106.38	113.18
1	A	144	VAL	N-CA-CB	5.62	118.05	111.87
1	d	162	THR	O-C-N	-5.62	117.20	123.04
1	f	98	ILE	N-CA-C	-5.62	105.05	110.72
2	j	95	SER	CA-C-O	-5.62	114.59	120.55
3	I	388	PRO	CA-C-N	5.62	129.60	121.68
3	I	388	PRO	C-N-CA	5.62	129.60	121.68
3	L	84	GLY	CA-C-O	-5.62	113.49	121.52
3	M	328	MET	N-CA-C	-5.62	102.44	110.59
3	H	126	MET	O-C-N	5.62	130.06	122.59
2	5	46	TYR	CA-CB-CG	-5.62	103.79	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	182	GLY	O-C-N	5.62	127.39	121.77
2	h	23	VAL	N-CA-C	-5.61	99.97	108.17
2	i	125	ILE	CA-CB-CG1	5.61	119.94	110.40
3	I	311	LEU	CB-CA-C	-5.61	102.41	109.31
1	a	122	GLN	CA-C-O	5.61	126.50	120.55
2	4	204	VAL	CA-C-N	5.61	128.57	120.38
2	4	204	VAL	C-N-CA	5.61	128.57	120.38
2	l	193	GLU	N-CA-CB	5.61	119.97	110.49
3	J	140	TYR	CB-CG-CD1	5.61	129.21	120.80
1	B	226	PRO	O-C-N	5.61	129.45	122.22
3	K	305	ARG	NE-CZ-NH2	-5.61	114.15	119.20
2	2	63	ALA	N-CA-CB	5.61	118.36	110.12
1	g	20	ARG	N-CA-C	-5.60	102.22	110.52
2	i	139	ALA	N-CA-C	-5.60	100.79	109.14
2	j	113	GLY	O-C-N	5.60	129.23	123.29
2	k	191	ILE	N-CA-CB	5.60	119.44	111.82
2	7	125	ILE	N-CA-C	-5.60	100.11	108.46
3	I	275	PHE	CA-C-O	5.60	126.33	119.05
1	F	64	ILE	CA-C-N	5.60	130.92	120.95
1	F	64	ILE	C-N-CA	5.60	130.92	120.95
1	F	135	SER	N-CA-C	-5.60	100.76	109.72
1	F	167	GLY	CA-C-N	5.60	127.72	120.44
1	F	167	GLY	C-N-CA	5.60	127.72	120.44
2	2	104	PHE	CA-CB-CG	-5.60	108.20	113.80
3	M	216	ILE	CA-C-O	5.60	126.52	120.53
3	J	263	ARG	N-CA-C	5.60	117.46	111.36
1	c	40	ILE	CB-CA-C	-5.60	102.28	110.62
3	H	326	ARG	NH1-CZ-NH2	-5.60	112.03	119.30
1	B	116	ILE	N-CA-C	5.59	116.37	110.72
1	c	168	ARG	NE-CZ-NH1	5.59	127.09	121.50
2	5	143	GLY	CA-C-N	5.59	128.04	120.38
2	5	143	GLY	C-N-CA	5.59	128.04	120.38
2	l	33	MET	N-CA-C	-5.59	99.30	108.76
3	M	28	ARG	O-C-N	5.59	127.83	122.07
1	E	13	THR	CA-C-N	5.59	127.99	120.50
1	E	13	THR	C-N-CA	5.59	127.99	120.50
1	F	185	PHE	CA-C-N	5.59	127.71	120.44
1	F	185	PHE	C-N-CA	5.59	127.71	120.44
2	3	195	GLU	N-CA-C	-5.59	100.80	109.24
2	l	116	ASP	CA-C-O	-5.59	115.43	121.36
2	m	123	TYR	CD1-CG-CD2	5.59	126.49	118.10
3	M	253	SER	N-CA-C	-5.59	100.87	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	130	ARG	CA-C-O	-5.59	114.90	120.66
1	c	200	ILE	CA-CB-CG1	5.59	119.90	110.40
3	L	189	THR	CA-C-N	5.59	128.23	120.29
3	L	189	THR	C-N-CA	5.59	128.23	120.29
1	B	90	ASP	CA-CB-CG	-5.59	107.01	112.60
1	B	160	LYS	N-CA-C	-5.59	105.06	113.89
2	5	204	VAL	O-C-N	5.59	127.59	121.83
1	d	77	ALA	CB-CA-C	-5.59	98.32	109.33
1	F	108	THR	CA-CB-OG1	5.59	117.98	109.60
2	6	185	GLY	N-CA-C	-5.59	99.94	113.18
3	H	80	LYS	O-C-N	-5.59	115.23	122.77
2	1	37	ILE	O-C-N	5.58	128.99	123.18
3	I	60	SER	CA-C-N	5.58	126.13	120.38
3	I	60	SER	C-N-CA	5.58	126.13	120.38
1	a	53	ARG	CA-C-N	5.58	132.02	121.97
1	a	53	ARG	C-N-CA	5.58	132.02	121.97
1	g	229	LEU	O-C-N	5.58	128.04	122.12
2	2	153	ASP	CA-C-O	-5.58	113.79	120.10
2	7	21	ASP	CA-CB-CG	-5.58	107.02	112.60
2	7	192	THR	CB-CA-C	5.58	119.41	110.09
3	L	135	LYS	CA-C-N	5.58	125.57	120.21
3	L	135	LYS	C-N-CA	5.58	125.57	120.21
3	L	361	PHE	O-C-N	-5.58	116.20	122.12
3	M	258	ASP	CA-C-N	5.58	128.22	120.29
3	M	258	ASP	C-N-CA	5.58	128.22	120.29
1	g	86	ARG	CD-NE-CZ	-5.58	116.59	124.40
2	6	159	ILE	CA-C-N	5.58	129.33	121.30
2	6	159	ILE	C-N-CA	5.58	129.33	121.30
3	M	202	THR	N-CA-CB	5.58	119.92	110.49
1	E	237	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	F	136	LEU	CA-C-N	5.58	130.78	122.86
1	F	136	LEU	C-N-CA	5.58	130.78	122.86
2	m	74	ALA	CA-C-N	5.58	127.69	120.44
2	m	74	ALA	C-N-CA	5.58	127.69	120.44
1	a	222	LYS	CA-C-N	5.57	130.85	123.05
1	a	222	LYS	C-N-CA	5.57	130.85	123.05
1	F	57	LYS	N-CA-CB	5.57	118.74	110.49
2	2	164	ALA	N-CA-C	-5.57	105.60	112.90
2	5	120	LYS	CB-CA-C	-5.57	97.73	109.38
3	H	117	ASN	OD1-CG-ND2	5.57	128.17	122.60
3	H	174	PRO	CA-C-O	-5.57	112.48	120.56
3	H	322	LYS	N-CA-CB	5.57	118.09	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	88	VAL	N-CA-CB	5.57	117.73	111.21
1	C	91	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	d	89	ILE	CA-C-N	5.57	128.02	120.44
1	d	89	ILE	C-N-CA	5.57	128.02	120.44
2	j	201	PRO	CA-C-N	5.57	127.68	120.44
2	j	201	PRO	C-N-CA	5.57	127.68	120.44
1	C	113	ALA	CA-C-N	5.57	127.74	120.28
1	C	113	ALA	C-N-CA	5.57	127.74	120.28
1	g	232	TYR	CB-CA-C	-5.57	100.51	110.70
1	C	118	ASP	CB-CA-C	-5.57	101.38	110.85
1	E	19	GLY	O-C-N	-5.57	115.93	122.50
2	m	198	GLN	N-CA-C	-5.57	99.33	108.41
3	L	74	ASP	CA-CB-CG	5.57	118.17	112.60
3	M	234	ALA	CA-C-O	-5.57	114.38	120.17
1	E	142	ASP	CB-CA-C	-5.57	108.41	116.54
2	5	99	ASN	N-CA-C	-5.57	105.36	111.82
3	K	61	PRO	CA-C-O	-5.57	112.49	120.56
3	L	225	GLU	N-CA-CB	5.57	118.08	110.01
1	C	196	MET	N-CA-CB	5.57	118.40	110.16
1	e	57	LYS	N-CA-C	-5.57	105.26	113.61
3	H	29	ARG	NE-CZ-NH2	5.57	124.21	119.20
3	I	21	TYR	O-C-N	-5.57	116.34	122.07
3	M	17	GLU	CA-C-N	5.57	128.19	120.29
3	M	17	GLU	C-N-CA	5.57	128.19	120.29
3	J	341	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	a	194	VAL	CA-CB-CG1	5.56	119.86	110.40
1	g	168	ARG	O-C-N	-5.56	115.19	122.59
2	n	181	ALA	CA-C-N	5.56	130.67	121.99
2	n	181	ALA	C-N-CA	5.56	130.67	121.99
3	K	71	ILE	N-CA-C	-5.56	100.68	108.80
2	2	42	ALA	O-C-N	5.56	129.97	122.96
1	C	35	ALA	CA-C-O	-5.56	114.37	120.43
3	I	109	ASN	CA-C-N	5.56	127.73	120.28
3	I	109	ASN	C-N-CA	5.56	127.73	120.28
1	A	217	ASP	CA-CB-CG	5.56	118.16	112.60
2	i	148	TYR	O-C-N	-5.56	116.23	122.12
3	H	10	LEU	N-CA-C	-5.56	105.23	112.23
2	n	43	LYS	CA-C-O	-5.56	114.64	120.58
3	H	388	PRO	CA-C-O	-5.56	114.89	121.67
3	L	66	GLY	CA-C-O	-5.56	115.00	121.61
2	5	24	VAL	N-CA-C	-5.55	100.48	108.48
2	6	110	LEU	N-CA-C	-5.55	100.83	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	176	MET	N-CA-C	-5.55	105.23	111.28
3	I	30	LEU	CA-C-N	5.55	127.66	120.44
3	I	30	LEU	C-N-CA	5.55	127.66	120.44
1	F	12	ILE	CA-C-O	-5.55	114.25	120.25
2	2	115	ILE	N-CA-C	-5.55	100.48	108.48
3	I	315	GLU	O-C-N	-5.55	115.82	122.15
3	J	335	ASP	CA-CB-CG	5.55	118.15	112.60
3	I	38	GLU	CA-C-N	5.55	127.72	120.28
3	I	38	GLU	C-N-CA	5.55	127.72	120.28
3	K	242	GLU	N-CA-C	-5.55	95.46	111.00
3	K	380	GLU	CA-C-N	5.55	127.65	120.44
3	K	380	GLU	C-N-CA	5.55	127.65	120.44
3	J	46	ARG	CB-CA-C	-5.55	101.42	110.85
1	G	92	ALA	CA-C-O	5.55	126.43	120.55
2	1	69	ILE	CA-C-N	5.55	129.83	120.29
2	1	69	ILE	C-N-CA	5.55	129.83	120.29
2	2	28	GLU	N-CA-C	-5.55	102.31	110.52
3	K	29	ARG	CB-CG-CD	5.54	124.05	111.30
3	K	134	GLU	CA-C-O	-5.54	114.06	120.49
3	M	226	VAL	N-CA-CB	5.54	120.81	110.77
1	f	150	THR	N-CA-CB	5.54	118.54	109.95
2	2	65	PHE	CA-C-N	5.54	128.26	120.28
2	2	65	PHE	C-N-CA	5.54	128.26	120.28
3	H	250	ARG	N-CA-CB	5.54	121.53	111.11
1	e	74	ILE	CB-CA-C	5.54	118.42	110.33
1	f	24	VAL	O-C-N	5.54	127.34	121.91
2	k	89	ALA	CA-C-O	5.54	126.64	120.82
3	H	49	ARG	NE-CZ-NH2	-5.54	114.22	119.20
3	H	80	LYS	CA-C-O	5.54	127.21	120.62
3	I	315	GLU	N-CA-CB	5.54	118.36	110.16
3	I	332	GLU	CB-CG-CD	5.54	122.01	112.60
3	M	131	GLU	CA-C-O	-5.54	115.30	121.23
1	A	44	GLU	CA-C-O	5.54	124.89	119.08
1	E	224	VAL	O-C-N	-5.54	116.64	122.95
1	e	47	ILE	CB-CA-C	5.54	118.83	110.63
1	G	116	ILE	CA-C-O	5.54	126.45	120.47
2	n	103	TYR	N-CA-C	-5.54	106.53	113.28
3	H	19	ASP	CB-CA-C	-5.54	101.44	110.85
3	I	16	LEU	CA-C-N	5.54	128.01	120.54
3	I	16	LEU	C-N-CA	5.54	128.01	120.54
1	E	142	ASP	N-CA-C	-5.53	100.21	108.34
1	f	142	ASP	N-CA-C	-5.53	104.65	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	212	ARG	NE-CZ-NH2	-5.53	114.22	119.20
3	M	269	LEU	CA-C-N	5.53	132.11	121.54
3	M	269	LEU	C-N-CA	5.53	132.11	121.54
3	M	324	HIS	CG-CD2-NE2	5.53	112.73	107.20
1	b	140	GLY	N-CA-C	5.53	118.57	110.38
1	C	102	THR	O-C-N	-5.53	115.50	122.19
3	K	101	LYS	N-CA-CB	5.53	116.47	111.27
1	a	82	VAL	CA-CB-CG1	5.53	119.80	110.40
1	B	161	ALA	N-CA-CB	5.53	119.84	110.49
3	I	109	ASN	OD1-CG-ND2	5.53	128.13	122.60
3	M	227	PHE	CA-CB-CG	-5.53	108.27	113.80
1	B	172	THR	CA-C-O	-5.53	115.00	120.70
3	I	299	ARG	N-CA-C	5.53	118.03	110.01
1	B	71	ASP	CA-C-O	-5.53	115.50	121.36
1	c	18	ASP	CA-CB-CG	-5.53	107.07	112.60
2	4	62	ASP	N-CA-C	-5.53	105.16	111.07
3	L	186	THR	CA-CB-CG2	-5.53	101.10	110.50
2	i	87	VAL	CA-C-N	5.53	127.68	120.28
2	i	87	VAL	C-N-CA	5.53	127.68	120.28
2	l	175	ALA	CA-C-N	5.53	128.24	120.28
2	l	175	ALA	C-N-CA	5.53	128.24	120.28
2	l	209	ALA	N-CA-C	-5.53	105.85	112.59
3	H	136	PRO	CB-CA-C	-5.53	102.44	111.56
3	I	51	LEU	N-CA-C	5.53	118.23	111.82
3	J	207	VAL	CA-CB-CG1	-5.53	101.01	110.40
1	b	193	LEU	CA-C-N	5.52	127.52	120.56
1	b	193	LEU	C-N-CA	5.52	127.52	120.56
1	C	24	VAL	O-C-N	5.52	128.04	121.80
3	I	359	GLY	CA-C-N	5.52	128.71	120.31
3	I	359	GLY	C-N-CA	5.52	128.71	120.31
1	G	171	VAL	O-C-N	5.52	127.52	121.83
3	K	224	ARG	CA-C-O	-5.52	114.70	120.55
1	F	209	ILE	CA-C-O	-5.52	115.50	121.19
1	G	14	VAL	CA-CB-CG2	5.52	119.78	110.40
2	l	50	ASP	N-CA-C	5.52	116.98	111.07
1	b	194	VAL	CB-CA-C	-5.52	104.91	111.97
1	d	14	VAL	O-C-N	-5.52	116.71	123.00
1	e	170	ALA	N-CA-C	5.52	116.98	111.07
3	M	349	ALA	CA-C-O	5.52	126.40	120.55
3	J	158	GLU	CA-C-N	5.52	126.99	120.09
3	J	158	GLU	C-N-CA	5.52	126.99	120.09
3	J	174	PRO	CA-C-N	5.52	125.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	174	PRO	C-N-CA	5.52	125.53	119.90
1	E	62	ASP	N-CA-C	-5.52	99.42	108.41
3	K	16	LEU	CA-C-O	-5.52	114.70	120.55
2	k	212	ARG	N-CA-C	-5.51	105.24	112.41
2	7	170	ARG	CA-C-N	5.51	127.94	120.44
2	7	170	ARG	C-N-CA	5.51	127.94	120.44
2	h	117	SER	CA-CB-OG	5.51	122.13	111.10
2	l	161	VAL	CA-CB-CG1	-5.51	101.03	110.40
2	m	144	SER	CA-C-O	-5.51	114.71	120.55
1	A	151	ASP	CA-C-N	5.51	125.34	119.28
1	A	151	ASP	C-N-CA	5.51	125.34	119.28
1	F	42	CYS	N-CA-C	-5.51	101.03	109.41
2	k	29	LYS	CA-C-O	5.51	126.61	120.77
3	I	113	LEU	CB-CA-C	5.51	119.24	111.86
3	J	41	ARG	O-C-N	5.51	128.43	122.15
1	A	161	ALA	CA-C-O	-5.51	114.83	120.89
1	g	80	GLY	N-CA-C	-5.51	102.56	110.60
2	2	187	ASP	N-CA-CB	5.51	119.25	110.16
2	j	99	ASN	CA-C-O	-5.51	115.03	120.70
2	1	35	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	74	ILE	CA-C-O	5.51	126.82	120.76
2	1	102	ARG	CD-NE-CZ	-5.51	116.69	124.40
3	L	98	GLU	CA-C-N	5.51	128.11	120.29
3	L	98	GLU	C-N-CA	5.51	128.11	120.29
3	H	35	LYS	CA-C-N	5.50	127.66	120.28
3	H	35	LYS	C-N-CA	5.50	127.66	120.28
1	f	233	VAL	CA-C-N	5.50	127.59	120.44
1	f	233	VAL	C-N-CA	5.50	127.59	120.44
1	G	151	ASP	N-CA-C	-5.50	103.80	110.13
1	g	182	ASP	N-CA-C	-5.50	105.19	113.89
3	I	205	ARG	N-CA-C	-5.50	99.55	108.52
3	K	392	LEU	CA-C-O	-5.50	115.32	122.14
3	J	169	GLU	N-CA-C	5.50	117.28	111.28
2	7	133	GLU	CB-CG-CD	-5.50	103.25	112.60
1	d	79	SER	N-CA-C	-5.50	98.58	108.48
1	F	18	ASP	N-CA-C	-5.50	105.36	111.36
1	f	99	ASN	N-CA-C	5.50	116.95	111.07
1	d	11	ALA	CA-C-O	-5.50	114.76	120.70
3	H	148	VAL	CA-C-O	-5.50	115.23	120.95
1	D	197	GLY	O-C-N	5.50	127.46	122.18
1	G	218	ASP	N-CA-C	-5.50	105.87	113.18
2	6	155	PHE	CA-CB-CG	-5.50	108.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	233	LYS	N-CA-C	-5.50	106.16	112.92
3	L	344	GLU	CA-C-N	5.50	131.26	122.25
3	L	344	GLU	C-N-CA	5.50	131.26	122.25
1	E	238	GLU	N-CA-C	5.50	116.95	111.07
1	g	116	ILE	CB-CA-C	5.49	119.56	112.14
2	3	33	MET	CG-SD-CE	-5.49	88.81	100.90
2	3	142	SER	N-CA-C	-5.49	107.12	113.88
3	H	215	TYR	CA-C-N	5.49	129.49	121.80
3	H	215	TYR	C-N-CA	5.49	129.49	121.80
3	H	288	ASN	N-CA-C	-5.49	105.70	112.90
3	M	329	LYS	CA-C-N	5.49	132.03	121.54
3	M	329	LYS	C-N-CA	5.49	132.03	121.54
1	B	119	PHE	CB-CA-C	5.49	119.58	110.90
1	f	162	THR	O-C-N	-5.49	117.49	123.26
1	F	41	LYS	O-C-N	-5.49	116.77	123.30
2	7	161	VAL	N-CA-C	-5.49	104.87	112.50
3	I	165	GLU	N-CA-CB	5.49	119.65	110.32
3	K	102	PRO	CA-C-O	-5.49	115.34	121.32
3	K	166	LEU	CB-CA-C	-5.49	100.47	110.63
3	J	187	GLY	CA-C-N	5.49	127.90	120.38
3	J	187	GLY	C-N-CA	5.49	127.90	120.38
1	C	217	ASP	N-CA-CB	5.49	118.67	110.22
1	B	119	PHE	CA-CB-CG	-5.49	108.31	113.80
1	c	232	TYR	CB-CA-C	-5.49	101.52	110.85
1	d	194	VAL	N-CA-CB	5.49	118.81	110.58
2	1	105	PRO	O-C-N	5.49	129.23	123.03
2	l	169	VAL	CA-C-N	5.49	128.08	120.29
2	l	169	VAL	C-N-CA	5.49	128.08	120.29
3	K	25	GLU	N-CA-CB	-5.49	102.05	110.12
3	K	99	GLU	CA-C-O	-5.49	112.89	119.15
3	L	223	VAL	O-C-N	5.49	127.19	121.87
1	a	92	ALA	CA-C-N	5.48	127.63	120.28
1	a	92	ALA	C-N-CA	5.48	127.63	120.28
1	G	8	TYR	N-CA-C	-5.48	104.84	112.30
2	l	86	THR	CA-C-N	5.48	127.97	120.46
2	l	86	THR	C-N-CA	5.48	127.97	120.46
1	f	24	VAL	CA-C-O	-5.48	115.36	121.17
1	f	123	TYR	N-CA-C	-5.48	106.26	113.17
2	3	63	ALA	CB-CA-C	-5.48	101.69	110.79
2	5	61	GLY	N-CA-C	5.48	119.27	112.64
3	I	205	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	A	135	SER	CA-C-O	5.48	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	46	VAL	O-C-N	-5.48	116.73	123.03
2	n	40	LYS	CA-C-O	5.48	125.08	119.05
3	M	125	PRO	O-C-N	5.48	128.80	122.17
1	E	58	LEU	N-CA-C	-5.48	106.27	113.17
2	5	80	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	l	125	ILE	N-CA-CB	5.48	118.70	111.25
1	B	9	ASP	N-CA-CB	5.48	120.02	110.98
2	m	35	ASN	O-C-N	5.48	129.93	122.37
3	I	360	MET	N-CA-CB	5.48	118.77	110.28
3	M	367	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	194	VAL	CA-C-N	5.48	127.62	120.28
1	A	194	VAL	C-N-CA	5.48	127.62	120.28
1	b	217	ASP	O-C-N	5.48	129.67	122.33
3	H	233	LYS	N-CA-C	-5.48	106.18	112.92
3	I	159	LEU	O-C-N	-5.48	115.02	121.32
3	L	337	LYS	CA-C-N	5.48	127.56	120.44
3	L	337	LYS	C-N-CA	5.48	127.56	120.44
1	F	59	LEU	N-CA-CB	5.47	119.10	110.23
1	F	110	LYS	CA-C-N	5.47	128.06	120.29
1	F	110	LYS	C-N-CA	5.47	128.06	120.29
2	j	13	THR	N-CA-C	-5.47	100.98	109.14
3	H	24	ARG	CA-C-N	5.47	127.62	120.28
3	H	24	ARG	C-N-CA	5.47	127.62	120.28
3	L	363	ILE	O-C-N	5.47	127.18	121.87
1	e	38	ILE	CA-C-N	5.47	132.14	121.41
1	e	38	ILE	C-N-CA	5.47	132.14	121.41
1	G	73	HIS	CA-C-N	5.47	130.59	122.71
1	G	73	HIS	C-N-CA	5.47	130.59	122.71
2	4	156	THR	CA-C-N	5.47	125.56	119.87
2	4	156	THR	C-N-CA	5.47	125.56	119.87
3	K	397	PHE	O-C-N	5.47	130.58	122.81
3	J	360	MET	CA-C-N	5.47	127.61	120.28
3	J	360	MET	C-N-CA	5.47	127.61	120.28
1	D	184	SER	CA-C-N	5.47	127.55	120.44
1	D	184	SER	C-N-CA	5.47	127.55	120.44
1	E	213	TYR	CA-CB-CG	5.47	123.75	113.90
1	e	155	ALA	N-CA-C	-5.47	100.86	109.50
1	b	47	ILE	CA-C-O	5.47	126.13	120.39
1	d	40	ILE	CA-C-O	-5.47	114.93	121.28
1	E	37	ALA	CB-CA-C	-5.47	100.50	109.80
3	H	147	ASP	CA-C-N	5.47	127.95	120.46
3	H	147	ASP	C-N-CA	5.47	127.95	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	287	THR	CA-CB-OG1	5.47	117.80	109.60
3	I	223	VAL	CB-CA-C	-5.47	104.97	111.97
3	I	280	ASP	N-CA-C	-5.47	104.38	111.71
3	L	167	PHE	CA-C-N	5.47	127.61	120.28
3	L	167	PHE	C-N-CA	5.47	127.61	120.28
1	C	151	ASP	CA-C-N	5.47	125.08	119.56
1	C	151	ASP	C-N-CA	5.47	125.08	119.56
3	K	147	ASP	CA-C-N	5.47	129.60	120.64
3	K	147	ASP	C-N-CA	5.47	129.60	120.64
1	C	172	THR	N-CA-CB	5.46	118.25	110.16
1	D	151	ASP	CA-CB-CG	-5.46	107.14	112.60
1	f	235	ARG	CA-C-O	-5.46	114.76	120.55
2	4	74	ALA	CB-CA-C	-5.46	101.56	110.85
1	g	91	ARG	CA-C-N	5.46	128.05	120.29
1	g	91	ARG	C-N-CA	5.46	128.05	120.29
3	M	20	TYR	CB-CG-CD2	-5.46	112.61	120.80
1	e	122	GLN	N-CA-C	-5.46	105.88	112.54
2	3	73	GLU	N-CA-C	-5.46	105.48	111.82
3	H	78	VAL	CA-C-O	5.46	126.54	120.59
3	H	126	MET	CA-C-O	-5.46	112.70	120.51
3	H	178	VAL	N-CA-C	-5.46	98.60	107.28
1	B	226	PRO	CA-C-O	-5.46	111.25	119.55
1	A	153	SER	N-CA-C	-5.46	105.25	111.14
1	c	20	ARG	N-CA-C	-5.46	98.65	108.48
1	D	229	LEU	CA-C-N	5.46	129.05	120.97
1	D	229	LEU	C-N-CA	5.46	129.05	120.97
1	e	101	LEU	N-CA-C	-5.46	105.25	111.14
1	e	230	LYS	CA-C-N	5.46	125.11	119.05
1	e	230	LYS	C-N-CA	5.46	125.11	119.05
2	h	21	ASP	CA-CB-CG	5.46	118.06	112.60
2	i	57	ALA	O-C-N	-5.46	116.80	123.30
2	i	87	VAL	O-C-N	5.46	127.17	121.87
2	4	139	ALA	CB-CA-C	-5.46	100.17	110.16
1	A	94	ILE	CA-C-N	5.46	128.60	120.31
1	A	94	ILE	C-N-CA	5.46	128.60	120.31
1	f	86	ARG	CB-CG-CD	5.46	123.85	111.30
2	3	85	PRO	N-CA-C	-5.46	102.62	111.19
3	M	117	ASN	CA-CB-CG	5.46	118.06	112.60
1	C	200	ILE	O-C-N	-5.46	115.74	122.18
2	3	65	PHE	CA-CB-CG	-5.46	108.34	113.80
2	6	45	ILE	CA-CB-CG1	5.46	119.67	110.40
3	I	263	ARG	N-CA-C	-5.46	106.40	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	SER	CA-C-N	5.45	125.28	119.28
1	B	225	SER	C-N-CA	5.45	125.28	119.28
1	c	73	HIS	CG-CD2-NE2	5.45	112.65	107.20
1	E	79	SER	O-C-N	-5.45	117.03	123.41
3	L	101	LYS	CA-C-O	-5.45	115.32	120.34
3	M	123	LYS	O-C-N	-5.45	117.38	121.47
3	L	196	ALA	CA-C-N	5.45	129.82	120.72
3	L	196	ALA	C-N-CA	5.45	129.82	120.72
1	B	90	ASP	N-CA-C	-5.45	105.42	111.36
1	C	210	GLU	N-CA-C	-5.45	100.14	109.24
3	L	52	ARG	O-C-N	5.45	127.68	122.07
3	M	19	ASP	CA-C-O	5.45	126.33	120.55
1	b	200	ILE	CA-C-N	5.45	129.87	122.19
1	b	200	ILE	C-N-CA	5.45	129.87	122.19
1	F	216	VAL	N-CA-C	-5.45	105.06	111.00
3	K	371	THR	N-CA-C	-5.45	99.19	110.80
3	M	175	PRO	O-C-N	-5.45	116.35	123.00
3	H	321	PHE	CA-CB-CG	-5.45	108.35	113.80
1	d	216	VAL	CB-CA-C	-5.45	105.00	111.97
1	G	112	LEU	CB-CA-C	5.45	120.11	110.85
1	G	185	PHE	CA-C-N	5.45	127.85	120.44
1	G	185	PHE	C-N-CA	5.45	127.85	120.44
2	2	55	THR	CA-CB-OG1	5.45	117.77	109.60
3	L	40	GLU	CA-C-N	5.45	127.58	120.28
3	L	40	GLU	C-N-CA	5.45	127.58	120.28
1	d	168	ARG	O-C-N	-5.44	116.25	122.08
1	A	215	LYS	N-CA-CB	5.44	118.82	110.49
1	a	25	GLU	CA-C-N	5.44	127.57	120.28
1	a	25	GLU	C-N-CA	5.44	127.57	120.28
1	B	138	ILE	CB-CA-C	-5.44	104.38	110.96
2	1	147	ALA	N-CA-CB	5.44	118.12	110.12
2	h	174	SER	CA-C-N	5.44	129.89	120.58
2	h	174	SER	C-N-CA	5.44	129.89	120.58
2	4	30	ARG	CA-C-O	-5.44	114.01	120.43
3	J	303	PHE	CB-CA-C	-5.44	104.68	111.43
1	C	233	VAL	N-CA-C	5.44	117.89	111.09
1	e	230	LYS	N-CA-C	5.44	120.95	113.77
2	7	44	LYS	O-C-N	5.44	127.70	121.93
3	H	128	TYR	N-CA-C	-5.44	106.50	114.39
3	K	41	ARG	CB-CG-CD	5.44	123.81	111.30
3	L	199	THR	N-CA-C	-5.44	105.35	111.28
1	a	29	GLU	N-CA-CB	5.44	118.12	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	15	VAL	CA-C-N	5.44	128.45	121.27
2	5	15	VAL	C-N-CA	5.44	128.45	121.27
3	M	348	GLY	CA-C-N	5.44	127.57	120.28
3	M	348	GLY	C-N-CA	5.44	127.57	120.28
2	1	75	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	1	163	GLU	CA-C-O	5.44	126.21	119.79
2	3	42	ALA	CA-C-O	-5.44	115.10	121.46
2	j	165	VAL	CA-CB-CG2	5.44	119.64	110.40
3	M	156	ALA	CA-C-N	-5.44	117.40	123.16
3	M	156	ALA	C-N-CA	-5.44	117.40	123.16
1	A	143	GLU	CB-CG-CD	-5.44	103.36	112.60
1	A	74	ILE	N-CA-CB	5.43	120.36	111.45
1	F	75	CYS	CA-C-O	-5.43	115.27	121.68
3	H	47	GLU	CA-C-N	5.43	127.90	120.46
3	H	47	GLU	C-N-CA	5.43	127.90	120.46
3	M	110	GLN	CA-C-N	5.43	128.01	120.29
3	M	110	GLN	C-N-CA	5.43	128.01	120.29
1	B	191	LEU	O-C-N	5.43	127.88	122.12
2	6	205	GLU	CA-C-N	5.43	129.92	120.68
2	6	205	GLU	C-N-CA	5.43	129.92	120.68
2	7	84	LYS	N-CA-C	5.43	116.54	109.64
3	K	19	ASP	CA-C-N	5.43	128.57	120.31
3	K	19	ASP	C-N-CA	5.43	128.57	120.31
3	K	195	VAL	CB-CA-C	-5.43	104.72	112.22
3	J	200	ARG	N-CA-CB	5.43	120.17	111.91
2	m	176	MET	CG-SD-CE	-5.43	88.95	100.90
1	B	125	GLN	OE1-CD-NE2	-5.43	117.17	122.60
2	n	195	GLU	CA-C-O	-5.43	115.27	121.40
3	I	377	LYS	CB-CA-C	-5.43	101.62	110.85
1	A	52	LYS	N-CA-C	-5.43	104.34	112.54
1	d	91	ARG	CA-C-O	-5.43	115.12	120.82
2	i	164	ALA	CA-C-O	-5.43	113.73	119.97
2	3	147	ALA	CB-CA-C	-5.43	101.78	110.79
2	k	204	VAL	CA-C-N	5.43	128.10	120.28
2	k	204	VAL	C-N-CA	5.43	128.10	120.28
1	B	92	ALA	CA-C-N	5.43	127.55	120.28
1	B	92	ALA	C-N-CA	5.43	127.55	120.28
1	E	220	THR	CA-CB-OG1	5.43	117.74	109.60
1	g	177	LYS	N-CA-C	-5.43	105.46	112.68
2	h	186	ILE	N-CA-C	-5.43	100.31	108.12
2	5	28	GLU	O-C-N	-5.43	117.14	123.27
2	m	45	ILE	N-CA-C	-5.43	100.51	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	159	LEU	CA-C-N	5.43	126.62	119.84
3	M	159	LEU	C-N-CA	5.43	126.62	119.84
1	E	39	GLY	CA-C-O	5.42	125.17	120.94
1	F	227	GLU	CA-C-N	5.42	132.15	122.06
1	F	227	GLU	C-N-CA	5.42	132.15	122.06
2	1	27	THR	O-C-N	5.42	129.74	123.17
2	1	109	GLN	OE1-CD-NE2	5.42	128.02	122.60
2	3	142	SER	O-C-N	5.42	129.63	122.36
3	M	121	THR	CA-C-N	5.42	131.46	121.70
3	M	121	THR	C-N-CA	5.42	131.46	121.70
3	K	273	ASP	CA-C-N	5.42	126.92	120.14
3	K	273	ASP	C-N-CA	5.42	126.92	120.14
3	I	78	VAL	CA-C-N	5.42	130.24	123.14
3	I	78	VAL	C-N-CA	5.42	130.24	123.14
3	K	314	PHE	CA-C-N	5.42	127.99	120.29
3	K	314	PHE	C-N-CA	5.42	127.99	120.29
3	L	65	VAL	CA-CB-CG2	5.42	119.62	110.40
3	J	111	GLN	CG-CD-NE2	-5.42	108.27	116.40
1	a	65	GLU	N-CA-CB	5.42	120.18	110.80
3	H	206	VAL	O-C-N	-5.42	117.02	123.04
2	4	62	ASP	CA-C-N	5.42	127.86	120.54
2	4	62	ASP	C-N-CA	5.42	127.86	120.54
3	I	370	VAL	N-CA-CB	5.42	117.55	111.21
3	M	212	VAL	N-CA-CB	5.42	120.17	111.23
3	J	58	LEU	CA-C-N	5.42	130.62	121.14
3	J	58	LEU	C-N-CA	5.42	130.62	121.14
1	B	150	THR	CA-CB-OG1	5.42	117.73	109.60
1	d	156	LEU	CB-CA-C	5.42	118.58	109.48
1	d	170	ALA	CA-C-N	5.42	128.11	120.42
1	d	170	ALA	C-N-CA	5.42	128.11	120.42
2	m	58	GLY	CA-C-N	5.42	128.40	120.71
2	m	58	GLY	C-N-CA	5.42	128.40	120.71
3	H	97	GLU	O-C-N	5.42	129.84	122.37
1	G	81	LEU	CB-CA-C	-5.41	101.46	109.90
2	m	123	TYR	CG-CD1-CE1	-5.41	113.08	121.20
3	M	386	THR	N-CA-C	-5.41	107.93	114.75
2	l	129	GLY	CA-C-N	5.41	132.02	121.41
2	l	129	GLY	C-N-CA	5.41	132.02	121.41
3	K	315	GLU	CA-C-N	5.41	125.95	119.94
3	K	315	GLU	C-N-CA	5.41	125.95	119.94
1	e	70	ILE	N-CA-C	-5.41	105.84	111.58
2	k	198	GLN	N-CA-C	-5.41	99.28	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	343	THR	CA-CB-OG1	5.41	117.71	109.60
1	A	92	ALA	CB-CA-C	-5.41	102.39	110.88
1	G	29	GLU	CA-CB-CG	-5.41	103.28	114.10
2	j	175	ALA	N-CA-C	5.41	117.17	111.28
2	k	124	SER	N-CA-C	-5.41	100.42	109.24
2	6	73	GLU	N-CA-CB	5.41	119.22	110.40
3	J	152	GLU	CA-C-N	5.41	128.10	120.42
3	J	152	GLU	C-N-CA	5.41	128.10	120.42
1	D	206	PRO	CA-C-N	5.41	127.53	120.28
1	D	206	PRO	C-N-CA	5.41	127.53	120.28
1	E	157	LEU	N-CA-C	-5.41	99.50	108.75
2	j	116	ASP	CA-C-N	5.41	127.97	120.29
2	j	116	ASP	C-N-CA	5.41	127.97	120.29
2	4	198	GLN	CA-C-N	5.41	128.53	120.31
2	4	198	GLN	C-N-CA	5.41	128.53	120.31
2	k	116	ASP	N-CA-C	-5.41	101.28	108.74
3	J	330	LEU	CA-C-N	5.41	129.02	121.02
3	J	330	LEU	C-N-CA	5.41	129.02	121.02
1	e	45	GLY	CA-C-O	-5.41	115.25	121.47
1	F	190	VAL	CB-CA-C	-5.41	104.76	112.22
3	H	263	ARG	NE-CZ-NH1	5.41	126.91	121.50
3	J	275	PHE	CA-CB-CG	-5.41	108.39	113.80
3	M	165	GLU	N-CA-C	5.40	117.17	111.28
1	c	90	ASP	CA-C-N	5.40	127.52	120.28
1	c	90	ASP	C-N-CA	5.40	127.52	120.28
1	G	72	GLU	N-CA-CB	5.40	118.75	110.70
1	g	194	VAL	CA-C-N	5.40	127.96	120.29
1	g	194	VAL	C-N-CA	5.40	127.96	120.29
2	2	78	GLU	N-CA-C	-5.40	105.47	111.36
2	5	154	ARG	NE-CZ-NH1	-5.40	116.10	121.50
3	L	252	ASN	OD1-CG-ND2	5.40	128.00	122.60
2	k	145	LEU	CA-C-N	5.40	127.96	120.29
2	k	145	LEU	C-N-CA	5.40	127.96	120.29
2	5	164	ALA	N-CA-C	-5.40	105.43	112.23
1	f	185	PHE	CB-CG-CD2	-5.40	111.52	120.70
3	J	188	LYS	CA-C-N	5.40	127.51	120.28
3	J	188	LYS	C-N-CA	5.40	127.51	120.28
3	J	302	ARG	NE-CZ-NH1	-5.40	116.10	121.50
2	6	163	GLU	N-CA-C	-5.40	106.70	113.28
1	b	102	THR	CA-CB-CG2	5.39	119.67	110.50
1	g	207	GLU	CB-CG-CD	5.39	121.77	112.60
2	i	169	VAL	N-CA-C	-5.39	105.24	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ARG	CA-C-N	5.39	127.61	122.27
1	C	33	ARG	C-N-CA	5.39	127.61	122.27
1	G	86	ARG	CA-C-N	5.39	129.14	120.30
1	G	86	ARG	C-N-CA	5.39	129.14	120.30
2	j	57	ALA	CA-C-O	5.39	126.86	120.66
2	m	88	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	E	218	ASP	CA-CB-CG	5.39	117.99	112.60
2	3	55	THR	N-CA-CB	5.39	119.48	110.85
3	K	93	GLN	CA-C-N	5.39	130.69	122.23
3	K	93	GLN	C-N-CA	5.39	130.69	122.23
3	L	131	GLU	CB-CG-CD	-5.39	103.44	112.60
1	a	200	ILE	CA-C-N	5.39	130.50	122.74
1	a	200	ILE	C-N-CA	5.39	130.50	122.74
1	e	232	TYR	N-CA-CB	5.39	118.14	110.16
1	F	66	LYS	N-CA-CB	5.39	118.16	110.67
1	F	143	GLU	CB-CA-C	-5.39	99.69	110.42
2	h	132	ILE	CA-C-O	-5.39	114.85	120.51
2	l	20	LYS	N-CA-C	-5.39	106.70	113.28
3	H	136	PRO	CA-CB-CG	-5.39	94.26	104.50
1	c	50	ALA	N-CA-C	-5.39	99.90	109.06
1	F	82	VAL	CA-C-O	5.39	126.56	120.85
1	f	215	LYS	CA-C-O	-5.39	114.90	121.36
2	4	134	GLU	N-CA-C	-5.39	101.38	109.95
2	5	104	PHE	N-CA-C	-5.39	96.87	107.91
2	7	21	ASP	CA-C-N	-5.39	114.83	121.83
2	7	21	ASP	C-N-CA	-5.39	114.83	121.83
2	l	68	ARG	CB-CA-C	-5.38	101.70	110.85
1	e	130	ARG	O-C-N	-5.38	115.40	121.43
2	3	76	LEU	N-CA-C	5.38	117.57	111.11
2	7	135	LYS	CA-C-O	5.38	125.11	119.51
3	K	165	GLU	CA-C-N	5.38	128.03	120.28
3	K	165	GLU	C-N-CA	5.38	128.03	120.28
3	I	195	VAL	N-CA-C	-5.38	105.13	110.62
3	M	368	ALA	CA-C-N	5.38	129.19	121.50
3	M	368	ALA	C-N-CA	5.38	129.19	121.50
1	a	180	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	c	119	PHE	N-CA-CB	5.38	118.03	110.12
1	G	208	ASN	CA-C-O	5.38	124.82	118.90
3	M	141	GLU	N-CA-C	-5.38	106.09	113.30
1	b	93	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	j	46	TYR	CA-CB-CG	-5.38	104.22	113.90
2	k	161	VAL	CA-C-O	-5.38	114.81	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	148	TYR	O-C-N	-5.38	116.53	122.07
3	H	170	VAL	N-CA-C	-5.38	105.60	110.82
3	L	51	LEU	N-CA-CB	5.38	118.12	110.16
1	a	45	GLY	N-CA-C	-5.38	103.17	110.43
1	F	82	VAL	N-CA-C	-5.38	105.29	110.72
2	7	75	ASN	CB-CA-C	-5.38	101.71	110.85
1	C	74	ILE	CB-CG1-CD1	5.38	125.09	113.80
1	A	12	ILE	N-CA-C	-5.37	106.61	113.22
1	b	199	SER	CA-CB-OG	-5.37	100.35	111.10
1	c	38	ILE	CB-CG1-CD1	5.37	125.08	113.80
2	4	13	THR	O-C-N	5.37	129.38	123.25
3	J	266	MET	CG-SD-CE	-5.37	89.08	100.90
2	h	139	ALA	N-CA-CB	5.37	119.57	110.49
2	m	144	SER	N-CA-C	5.37	117.14	111.28
2	n	32	THR	CA-C-O	-5.37	115.35	121.58
3	M	221	ARG	N-CA-CB	5.37	119.57	110.49
1	F	114	LYS	N-CA-CB	5.37	118.02	110.12
1	C	91	ARG	N-CA-C	-5.37	105.33	111.07
1	e	15	PHE	CA-C-N	5.37	127.85	120.39
1	e	15	PHE	C-N-CA	5.37	127.85	120.39
1	g	19	GLY	CA-C-N	5.37	132.86	122.07
1	g	19	GLY	C-N-CA	5.37	132.86	122.07
2	2	179	ASP	N-CA-CB	5.37	118.93	110.56
2	5	20	LYS	CA-C-N	5.37	129.74	121.53
2	5	20	LYS	C-N-CA	5.37	129.74	121.53
2	5	143	GLY	N-CA-C	-5.37	106.71	115.46
3	I	88	VAL	N-CA-CB	5.37	117.43	110.99
1	a	218	ASP	N-CA-C	-5.37	107.39	114.04
1	b	17	PRO	CA-C-N	5.37	130.91	122.11
1	b	17	PRO	C-N-CA	5.37	130.91	122.11
3	K	164	PRO	N-CA-C	-5.37	107.18	114.80
1	B	229	LEU	CB-CA-C	-5.37	101.73	110.85
1	b	115	LYS	N-CA-C	5.37	117.21	111.36
1	b	230	LYS	N-CA-CB	5.37	119.92	110.37
1	G	122	GLN	O-C-N	5.37	128.27	122.15
2	j	211	PHE	N-CA-C	-5.37	104.44	112.54
2	m	70	ILE	CA-CB-CG1	-5.37	101.28	110.40
3	H	231	LYS	CA-C-N	5.37	127.91	120.29
3	H	231	LYS	C-N-CA	5.37	127.91	120.29
1	a	52	LYS	N-CA-C	-5.36	105.96	112.88
1	a	234	GLU	CB-CG-CD	-5.36	103.48	112.60
1	D	128	GLY	N-CA-C	-5.36	107.92	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	181	ASP	N-CA-CB	5.36	118.48	110.22
1	E	65	GLU	N-CA-CB	5.36	119.62	110.50
2	2	122	ILE	N-CA-CB	5.36	120.25	111.45
3	H	148	VAL	CA-C-N	5.36	127.47	120.28
3	H	148	VAL	C-N-CA	5.36	127.47	120.28
1	C	103	TYR	CA-C-N	5.36	130.18	122.40
1	C	103	TYR	C-N-CA	5.36	130.18	122.40
3	L	107	ALA	N-CA-C	-5.36	100.50	109.24
3	K	66	GLY	N-CA-C	-5.36	103.31	111.14
3	J	119	LEU	CA-C-O	-5.36	114.92	120.87
3	J	198	GLN	CB-CA-C	-5.36	101.74	110.85
1	b	217	ASP	N-CA-CB	5.36	118.55	110.30
2	n	102	ARG	CA-C-N	5.36	132.03	122.06
2	n	102	ARG	C-N-CA	5.36	132.03	122.06
1	a	172	THR	CA-C-N	5.36	127.41	120.44
1	a	172	THR	C-N-CA	5.36	127.41	120.44
1	b	82	VAL	CA-C-N	5.36	127.90	120.29
1	b	82	VAL	C-N-CA	5.36	127.90	120.29
1	d	33	ARG	CA-C-O	5.36	125.03	119.14
1	F	242	GLU	CA-C-O	-5.36	113.81	119.97
2	3	158	GLU	CB-CA-C	-5.36	100.33	109.65
2	4	38	ALA	N-CA-C	-5.36	107.11	113.97
3	H	142	ASP	N-CA-CB	5.36	119.36	110.47
2	3	165	VAL	N-CA-CB	5.36	118.61	110.58
2	3	183	GLY	N-CA-C	-5.36	107.63	115.72
2	l	42	ALA	CB-CA-C	-5.36	100.48	109.53
3	I	236	SER	N-CA-C	-5.36	100.30	108.76
1	b	103	TYR	N-CA-CB	5.35	118.27	110.88
1	d	215	LYS	CA-C-O	-5.35	114.96	121.28
3	J	26	LEU	CB-CA-C	-5.35	102.47	110.88
1	A	177	LYS	N-CA-C	-5.35	104.33	112.04
1	a	27	ALA	CA-C-N	5.35	127.89	120.29
1	a	27	ALA	C-N-CA	5.35	127.89	120.29
1	E	39	GLY	O-C-N	-5.35	119.21	123.49
2	k	58	GLY	CA-C-N	5.35	128.37	120.82
2	k	58	GLY	C-N-CA	5.35	128.37	120.82
2	5	103	TYR	N-CA-C	-5.35	105.89	112.90
2	6	148	TYR	CA-C-O	-5.35	114.88	120.55
3	K	146	LEU	N-CA-C	-5.35	103.57	111.81
2	2	170	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	8	TYR	N-CA-C	-5.35	106.43	113.17
2	k	102	ARG	N-CA-C	-5.35	106.71	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	88	VAL	CA-C-N	5.35	131.40	122.57
3	H	88	VAL	C-N-CA	5.35	131.40	122.57
1	D	21	LEU	N-CA-CB	5.35	119.51	110.69
1	G	152	PRO	N-CA-CB	5.35	108.44	103.41
1	G	222	LYS	N-CA-C	-5.35	100.59	108.99
2	l	49	ALA	N-CA-C	-5.35	101.71	108.45
2	k	124	SER	O-C-N	5.35	129.31	123.27
2	l	85	PRO	CB-CA-C	-5.35	104.39	111.23
1	d	37	ALA	CA-C-O	5.34	127.26	121.06
1	e	235	ARG	CG-CD-NE	-5.34	100.24	112.00
1	f	186	ASP	CA-CB-CG	-5.34	107.26	112.60
3	H	182	GLY	CA-C-N	5.34	125.88	120.38
3	H	182	GLY	C-N-CA	5.34	125.88	120.38
1	G	74	ILE	CA-CB-CG1	5.34	119.48	110.40
2	m	21	ASP	CA-CB-CG	5.34	117.94	112.60
2	m	90	ILE	CA-C-N	5.34	127.70	120.44
2	m	90	ILE	C-N-CA	5.34	127.70	120.44
3	H	100	LEU	N-CA-CB	5.34	120.12	110.83
3	H	174	PRO	CB-CA-C	-5.34	104.40	110.92
3	I	126	MET	O-C-N	-5.34	116.67	123.24
3	K	188	LYS	CA-C-N	5.34	127.97	120.28
3	K	188	LYS	C-N-CA	5.34	127.97	120.28
1	D	15	PHE	CA-C-O	-5.34	115.13	121.16
1	G	180	ARG	NE-CZ-NH1	-5.34	116.16	121.50
2	3	64	GLN	CA-C-N	5.34	127.44	120.28
2	3	64	GLN	C-N-CA	5.34	127.44	120.28
2	n	182	SER	CA-C-N	5.34	128.13	121.83
2	n	182	SER	C-N-CA	5.34	128.13	121.83
3	I	373	LEU	CD1-CG-CD2	5.34	122.55	110.80
1	b	130	ARG	N-CA-CB	5.34	119.94	110.39
1	b	123	TYR	N-CA-C	-5.34	106.54	113.16
1	E	199	SER	N-CA-CB	5.34	118.06	110.16
2	i	134	GLU	N-CA-CB	5.34	118.22	109.95
2	i	143	GLY	CA-C-N	5.34	127.43	120.28
2	i	143	GLY	C-N-CA	5.34	127.43	120.28
2	n	175	ALA	N-CA-C	5.34	117.10	111.28
3	H	138	VAL	CA-C-O	5.34	126.93	120.74
3	K	264	THR	N-CA-CB	5.34	117.81	110.07
3	I	82	SER	N-CA-CB	5.33	117.96	110.12
3	L	65	VAL	CB-CA-C	5.33	118.52	111.21
1	B	113	ALA	CA-C-N	5.33	127.43	120.28
1	B	113	ALA	C-N-CA	5.33	127.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	64	GLN	CB-CA-C	-5.33	101.78	110.85
3	I	41	ARG	CA-C-N	5.33	127.77	120.46
3	I	41	ARG	C-N-CA	5.33	127.77	120.46
3	I	381	LYS	O-C-N	5.33	127.58	122.03
3	L	372	MET	CA-C-N	5.33	127.69	120.38
3	L	372	MET	C-N-CA	5.33	127.69	120.38
3	J	352	LYS	CA-C-N	5.33	127.86	120.29
3	J	352	LYS	C-N-CA	5.33	127.86	120.29
3	I	173	GLU	CB-CA-C	-5.33	100.75	108.91
3	I	303	PHE	CA-C-N	5.33	127.42	120.28
3	I	303	PHE	C-N-CA	5.33	127.42	120.28
1	F	70	ILE	CA-C-N	5.33	130.61	121.87
1	F	70	ILE	C-N-CA	5.33	130.61	121.87
2	4	117	SER	CA-C-N	5.33	128.41	120.31
2	4	117	SER	C-N-CA	5.33	128.41	120.31
3	M	68	VAL	CA-CB-CG2	-5.33	101.34	110.40
2	m	128	ILE	N-CA-C	-5.33	107.78	112.90
3	L	57	ARG	CA-C-O	5.33	126.07	120.42
1	D	182	ASP	N-CA-C	-5.33	106.55	113.16
1	d	127	GLY	N-CA-C	-5.33	106.53	115.80
1	d	224	VAL	N-CA-CB	5.33	116.91	110.95
1	E	119	PHE	CA-C-N	5.33	127.36	120.44
1	E	119	PHE	C-N-CA	5.33	127.36	120.44
2	4	88	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	n	144	SER	N-CA-C	5.33	117.77	111.33
3	H	353	ALA	CA-C-N	5.33	127.75	120.46
3	H	353	ALA	C-N-CA	5.33	127.75	120.46
1	b	225	SER	N-CA-CB	5.32	117.13	109.78
1	F	73	HIS	CA-C-N	5.32	130.47	122.75
1	F	73	HIS	C-N-CA	5.32	130.47	122.75
1	f	203	GLU	O-C-N	-5.32	116.98	123.16
2	h	102	ARG	CA-C-N	5.32	127.41	120.28
2	h	102	ARG	C-N-CA	5.32	127.41	120.28
2	i	154	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	n	33	MET	N-CA-C	-5.32	105.43	112.94
3	L	281	VAL	CA-C-O	-5.32	114.85	120.39
1	E	185	PHE	CA-C-O	5.32	126.06	120.42
2	3	206	GLN	N-CA-C	-5.32	106.63	113.23
1	C	210	GLU	O-C-N	-5.32	116.78	123.27
1	G	184	SER	CA-C-N	5.32	127.41	120.28
1	G	184	SER	C-N-CA	5.32	127.41	120.28
2	2	116	ASP	CA-C-O	-5.32	115.72	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	71	LYS	O-C-N	5.32	127.76	122.12
1	b	136	LEU	CA-C-O	-5.32	114.89	121.11
3	M	305	ARG	CA-C-O	5.32	126.05	120.36
3	J	357	GLU	CA-C-N	5.32	127.84	120.29
3	J	357	GLU	C-N-CA	5.32	127.84	120.29
3	H	331	ALA	O-C-N	-5.32	115.52	122.59
3	K	120	PRO	CA-C-O	-5.32	115.18	121.67
3	M	9	LEU	CA-C-N	5.32	127.41	120.28
3	M	9	LEU	C-N-CA	5.32	127.41	120.28
1	a	178	GLU	CB-CG-CD	5.32	121.64	112.60
1	d	59	LEU	CA-C-O	5.32	126.61	120.60
1	E	206	PRO	N-CA-C	5.32	120.75	113.84
1	G	80	GLY	N-CA-C	-5.32	100.58	113.18
2	3	143	GLY	CA-C-N	5.32	127.40	120.28
2	3	143	GLY	C-N-CA	5.32	127.40	120.28
2	k	202	GLU	CA-C-O	-5.32	115.21	120.90
3	I	186	THR	O-C-N	-5.32	115.81	122.24
3	J	287	THR	CA-C-N	5.32	128.36	120.17
3	J	287	THR	C-N-CA	5.32	128.36	120.17
2	1	200	SER	CA-C-N	5.31	126.48	119.84
2	1	200	SER	C-N-CA	5.31	126.48	119.84
2	h	77	TYR	CA-C-N	5.31	127.35	120.44
2	h	77	TYR	C-N-CA	5.31	127.35	120.44
2	7	131	ALA	O-C-N	-5.31	116.91	123.44
3	J	131	GLU	N-CA-CB	5.31	118.73	110.44
1	C	33	ARG	N-CA-C	-5.31	106.48	113.17
2	i	25	MET	CG-SD-CE	-5.31	89.22	100.90
1	A	57	LYS	O-C-N	-5.31	114.68	122.43
1	A	199	SER	CA-C-O	-5.31	115.25	120.82
1	D	134	VAL	CA-CB-CG1	5.31	119.42	110.40
1	g	208	ASN	CB-CG-ND2	-5.31	108.44	116.40
2	2	41	ALA	CA-C-N	5.31	128.89	121.24
2	2	41	ALA	C-N-CA	5.31	128.89	121.24
2	j	132	ILE	N-CA-CB	5.31	118.74	111.41
3	L	78	VAL	CA-CB-CG2	-5.31	101.38	110.40
3	M	137	GLU	N-CA-C	5.31	117.98	111.82
1	C	168	ARG	CA-C-O	-5.31	115.22	120.90
1	E	234	GLU	CA-C-N	5.31	127.39	120.28
1	E	234	GLU	C-N-CA	5.31	127.39	120.28
2	i	111	LEU	N-CA-C	-5.31	99.76	108.41
2	j	156	THR	CA-CB-OG1	5.31	117.56	109.60
2	k	53	ALA	N-CA-C	-5.31	101.23	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	269	LEU	N-CA-CB	5.31	117.92	110.12
1	a	116	ILE	CA-C-N	5.31	127.34	120.44
1	a	116	ILE	C-N-CA	5.31	127.34	120.44
1	g	46	VAL	CA-CB-CG1	5.31	119.42	110.40
2	h	150	VAL	N-CA-C	5.31	116.08	110.72
2	i	86	THR	CA-C-N	5.31	127.73	120.46
2	i	86	THR	C-N-CA	5.31	127.73	120.46
3	I	70	ASP	CA-C-O	-5.31	115.63	121.31
3	K	241	ASP	N-CA-C	-5.31	101.63	110.17
1	A	70	ILE	CA-C-O	5.30	126.26	120.69
1	e	102	THR	CA-C-O	-5.30	112.87	119.18
1	f	57	LYS	N-CA-CB	5.30	118.56	110.44
1	G	67	ILE	N-CA-C	-5.30	97.17	106.61
1	C	219	ARG	N-CA-C	5.30	118.90	111.90
2	i	30	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	H	272	LEU	N-CA-C	5.30	116.87	111.14
3	I	192	ALA	N-CA-CB	5.30	118.01	110.16
1	A	200	ILE	N-CA-C	-5.30	105.81	113.07
2	5	157	PRO	N-CA-C	-5.30	107.27	114.80
3	H	111	GLN	O-C-N	-5.30	116.48	122.10
1	F	104	ASP	CA-CB-CG	5.30	117.90	112.60
2	k	182	SER	N-CA-C	-5.30	104.54	112.54
2	m	103	TYR	N-CA-C	-5.30	105.17	111.69
2	7	74	ALA	N-CA-CB	5.30	117.76	110.07
3	L	78	VAL	N-CA-C	-5.30	100.25	107.99
1	b	69	LYS	CA-C-O	-5.30	114.65	120.69
1	f	25	GLU	CA-C-N	5.30	127.81	120.29
1	f	25	GLU	C-N-CA	5.30	127.81	120.29
1	B	237	ASN	CA-C-N	5.30	127.38	120.28
1	B	237	ASN	C-N-CA	5.30	127.38	120.28
1	G	122	GLN	N-CA-CB	5.30	118.00	110.16
2	4	188	VAL	CA-CB-CG2	5.30	119.41	110.40
2	k	24	VAL	CA-CB-CG2	-5.30	101.39	110.40
3	I	12	LYS	CA-C-N	5.30	127.81	120.29
3	I	12	LYS	C-N-CA	5.30	127.81	120.29
3	L	331	ALA	N-CA-C	-5.30	101.06	109.59
1	D	211	VAL	CA-CB-CG1	5.29	119.40	110.40
1	a	155	ALA	N-CA-CB	5.29	118.34	110.29
1	D	102	THR	CA-C-O	5.29	124.63	118.97
3	K	192	ALA	CA-C-N	5.29	127.81	120.29
3	K	192	ALA	C-N-CA	5.29	127.81	120.29
3	J	279	GLY	CA-C-N	5.29	129.70	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	279	GLY	C-N-CA	5.29	129.70	122.34
1	d	58	LEU	N-CA-C	-5.29	105.10	112.45
1	E	130	ARG	O-C-N	-5.29	115.50	121.43
2	n	71	LYS	CA-C-N	5.29	127.93	120.42
2	n	71	LYS	C-N-CA	5.29	127.93	120.42
1	C	132	PHE	CA-CB-CG	-5.29	108.51	113.80
2	5	83	ARG	CB-CA-C	-5.29	99.89	110.42
2	m	188	VAL	O-C-N	5.29	128.76	123.10
1	F	98	ILE	CA-C-N	5.29	127.37	120.28
1	F	98	ILE	C-N-CA	5.29	127.37	120.28
1	g	140	GLY	O-C-N	-5.29	117.26	123.55
2	l	135	LYS	CA-C-O	5.29	125.39	119.41
2	6	66	LEU	CA-C-N	5.29	127.80	120.29
2	6	66	LEU	C-N-CA	5.29	127.80	120.29
1	c	151	ASP	CA-C-O	-5.29	115.42	120.97
1	G	52	LYS	N-CA-C	-5.29	99.54	110.80
1	g	175	PHE	CB-CG-CD2	-5.29	111.71	120.70
2	5	89	ALA	N-CA-C	-5.29	105.19	111.69
2	3	79	ILE	CB-CA-C	-5.29	105.01	112.14
3	J	141	GLU	CA-C-O	5.29	125.53	119.35
1	a	116	ILE	N-CA-C	5.28	116.06	110.72
1	B	31	VAL	O-C-N	5.28	127.27	121.83
1	F	31	VAL	N-CA-C	-5.28	105.23	110.62
2	7	187	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	153	SER	CB-CA-C	-5.28	101.87	110.85
3	K	236	SER	CA-C-O	5.28	126.66	120.43
3	J	114	ALA	O-C-N	5.28	129.59	123.41
1	F	149	GLU	CB-CG-CD	-5.28	103.63	112.60
2	j	76	LEU	N-CA-CB	5.28	118.46	110.28
2	l	153	ASP	O-C-N	5.28	128.17	122.15
2	6	23	VAL	N-CA-C	-5.28	100.60	108.46
1	A	131	PRO	N-CA-CB	-5.28	98.42	103.33
1	F	194	VAL	O-C-N	5.28	127.76	121.80
2	l	104	PHE	N-CA-C	-5.28	102.55	110.73
3	H	231	LYS	CB-CA-C	-5.28	102.03	110.79
1	A	5	GLN	O-C-N	-5.27	114.56	123.00
2	m	49	ALA	CA-C-N	5.27	127.30	120.44
2	m	49	ALA	C-N-CA	5.27	127.30	120.44
2	n	50	ASP	N-CA-C	-5.27	107.02	112.93
1	B	44	GLU	CA-C-O	-5.27	112.97	120.51
1	e	29	GLU	CA-C-N	5.27	129.60	120.58
1	e	29	GLU	C-N-CA	5.27	129.60	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	43	LYS	O-C-N	5.27	129.33	122.42
1	G	161	ALA	N-CA-C	-5.27	100.71	108.99
2	5	16	GLY	CA-C-O	5.27	125.81	121.06
2	6	112	ILE	N-CA-C	-5.27	100.53	108.12
2	7	191	ILE	N-CA-C	-5.27	98.37	109.34
3	L	236	SER	CA-C-N	5.27	131.46	121.97
3	L	236	SER	C-N-CA	5.27	131.46	121.97
3	J	185	GLY	CA-C-N	5.27	127.78	120.29
3	J	185	GLY	C-N-CA	5.27	127.78	120.29
1	a	154	GLY	N-CA-C	-5.27	107.52	115.32
1	d	186	ASP	O-C-N	5.27	128.16	122.15
2	2	170	ARG	CA-C-N	5.27	127.78	120.29
2	2	170	ARG	C-N-CA	5.27	127.78	120.29
2	3	100	SER	CA-C-O	-5.27	115.27	120.70
2	k	188	VAL	O-C-N	5.27	128.64	123.00
1	g	131	PRO	CB-CA-C	-5.27	104.05	110.95
2	5	70	ILE	CA-C-N	5.27	127.29	120.44
2	5	70	ILE	C-N-CA	5.27	127.29	120.44
3	H	324	HIS	CB-CG-CD2	-5.27	124.35	131.20
3	K	49	ARG	O-C-N	5.27	128.16	122.15
1	C	120	LYS	CA-C-N	5.27	127.34	120.28
1	C	120	LYS	C-N-CA	5.27	127.34	120.28
2	1	204	VAL	N-CA-CB	5.27	117.70	110.54
2	i	156	THR	O-C-N	-5.27	118.14	121.88
2	k	21	ASP	CA-CB-CG	-5.27	107.33	112.60
3	K	367	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	3	65	PHE	CA-C-N	5.27	127.34	120.28
2	3	65	PHE	C-N-CA	5.27	127.34	120.28
1	b	239	ARG	CA-C-N	5.26	127.67	120.46
1	b	239	ARG	C-N-CA	5.26	127.67	120.46
1	E	126	TYR	N-CA-CB	-5.26	102.11	110.06
2	i	59	SER	CA-C-N	5.26	127.14	120.72
2	i	59	SER	C-N-CA	5.26	127.14	120.72
3	H	210	GLU	CA-C-N	5.26	128.19	120.71
3	H	210	GLU	C-N-CA	5.26	128.19	120.71
3	K	62	PRO	N-CA-CB	5.26	108.39	102.60
3	J	332	GLU	N-CA-CB	5.26	117.70	110.07
1	d	168	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	F	83	ALA	CA-C-N	5.26	127.33	120.28
1	F	83	ALA	C-N-CA	5.26	127.33	120.28
2	2	156	THR	CA-C-O	-5.26	115.26	120.26
2	5	212	ARG	N-CA-CB	5.26	119.38	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	304	ASP	CA-C-O	5.26	126.00	120.42
1	D	70	ILE	CB-CA-C	-5.26	102.66	111.29
2	h	49	ALA	N-CA-C	-5.26	101.48	108.74
3	H	273	ASP	CA-CB-CG	5.26	117.86	112.60
3	J	327	LYS	N-CA-C	-5.26	106.37	112.89
1	e	84	ASP	CA-C-N	5.26	127.33	120.28
1	e	84	ASP	C-N-CA	5.26	127.33	120.28
1	a	163	ALA	CA-C-N	5.26	130.16	122.69
1	a	163	ALA	C-N-CA	5.26	130.16	122.69
3	I	328	MET	N-CA-CB	5.26	117.58	110.38
3	M	374	ASP	CB-CA-C	-5.26	102.06	110.79
1	g	36	THR	CA-CB-OG1	5.25	117.48	109.60
1	B	73	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
2	l	85	PRO	O-C-N	5.25	129.52	123.01
2	6	62	ASP	CA-C-O	5.25	125.99	120.42
3	L	29	ARG	CA-C-N	5.25	127.32	120.28
3	L	29	ARG	C-N-CA	5.25	127.32	120.28
3	M	228	GLN	N-CA-CB	5.25	117.94	110.16
1	c	56	SER	O-C-N	5.25	128.96	123.03
1	D	216	VAL	CB-CA-C	-5.25	104.97	112.22
1	f	40	ILE	CA-CB-CG1	5.25	119.33	110.40
2	l	142	SER	N-CA-CB	5.25	119.36	110.49
1	e	221	PHE	N-CA-CB	5.25	119.19	110.47
3	J	311	LEU	CA-C-O	5.25	126.68	120.96
1	g	135	SER	N-CA-C	-5.25	101.21	109.50
2	h	38	ALA	N-CA-C	-5.25	107.25	113.97
2	3	146	THR	CA-CB-CG2	-5.25	101.58	110.50
2	j	181	ALA	CA-C-O	5.25	125.13	119.15
2	i	100	SER	CA-C-N	5.25	130.89	122.86
2	i	100	SER	C-N-CA	5.25	130.89	122.86
2	6	165	VAL	N-CA-C	-5.25	105.42	110.72
3	H	162	LEU	N-CA-C	-5.25	106.03	112.90
3	L	113	LEU	N-CA-CB	5.25	119.36	110.49
2	1	112	ILE	N-CA-C	-5.25	100.77	108.11
2	j	155	PHE	N-CA-CB	5.25	118.85	110.46
3	I	315	GLU	CA-C-O	5.25	125.98	120.42
1	B	157	LEU	CA-C-N	5.24	130.46	122.65
1	B	157	LEU	C-N-CA	5.24	130.46	122.65
1	b	235	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	c	59	LEU	N-CA-C	-5.24	102.01	110.14
1	c	239	ARG	O-C-N	5.24	128.13	122.15
1	F	183	LEU	N-CA-CB	5.24	117.75	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	133	GLU	CB-CG-CD	-5.24	103.69	112.60
2	6	184	ASP	N-CA-C	-5.24	102.29	110.42
3	L	391	ASP	CA-C-N	5.24	131.14	121.70
3	L	391	ASP	C-N-CA	5.24	131.14	121.70
1	e	22	PHE	CA-C-N	5.24	127.83	120.28
1	e	22	PHE	C-N-CA	5.24	127.83	120.28
1	e	52	LYS	N-CA-C	-5.24	105.97	114.09
2	i	192	THR	CA-C-N	5.24	131.55	121.54
2	i	192	THR	C-N-CA	5.24	131.55	121.54
1	E	197	GLY	CA-C-O	-5.24	114.74	120.40
3	K	160	PRO	CA-C-N	5.24	129.54	120.58
3	K	160	PRO	C-N-CA	5.24	129.54	120.58
1	e	83	ALA	CA-C-N	5.24	127.73	120.29
1	e	83	ALA	C-N-CA	5.24	127.73	120.29
2	h	161	VAL	CA-C-O	5.24	124.23	119.20
2	4	206	GLN	OE1-CD-NE2	5.24	127.84	122.60
2	l	93	LEU	N-CA-CB	5.24	117.82	110.12
1	c	239	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	E	210	GLU	N-CA-CB	5.24	119.86	110.80
1	G	79	SER	N-CA-C	-5.24	100.77	108.99
1	g	27	ALA	CA-C-O	5.24	125.97	119.79
2	4	174	SER	CA-C-N	5.24	128.27	120.31
2	4	174	SER	C-N-CA	5.24	128.27	120.31
3	K	107	ALA	O-C-N	-5.24	117.11	123.29
3	L	33	GLU	N-CA-C	5.24	117.89	111.82
3	L	157	VAL	CA-C-N	5.24	127.30	120.28
3	L	157	VAL	C-N-CA	5.24	127.30	120.28
2	4	201	PRO	CA-C-N	5.23	128.06	120.79
2	4	201	PRO	C-N-CA	5.23	128.06	120.79
1	a	40	ILE	N-CA-C	-5.23	100.70	108.45
1	B	218	ASP	CA-C-N	5.23	129.61	122.34
1	B	218	ASP	C-N-CA	5.23	129.61	122.34
1	D	122	GLN	CA-C-N	5.23	129.46	120.72
1	D	122	GLN	C-N-CA	5.23	129.46	120.72
1	d	241	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	E	83	ALA	N-CA-C	5.23	116.67	111.07
2	i	122	ILE	CB-CG1-CD1	5.23	124.79	113.80
2	3	50	ASP	O-C-N	5.23	128.17	122.20
2	6	138	VAL	CA-C-O	-5.23	116.51	121.64
2	7	30	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	27	ALA	CA-C-N	5.23	128.26	120.31
1	A	27	ALA	C-N-CA	5.23	128.26	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	102	THR	O-C-N	5.23	128.57	122.24
2	1	201	PRO	N-CD-CG	5.23	111.05	103.20
2	6	111	LEU	N-CA-CB	5.23	119.85	110.80
3	M	295	PRO	CA-C-O	-5.23	111.70	119.18
3	J	22	LYS	CB-CG-CD	5.23	123.33	111.30
1	e	12	ILE	CB-CA-C	5.23	118.71	111.49
3	H	288	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	d	36	THR	CA-CB-OG1	5.23	117.44	109.60
1	e	10	ARG	CD-NE-CZ	-5.23	117.08	124.40
2	m	46	TYR	N-CA-C	-5.23	101.13	109.23
3	I	266	MET	CA-C-N	5.23	127.71	120.29
3	I	266	MET	C-N-CA	5.23	127.71	120.29
3	M	29	ARG	O-C-N	-5.23	116.19	122.15
3	J	14	LYS	CA-C-N	5.23	127.81	120.28
3	J	14	LYS	C-N-CA	5.23	127.81	120.28
3	J	120	PRO	N-CA-C	5.23	123.24	112.47
2	5	144	SER	N-CA-CB	5.23	117.90	110.06
2	n	87	VAL	CA-C-N	5.23	127.28	120.28
2	n	87	VAL	C-N-CA	5.23	127.28	120.28
3	I	82	SER	N-CA-C	-5.23	105.58	111.28
3	K	260	GLU	CB-CG-CD	-5.23	103.72	112.60
1	f	171	VAL	O-C-N	-5.22	115.89	121.80
2	m	68	ARG	CA-C-N	5.22	127.25	120.56
2	m	68	ARG	C-N-CA	5.22	127.25	120.56
3	K	241	ASP	N-CA-CB	5.22	119.15	110.63
1	G	22	PHE	N-CA-C	5.22	117.88	111.82
1	G	82	VAL	N-CA-C	-5.22	105.97	113.07
2	m	94	THR	O-C-N	-5.22	116.20	122.15
1	e	107	ILE	CA-C-N	5.22	128.12	120.71
1	e	107	ILE	C-N-CA	5.22	128.12	120.71
1	A	55	GLY	CA-C-O	5.22	129.65	120.57
1	E	60	GLU	CA-C-O	-5.22	116.13	121.87
1	E	118	ASP	CA-C-O	-5.22	115.02	120.55
3	I	242	GLU	N-CA-CB	5.22	119.31	110.49
1	d	73	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	e	192	GLY	CA-C-N	5.22	127.70	120.29
1	e	192	GLY	C-N-CA	5.22	127.70	120.29
2	h	36	PHE	CA-C-O	5.22	126.06	120.32
1	A	120	LYS	CA-C-N	5.22	127.70	120.29
1	A	120	LYS	C-N-CA	5.22	127.70	120.29
1	B	221	PHE	CB-CG-CD1	-5.22	111.83	120.70
1	d	17	PRO	N-CA-CB	-5.22	98.51	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	169	VAL	CA-C-O	-5.22	115.64	121.17
2	l	210	LYS	CA-C-O	5.22	124.79	119.05
3	J	87	PHE	N-CA-C	-5.22	101.26	109.50
1	d	14	VAL	CA-C-N	5.21	128.27	120.87
1	d	14	VAL	C-N-CA	5.21	128.27	120.87
2	5	95	SER	N-CA-C	5.21	116.96	111.28
3	H	46	ARG	NE-CZ-NH2	-5.21	114.51	119.20
3	H	324	HIS	CG-CD2-NE2	5.21	112.41	107.20
3	K	52	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	D	61	ALA	CA-C-N	5.21	130.73	122.60
1	D	61	ALA	C-N-CA	5.21	130.73	122.60
1	d	95	GLU	O-C-N	-5.21	116.59	122.12
2	6	148	TYR	O-C-N	5.21	127.64	122.12
3	I	388	PRO	N-CD-CG	5.21	110.05	103.80
3	M	232	GLU	N-CA-C	-5.21	105.67	112.23
1	D	171	VAL	CA-CB-CG1	5.21	119.26	110.40
2	1	139	ALA	CA-C-O	5.21	127.10	121.06
2	6	161	VAL	N-CA-C	5.21	115.98	110.72
3	M	183	PRO	CA-C-N	5.21	125.15	119.78
3	M	183	PRO	C-N-CA	5.21	125.15	119.78
2	2	81	ARG	NH1-CZ-NH2	5.21	126.07	119.30
2	j	106	TYR	N-CA-CB	5.21	118.86	111.05
2	7	64	GLN	CA-C-N	5.21	127.21	120.44
2	7	64	GLN	C-N-CA	5.21	127.21	120.44
3	K	146	LEU	CA-C-N	5.21	127.21	120.44
3	K	146	LEU	C-N-CA	5.21	127.21	120.44
3	K	147	ASP	CA-C-O	-5.21	115.35	120.82
3	L	121	THR	CA-C-N	5.21	131.49	121.54
3	L	121	THR	C-N-CA	5.21	131.49	121.54
1	a	239	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	d	58	LEU	CA-C-N	5.21	129.75	121.99
1	d	58	LEU	C-N-CA	5.21	129.75	121.99
1	g	185	PHE	CA-C-N	5.21	127.26	120.28
1	g	185	PHE	C-N-CA	5.21	127.26	120.28
1	B	131	PRO	O-C-N	5.21	129.51	123.21
1	G	197	GLY	CA-C-N	5.20	127.25	120.28
1	G	197	GLY	C-N-CA	5.20	127.25	120.28
2	1	128	ILE	CA-C-O	5.20	125.06	119.91
2	1	206	GLN	OE1-CD-NE2	-5.20	117.40	122.60
2	h	50	ASP	CA-CB-CG	-5.20	107.40	112.60
2	5	114	GLY	CA-C-O	-5.20	116.37	121.05
3	I	184	PRO	CA-C-O	-5.20	115.32	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	238	ILE	CA-C-O	-5.20	114.96	120.48
1	c	75	CYS	N-CA-C	-5.20	101.53	108.86
2	k	123	TYR	N-CA-CB	5.20	119.80	110.80
2	l	40	LYS	N-CA-C	-5.20	99.72	110.80
3	L	49	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	b	50	ALA	CB-CA-C	-5.20	100.00	110.30
1	E	33	ARG	N-CA-C	-5.20	105.69	111.36
1	f	141	VAL	CA-C-O	5.20	125.41	120.31
2	j	203	GLU	N-CA-C	5.20	116.95	111.28
3	M	227	PHE	O-C-N	-5.20	115.47	122.23
1	C	190	VAL	CA-C-O	-5.20	115.54	120.95
1	D	120	LYS	CA-C-N	5.20	127.25	120.28
1	D	120	LYS	C-N-CA	5.20	127.25	120.28
1	E	11	ALA	O-C-N	-5.20	117.12	123.10
1	e	10	ARG	CG-CD-NE	-5.20	100.56	112.00
2	l	132	ILE	CB-CA-C	-5.20	104.03	111.31
3	H	283	VAL	CA-C-O	-5.20	114.92	120.59
3	K	336	PHE	CB-CA-C	-5.20	100.69	110.67
1	D	195	ALA	N-CA-CB	5.20	117.55	110.01
1	e	187	ASP	N-CA-C	-5.20	105.53	111.14
2	4	152	GLU	O-C-N	5.20	129.29	122.33
2	l	66	LEU	N-CA-CB	5.20	118.33	110.28
3	M	350	ASP	CA-C-O	5.20	125.93	120.42
1	A	28	ARG	O-C-N	5.20	128.66	122.27
3	I	76	ARG	O-C-N	-5.20	116.39	123.15
3	J	291	ASP	CA-CB-CG	-5.20	107.41	112.60
1	C	67	ILE	N-CA-CB	5.19	119.80	111.23
2	4	25	MET	CA-C-O	-5.19	115.24	121.11
2	n	28	GLU	CA-C-N	5.19	130.72	122.62
2	n	28	GLU	C-N-CA	5.19	130.72	122.62
3	J	262	GLN	N-CA-CB	5.19	117.75	110.12
1	f	53	ARG	CA-C-O	-5.19	115.00	120.92
1	g	15	PHE	N-CA-CB	5.19	120.40	111.00
2	7	202	GLU	CB-CG-CD	-5.19	103.77	112.60
1	A	232	TYR	N-CA-CB	5.19	117.84	110.16
1	a	12	ILE	CA-C-N	5.19	131.45	121.54
1	a	12	ILE	C-N-CA	5.19	131.45	121.54
1	B	231	PRO	N-CA-CB	5.19	109.00	103.39
1	F	206	PRO	N-CA-CB	5.19	106.17	102.28
2	6	133	GLU	N-CA-C	-5.19	101.65	109.85
2	n	186	ILE	N-CA-C	-5.19	100.73	108.46
3	M	122	SER	CA-CB-OG	5.19	121.48	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	339	LEU	O-C-N	5.19	127.42	122.07
1	d	218	ASP	CB-CA-C	-5.19	101.93	110.08
2	2	106	TYR	CB-CG-CD1	5.19	128.58	120.80
1	b	77	ALA	CB-CA-C	-5.19	99.08	109.35
2	l	170	ARG	CD-NE-CZ	5.19	131.66	124.40
3	I	233	LYS	O-C-N	-5.19	116.11	122.34
3	M	13	LEU	CA-C-O	-5.19	115.05	120.55
1	A	44	GLU	N-CA-C	-5.19	104.64	112.99
1	f	182	ASP	CA-CB-CG	5.19	117.79	112.60
1	G	57	LYS	N-CA-C	-5.19	106.64	113.17
2	j	126	ASP	CB-CA-C	5.19	117.74	109.96
3	K	326	ARG	CA-C-N	5.19	127.49	120.44
3	K	326	ARG	C-N-CA	5.19	127.49	120.44
1	F	177	LYS	CA-CB-CG	-5.18	103.73	114.10
3	I	84	GLY	CA-C-O	-5.18	114.11	121.52
3	K	38	GLU	O-C-N	5.18	127.61	122.12
3	K	332	GLU	CB-CG-CD	5.18	121.41	112.60
3	L	179	LEU	N-CA-CB	5.18	119.04	110.69
1	D	202	SER	N-CA-CB	5.18	119.44	111.46
1	F	168	ARG	N-CA-C	5.18	116.61	111.07
2	h	30	ARG	NE-CZ-NH1	-5.18	116.32	121.50
2	2	84	LYS	N-CA-C	5.18	117.23	110.08
2	i	185	GLY	N-CA-C	-5.18	100.90	113.18
3	L	164	PRO	CA-C-N	5.18	127.49	120.44
3	L	164	PRO	C-N-CA	5.18	127.49	120.44
3	M	42	ILE	CA-C-N	5.18	127.65	120.29
3	M	42	ILE	C-N-CA	5.18	127.65	120.29
3	J	297	ILE	CA-C-N	5.18	127.22	120.28
3	J	297	ILE	C-N-CA	5.18	127.22	120.28
1	A	191	LEU	O-C-N	-5.18	115.90	122.27
2	2	161	VAL	CA-CB-CG2	5.18	119.21	110.40
1	D	100	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	g	154	GLY	CA-C-N	5.18	129.29	122.30
1	g	154	GLY	C-N-CA	5.18	129.29	122.30
2	6	94	THR	CA-C-N	5.18	127.17	120.44
2	6	94	THR	C-N-CA	5.18	127.17	120.44
3	H	41	ARG	CA-C-O	-5.18	115.38	120.82
3	L	393	LYS	CA-C-N	5.18	127.04	122.43
3	L	393	LYS	C-N-CA	5.18	127.04	122.43
2	m	43	LYS	N-CA-CB	5.18	119.76	110.80
1	e	149	GLU	CA-C-O	-5.18	113.91	120.28
1	G	22	PHE	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	93	LEU	O-C-N	5.18	127.61	122.12
3	J	226	VAL	CA-C-O	-5.18	115.36	120.85
3	H	44	TYR	CA-C-N	5.17	127.21	120.28
3	H	44	TYR	C-N-CA	5.17	127.21	120.28
3	M	200	ARG	CD-NE-CZ	-5.17	117.16	124.40
3	J	382	VAL	CA-C-O	-5.17	115.17	120.71
1	B	161	ALA	N-CA-C	-5.17	99.78	110.80
1	G	48	LEU	CA-C-N	5.17	130.25	122.75
1	G	48	LEU	C-N-CA	5.17	130.25	122.75
2	k	169	VAL	CA-C-N	5.17	128.17	120.31
2	k	169	VAL	C-N-CA	5.17	128.17	120.31
2	6	200	SER	CA-C-N	5.17	126.31	119.84
2	6	200	SER	C-N-CA	5.17	126.31	119.84
3	H	261	VAL	CA-C-N	5.17	129.36	120.72
3	H	261	VAL	C-N-CA	5.17	129.36	120.72
1	A	68	TYR	CA-C-N	5.17	128.69	121.24
1	A	68	TYR	C-N-CA	5.17	128.69	121.24
1	B	84	ASP	CA-C-N	5.17	127.21	120.28
1	B	84	ASP	C-N-CA	5.17	127.21	120.28
1	C	93	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	c	121	GLN	N-CA-CB	5.17	118.18	110.22
1	d	119	PHE	N-CA-C	-5.17	105.54	111.07
2	3	74	ALA	N-CA-C	-5.17	105.72	111.36
2	k	168	ALA	CA-C-N	5.17	127.54	120.46
2	k	168	ALA	C-N-CA	5.17	127.54	120.46
3	J	334	VAL	N-CA-C	-5.17	100.97	108.36
1	a	159	TYR	CA-C-O	-5.17	115.58	121.58
1	E	79	SER	CA-C-O	5.17	126.90	120.54
1	F	8	TYR	N-CA-C	-5.17	104.26	110.88
1	f	107	ILE	O-C-N	-5.17	117.22	122.75
2	i	88	ARG	NE-CZ-NH1	-5.17	116.33	121.50
2	3	42	ALA	N-CA-CB	5.17	119.57	111.20
2	k	150	VAL	CA-C-N	5.17	127.63	120.29
2	k	150	VAL	C-N-CA	5.17	127.63	120.29
2	m	75	ASN	CB-CA-C	-5.17	102.77	110.88
3	H	67	VAL	CA-C-N	5.17	131.27	121.97
3	H	67	VAL	C-N-CA	5.17	131.27	121.97
1	A	180	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	E	50	ALA	O-C-N	-5.17	117.08	123.33
2	l	26	ALA	O-C-N	-5.17	117.28	123.27
2	6	170	ARG	NE-CZ-NH1	-5.17	116.33	121.50
3	K	224	ARG	CA-C-N	5.17	127.16	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	224	ARG	C-N-CA	5.17	127.16	120.44
3	K	287	THR	CA-CB-OG1	5.17	117.35	109.60
3	L	72	LEU	N-CA-CB	5.17	119.05	110.63
2	i	175	ALA	CA-C-N	5.17	127.72	120.28
2	i	175	ALA	C-N-CA	5.17	127.72	120.28
3	H	83	THR	N-CA-C	-5.17	105.34	111.69
3	M	309	VAL	O-C-N	-5.17	117.43	121.46
1	f	193	LEU	O-C-N	-5.16	116.26	122.15
1	G	240	ILE	O-C-N	5.16	127.15	121.83
2	3	165	VAL	N-CA-C	-5.16	105.50	110.72
3	I	35	LYS	O-C-N	-5.16	116.65	122.12
3	I	122	SER	N-CA-CB	5.16	119.28	110.50
3	L	310	PRO	N-CD-CG	5.16	110.94	103.20
3	M	225	GLU	O-C-N	-5.16	116.27	122.15
1	D	199	SER	N-CA-CB	-5.16	102.53	110.12
2	5	23	VAL	CA-CB-CG1	5.16	119.17	110.40
3	I	27	TYR	CA-C-N	5.16	127.20	120.28
3	I	27	TYR	C-N-CA	5.16	127.20	120.28
1	g	90	ASP	CA-C-O	5.16	125.89	120.42
2	i	45	ILE	N-CA-C	-5.16	100.89	108.11
2	4	46	TYR	N-CA-C	-5.16	99.69	108.26
2	l	48	ILE	CB-CA-C	5.16	118.80	112.04
2	m	172	ILE	CA-C-N	5.16	127.62	120.29
2	m	172	ILE	C-N-CA	5.16	127.62	120.29
1	E	19	GLY	CA-C-N	5.16	129.95	121.39
1	E	19	GLY	C-N-CA	5.16	129.95	121.39
1	e	185	PHE	CA-C-O	5.16	125.89	120.42
2	h	51	ARG	N-CA-C	-5.16	106.80	114.64
3	H	254	ASP	CA-CB-CG	-5.16	107.44	112.60
3	K	183	PRO	CA-CB-CG	5.16	114.30	104.50
3	M	203	PHE	N-CA-C	-5.16	98.86	107.99
3	J	311	LEU	N-CA-C	-5.16	103.45	110.36
3	J	353	ALA	CA-C-N	5.16	127.53	120.46
3	J	353	ALA	C-N-CA	5.16	127.53	120.46
1	G	12	ILE	N-CA-C	-5.16	106.87	112.80
2	5	170	ARG	CB-CA-C	-5.16	102.23	110.79
3	L	372	MET	CA-C-O	-5.16	114.95	120.42
1	D	23	GLN	CA-C-N	5.16	128.75	120.30
1	D	23	GLN	C-N-CA	5.16	128.75	120.30
1	d	10	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	f	60	GLU	CB-CG-CD	-5.16	103.83	112.60
2	k	163	GLU	CB-CG-CD	-5.16	103.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	45	ILE	CA-C-O	5.16	125.48	120.27
3	I	106	VAL	CA-C-O	5.16	126.05	120.43
3	K	193	LYS	CA-C-N	5.15	127.61	120.29
3	K	193	LYS	C-N-CA	5.15	127.61	120.29
1	D	229	LEU	N-CA-CB	5.15	117.78	110.16
2	2	159	ILE	N-CA-CB	5.15	116.54	110.82
2	l	171	ALA	O-C-N	5.15	127.58	122.12
2	h	180	SER	N-CA-C	-5.15	107.17	113.50
3	K	32	ASP	CA-C-N	5.15	127.61	120.29
3	K	32	ASP	C-N-CA	5.15	127.61	120.29
3	K	248	ALA	N-CA-CB	5.15	121.10	111.52
3	K	306	ILE	CA-C-N	5.15	130.29	122.98
3	K	306	ILE	C-N-CA	5.15	130.29	122.98
3	L	226	VAL	CB-CA-C	5.15	119.09	112.14
1	f	95	GLU	N-CA-C	5.15	117.79	111.82
2	1	76	LEU	CA-C-N	5.15	127.18	120.28
2	1	76	LEU	C-N-CA	5.15	127.18	120.28
2	3	148	TYR	CA-C-N	5.15	131.50	121.41
2	3	148	TYR	C-N-CA	5.15	131.50	121.41
3	L	254	ASP	CA-CB-CG	-5.15	107.45	112.60
1	G	165	GLY	O-C-N	5.15	127.15	122.88
2	j	133	GLU	N-CA-C	5.15	117.16	109.59
2	6	151	LEU	CA-C-O	-5.15	115.40	120.70
3	H	311	LEU	CA-C-O	-5.15	115.03	120.02
3	L	216	ILE	O-C-N	5.15	128.66	123.20
1	b	39	GLY	N-CA-C	-5.15	100.98	113.18
1	b	97	GLN	N-CA-CB	5.15	118.93	110.39
2	1	127	PRO	N-CA-C	5.15	120.62	113.98
2	h	196	PHE	CA-CB-CG	-5.15	108.65	113.80
2	4	194	ASP	CA-CB-CG	-5.15	107.45	112.60
1	g	20	ARG	N-CA-CB	5.14	118.69	110.46
1	g	94	ILE	CA-C-N	5.14	127.17	120.28
1	g	94	ILE	C-N-CA	5.14	127.17	120.28
2	1	30	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	5	128	ILE	CA-CB-CG2	-5.14	101.75	110.50
2	m	162	ASP	N-CA-C	-5.14	107.00	113.28
3	I	104	ALA	N-CA-CB	5.14	118.25	109.87
2	7	66	LEU	O-C-N	5.14	128.01	122.15
3	J	60	SER	CA-C-N	5.14	125.67	120.38
3	J	60	SER	C-N-CA	5.14	125.67	120.38
2	i	98	LEU	CA-C-O	-5.14	115.10	120.55
3	H	58	LEU	CA-C-N	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	58	LEU	C-N-CA	5.14	127.17	120.28
3	L	114	ALA	O-C-N	5.14	129.23	123.27
3	L	397	PHE	N-CA-C	-5.14	107.04	113.72
3	J	280	ASP	CA-C-N	5.14	130.28	122.98
3	J	280	ASP	C-N-CA	5.14	130.28	122.98
2	2	204	VAL	CA-CB-CG2	-5.14	101.67	110.40
3	J	386	THR	CA-CB-CG2	5.14	119.23	110.50
1	a	174	PHE	CA-CB-CG	5.13	118.94	113.80
1	e	144	VAL	CA-C-O	-5.13	113.07	119.95
1	e	245	LYS	O-C-N	-5.13	115.76	122.59
1	f	215	LYS	CA-C-N	5.13	127.71	120.42
1	f	215	LYS	C-N-CA	5.13	127.71	120.42
3	K	58	LEU	CA-C-N	5.13	128.12	120.31
3	K	58	LEU	C-N-CA	5.13	128.12	120.31
3	K	225	GLU	O-C-N	5.13	127.36	122.07
1	F	183	LEU	N-CA-C	5.13	117.33	110.35
2	7	206	GLN	N-CA-C	-5.13	107.02	113.28
1	f	53	ARG	O-C-N	5.13	129.31	122.95
1	G	96	ALA	CA-C-O	5.13	125.99	120.55
3	J	142	ASP	CA-CB-CG	5.13	117.73	112.60
2	4	152	GLU	N-CA-C	5.13	118.69	112.23
1	c	108	THR	N-CA-C	-5.13	102.10	110.20
1	g	133	GLY	O-C-N	5.13	129.37	122.70
2	1	111	LEU	N-CA-CB	5.13	118.82	110.77
2	h	90	ILE	CA-C-N	5.13	127.57	120.29
2	h	90	ILE	C-N-CA	5.13	127.57	120.29
3	M	105	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	C	52	LYS	N-CA-C	-5.13	106.61	112.92
1	E	73	HIS	CB-CG-CD2	-5.13	124.54	131.20
2	k	98	LEU	O-C-N	-5.13	115.97	122.27
1	e	226	PRO	CA-C-N	5.12	127.57	120.29
1	e	226	PRO	C-N-CA	5.12	127.57	120.29
1	B	58	LEU	CA-C-N	5.12	130.69	121.06
1	B	58	LEU	C-N-CA	5.12	130.69	121.06
1	d	129	VAL	CA-CB-CG2	5.12	119.11	110.40
2	1	93	LEU	CA-C-O	5.12	126.20	120.82
2	4	154	ARG	CB-CG-CD	5.12	123.08	111.30
2	k	37	ILE	CA-CB-CG1	5.12	119.11	110.40
2	7	158	GLU	CA-C-N	5.12	127.37	120.50
2	7	158	GLU	C-N-CA	5.12	127.37	120.50
2	7	174	SER	N-CA-C	5.12	116.86	111.28
3	M	236	SER	CA-C-O	-5.12	115.75	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ARG	CA-C-O	-5.12	115.59	120.92
1	e	236	ALA	CA-C-O	-5.12	115.12	120.55
1	F	85	ALA	CB-CA-C	-5.12	102.14	110.85
1	g	138	ILE	N-CA-C	-5.12	100.27	107.75
2	l	207	ILE	CA-C-O	-5.12	113.38	119.58
3	L	372	MET	N-CA-C	-5.12	105.78	111.36
3	L	390	PRO	CA-C-N	5.12	131.32	121.54
3	L	390	PRO	C-N-CA	5.12	131.32	121.54
1	a	80	GLY	CA-C-N	5.12	128.14	120.87
1	a	80	GLY	C-N-CA	5.12	128.14	120.87
3	H	343	THR	CA-C-O	-5.12	113.29	119.59
1	a	95	GLU	CA-C-O	5.12	125.86	119.97
1	B	72	GLU	N-CA-C	-5.12	106.81	113.16
2	n	51	ARG	N-CA-C	-5.12	106.58	114.16
3	M	264	THR	CA-C-O	5.12	125.84	120.42
2	l	131	ALA	CA-C-O	5.12	125.78	120.30
1	B	146	LYS	CB-CA-C	-5.12	98.20	109.56
1	C	114	LYS	O-C-N	-5.12	116.70	122.12
1	d	172	THR	CA-C-N	5.12	127.55	120.29
1	d	172	THR	C-N-CA	5.12	127.55	120.29
2	5	33	MET	N-CA-C	-5.12	107.42	113.97
2	n	185	GLY	CA-C-O	5.12	127.14	121.31
3	K	36	PHE	CB-CG-CD1	5.12	129.40	120.70
3	L	43	ARG	NE-CZ-NH2	-5.12	114.60	119.20
3	J	40	GLU	CA-C-N	5.12	127.55	120.29
3	J	40	GLU	C-N-CA	5.12	127.55	120.29
3	H	158	GLU	CB-CA-C	-5.11	100.85	110.67
2	n	107	LEU	N-CA-CB	5.11	119.13	110.49
2	n	194	ASP	N-CA-CB	-5.11	104.20	111.00
1	G	182	ASP	N-CA-CB	5.11	118.02	110.56
2	6	137	ILE	N-CA-CB	5.11	120.63	111.63
3	H	107	ALA	CB-CA-C	5.11	118.06	109.48
3	I	152	GLU	CA-C-N	5.11	128.73	120.55
3	I	152	GLU	C-N-CA	5.11	128.73	120.55
1	b	117	CYS	O-C-N	5.11	128.55	122.27
1	G	146	LYS	CA-C-O	-5.11	115.27	120.99
2	i	189	VAL	N-CA-CB	5.11	118.20	111.25
2	3	72	ILE	O-C-N	-5.11	116.91	121.87
2	4	134	GLU	N-CA-CB	5.11	119.03	110.85
1	a	151	ASP	CA-C-N	5.11	125.18	119.87
1	a	151	ASP	C-N-CA	5.11	125.18	119.87
1	E	31	VAL	CB-CA-C	-5.11	105.33	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	91	ARG	CB-CA-C	-5.11	102.86	110.88
1	e	181	ASP	CA-C-O	5.11	126.93	120.65
2	i	103	TYR	CA-C-N	5.11	128.70	122.42
2	i	103	TYR	C-N-CA	5.11	128.70	122.42
2	3	166	GLU	CA-C-N	5.11	127.12	120.28
2	3	166	GLU	C-N-CA	5.11	127.12	120.28
2	j	192	THR	CA-C-O	5.11	124.67	119.05
2	4	167	LEU	CA-C-N	5.11	127.08	120.44
2	4	167	LEU	C-N-CA	5.11	127.08	120.44
3	I	340	ALA	CA-C-O	5.11	125.84	119.97
3	L	263	ARG	N-CA-C	5.11	116.53	111.07
2	1	13	THR	CA-C-O	5.11	126.69	121.23
2	1	13	THR	N-CA-C	-5.11	100.98	108.79
2	j	46	TYR	N-CA-C	-5.11	101.08	109.40
2	5	148	TYR	CA-C-N	5.11	125.76	119.99
2	5	148	TYR	C-N-CA	5.11	125.76	119.99
3	H	85	PRO	N-CA-CB	5.11	108.61	103.25
3	L	294	ASP	CA-C-N	5.11	126.22	119.84
3	L	294	ASP	C-N-CA	5.11	126.22	119.84
3	L	344	GLU	O-C-N	-5.11	116.62	122.95
1	a	59	LEU	O-C-N	-5.10	117.23	123.10
1	D	8	TYR	N-CA-C	-5.10	104.35	110.88
1	E	209	ILE	CA-C-O	5.10	126.69	121.28
1	F	176	GLU	N-CA-CB	5.10	117.41	110.01
1	f	84	ASP	CA-C-N	5.10	127.07	120.44
1	f	84	ASP	C-N-CA	5.10	127.07	120.44
1	G	115	LYS	CA-C-O	-5.10	114.58	120.24
2	l	200	SER	CA-C-N	5.10	125.14	119.32
2	l	200	SER	C-N-CA	5.10	125.14	119.32
2	n	48	ILE	N-CA-C	-5.10	106.70	111.45
3	M	387	THR	CA-CB-OG1	5.10	117.25	109.60
1	f	240	ILE	N-CA-CB	5.10	116.17	110.51
1	G	241	ARG	CA-C-N	5.10	127.12	120.28
1	G	241	ARG	C-N-CA	5.10	127.12	120.28
1	g	135	SER	CB-CA-C	-5.10	98.72	109.38
3	L	375	PHE	N-CA-C	5.10	116.92	111.36
1	B	156	LEU	N-CA-C	-5.10	101.40	109.76
1	d	48	LEU	N-CA-C	-5.10	101.09	109.40
2	3	168	ALA	CB-CA-C	-5.10	102.33	110.79
3	K	299	ARG	CA-C-N	5.10	125.34	119.83
3	K	299	ARG	C-N-CA	5.10	125.34	119.83
2	1	115	ILE	CA-C-O	5.10	126.64	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	18	VAL	O-C-N	5.10	128.76	122.95
1	e	121	GLN	N-CA-C	-5.10	106.57	112.89
1	F	225	SER	CA-C-N	5.10	125.38	119.47
1	F	225	SER	C-N-CA	5.10	125.38	119.47
2	h	79	ILE	N-CA-C	-5.09	105.88	110.82
2	2	99	ASN	N-CA-CB	5.09	117.61	110.12
2	7	102	ARG	N-CA-CB	5.09	117.86	110.47
3	I	149	GLN	CA-C-O	-5.09	115.02	120.42
3	I	251	THR	CA-CB-OG1	5.09	117.24	109.60
2	i	102	ARG	CD-NE-CZ	-5.09	117.27	124.40
2	6	111	LEU	O-C-N	5.09	129.27	123.31
3	I	199	THR	CA-C-N	5.09	131.27	121.54
3	I	199	THR	C-N-CA	5.09	131.27	121.54
3	I	340	ALA	CA-C-N	5.09	127.06	120.44
3	I	340	ALA	C-N-CA	5.09	127.06	120.44
1	b	138	ILE	CA-C-N	5.09	130.90	121.94
1	b	138	ILE	C-N-CA	5.09	130.90	121.94
1	d	158	GLU	N-CA-C	-5.09	101.41	109.76
2	h	161	VAL	N-CA-C	-5.09	105.91	113.39
2	2	137	ILE	CA-CB-CG1	5.09	119.06	110.40
1	g	165	GLY	CA-C-N	5.09	127.52	120.29
1	g	165	GLY	C-N-CA	5.09	127.52	120.29
2	h	145	LEU	CA-C-O	-5.09	115.48	120.82
1	d	190	VAL	CA-C-N	5.09	127.10	120.28
1	d	190	VAL	C-N-CA	5.09	127.10	120.28
3	L	40	GLU	O-C-N	5.09	127.51	122.12
1	a	104	ASP	CA-CB-CG	-5.09	107.51	112.60
1	a	233	VAL	CA-C-N	5.09	127.05	120.44
1	a	233	VAL	C-N-CA	5.09	127.05	120.44
1	G	168	ARG	CD-NE-CZ	5.09	131.52	124.40
1	g	130	ARG	NE-CZ-NH1	-5.09	116.41	121.50
2	k	69	ILE	N-CA-C	5.09	115.31	110.53
2	k	113	GLY	CA-C-O	-5.09	116.12	121.56
2	6	125	ILE	CA-C-O	5.09	125.87	120.48
2	n	55	THR	O-C-N	-5.09	116.98	123.24
2	m	33	MET	CG-SD-CE	-5.08	89.71	100.90
3	K	215	TYR	CA-C-O	5.08	127.08	120.21
3	K	350	ASP	CA-C-N	5.08	127.43	120.46
3	K	350	ASP	C-N-CA	5.08	127.43	120.46
1	B	105	GLU	CA-C-O	-5.08	115.62	119.59
1	E	220	THR	O-C-N	-5.08	115.83	122.59
1	e	138	ILE	CB-CG1-CD1	-5.08	103.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	28	ARG	CA-CB-CG	-5.08	103.93	114.10
2	n	113	GLY	CA-C-O	-5.08	115.83	121.37
3	I	149	GLN	O-C-N	5.08	127.94	122.15
1	A	230	LYS	CA-C-O	-5.08	113.20	120.16
1	C	47	ILE	CA-C-O	-5.08	114.72	120.67
1	d	179	TYR	O-C-N	-5.08	117.19	123.44
2	l	202	GLU	O-C-N	-5.08	116.64	122.08
2	i	34	GLY	O-C-N	-5.08	116.98	122.62
2	k	33	MET	O-C-N	5.08	128.89	121.78
3	J	307	ILE	O-C-N	5.08	128.75	123.26
2	h	201	PRO	CA-C-N	5.08	127.40	120.54
2	h	201	PRO	C-N-CA	5.08	127.40	120.54
2	i	157	PRO	CA-C-O	-5.08	112.50	118.90
3	H	39	SER	N-CA-CB	5.08	117.38	110.01
1	f	174	PHE	N-CA-C	-5.08	105.75	111.28
2	l	205	GLU	N-CA-C	5.08	118.58	112.38
2	6	71	LYS	CA-C-N	5.08	127.63	120.42
2	6	71	LYS	C-N-CA	5.08	127.63	120.42
2	6	203	GLU	O-C-N	5.08	127.50	122.12
3	K	319	GLN	CB-CG-CD	-5.08	103.97	112.60
3	K	375	PHE	CA-C-N	5.08	127.08	120.28
3	K	375	PHE	C-N-CA	5.08	127.08	120.28
3	L	208	GLY	N-CA-C	-5.08	107.65	115.73
2	i	81	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	3	208	LEU	CA-C-N	5.08	128.03	120.31
2	3	208	LEU	C-N-CA	5.08	128.03	120.31
2	7	104	PHE	CA-C-O	-5.08	114.92	119.59
3	M	181	TYR	N-CA-C	-5.08	101.57	109.24
1	A	92	ALA	N-CA-CB	5.08	117.37	110.01
2	l	124	SER	N-CA-C	-5.08	101.44	109.76
3	H	263	ARG	CB-CA-C	-5.08	100.92	110.67
3	I	353	ALA	N-CA-CB	-5.08	102.65	110.16
3	K	228	GLN	OE1-CD-NE2	5.08	127.67	122.60
1	A	228	GLU	CA-C-N	5.07	127.59	120.28
1	A	228	GLU	C-N-CA	5.07	127.59	120.28
1	f	113	ALA	CB-CA-C	-5.07	102.92	110.88
2	h	179	ASP	CB-CA-C	-5.07	102.30	110.77
3	K	293	LEU	CA-C-N	5.07	128.36	120.60
3	K	293	LEU	C-N-CA	5.07	128.36	120.60
3	K	378	ALA	CA-C-N	5.07	126.95	120.56
3	K	378	ALA	C-N-CA	5.07	126.95	120.56
1	D	236	ALA	CA-C-O	-5.07	115.04	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	51	ARG	NH1-CZ-NH2	5.07	125.89	119.30
2	m	133	GLU	CB-CA-C	-5.07	104.03	111.23
3	L	285	GLY	N-CA-C	-5.07	103.32	111.59
3	J	143	ILE	N-CA-C	-5.07	101.65	108.35
1	b	86	ARG	CA-C-O	-5.07	115.50	120.82
1	f	86	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
2	j	58	GLY	CA-C-N	5.07	128.67	121.42
2	j	58	GLY	C-N-CA	5.07	128.67	121.42
3	K	11	GLU	CB-CG-CD	-5.07	103.98	112.60
3	L	56	GLU	CA-C-N	5.07	127.49	120.29
3	L	56	GLU	C-N-CA	5.07	127.49	120.29
3	L	192	ALA	CA-C-N	5.07	127.49	120.29
3	L	192	ALA	C-N-CA	5.07	127.49	120.29
3	J	122	SER	N-CA-C	5.07	117.82	110.42
3	I	383	LEU	N-CA-C	5.07	116.81	111.28
1	c	212	GLY	N-CA-C	-5.07	103.70	111.10
1	E	220	THR	N-CA-CB	5.07	119.05	110.49
1	F	35	ALA	CA-C-N	5.07	128.07	120.87
1	F	35	ALA	C-N-CA	5.07	128.07	120.87
2	4	68	ARG	NE-CZ-NH2	-5.07	114.64	119.20
2	k	44	LYS	N-CA-C	-5.07	106.66	114.16
2	6	37	ILE	CB-CA-C	5.07	117.69	111.25
3	H	237	ILE	N-CA-C	-5.07	100.82	108.12
3	K	203	PHE	N-CA-C	-5.07	101.45	109.96
3	J	60	SER	N-CA-CB	5.07	117.68	110.03
1	a	35	ALA	N-CA-CB	5.07	117.46	110.17
1	C	93	ARG	N-CA-C	-5.07	105.84	111.36
1	d	25	GLU	N-CA-CB	5.07	117.66	110.16
1	f	106	PRO	CA-C-O	-5.07	115.80	121.32
3	I	279	GLY	N-CA-C	-5.07	101.17	113.18
3	K	101	LYS	CA-C-N	5.07	125.35	119.93
3	K	101	LYS	C-N-CA	5.07	125.35	119.93
3	K	374	ASP	CA-C-O	5.07	125.92	120.55
3	M	37	ILE	CA-C-N	5.07	127.07	120.28
3	M	37	ILE	C-N-CA	5.07	127.07	120.28
3	M	78	VAL	N-CA-C	-5.07	100.48	108.23
2	5	170	ARG	CB-CG-CD	5.06	122.94	111.30
2	7	52	MET	CG-SD-CE	-5.06	89.77	100.90
3	I	381	LYS	CB-CG-CD	5.06	122.94	111.30
3	K	326	ARG	NE-CZ-NH2	-5.06	114.64	119.20
3	M	213	GLN	CB-CG-CD	5.06	121.21	112.60
1	A	149	GLU	CB-CG-CD	-5.06	104.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	169	ASN	N-CA-C	-5.06	105.76	111.28
2	2	201	PRO	N-CA-C	5.06	121.29	113.75
2	4	95	SER	CA-C-N	5.06	127.48	120.29
2	4	95	SER	C-N-CA	5.06	127.48	120.29
3	H	173	GLU	CA-CB-CG	-5.06	103.98	114.10
3	L	369	LYS	N-CA-C	-5.06	101.85	109.85
1	B	63	THR	CA-CB-CG2	-5.06	101.90	110.50
1	C	73	HIS	ND1-CE1-NE2	5.06	113.46	108.40
2	5	104	PHE	CB-CA-C	-5.06	102.68	110.62
1	B	14	VAL	CA-C-N	5.06	131.20	121.54
1	B	14	VAL	C-N-CA	5.06	131.20	121.54
1	B	209	ILE	CA-CB-CG2	-5.06	101.90	110.50
2	1	171	ALA	O-C-N	-5.06	116.39	122.15
2	6	212	ARG	CA-CB-CG	5.06	124.22	114.10
2	m	47	GLN	CA-C-N	5.06	128.66	120.82
2	m	47	GLN	C-N-CA	5.06	128.66	120.82
2	n	147	ALA	CA-C-N	5.06	127.06	120.28
2	n	147	ALA	C-N-CA	5.06	127.06	120.28
3	K	82	SER	CA-C-O	-5.06	113.16	119.38
3	K	229	LEU	CA-C-N	5.06	127.47	120.29
3	K	229	LEU	C-N-CA	5.06	127.47	120.29
3	M	355	CYS	N-CA-C	-5.06	105.77	111.28
1	F	109	VAL	CA-C-N	5.06	127.06	120.28
1	F	109	VAL	C-N-CA	5.06	127.06	120.28
1	G	108	THR	N-CA-C	-5.06	103.72	110.55
1	g	32	LYS	CA-C-N	5.06	128.00	120.31
1	g	32	LYS	C-N-CA	5.06	128.00	120.31
3	J	153	ILE	CA-C-N	5.06	127.05	120.28
3	J	153	ILE	C-N-CA	5.06	127.05	120.28
1	A	56	SER	CA-C-O	-5.05	115.18	121.50
1	g	45	GLY	CA-C-N	5.05	129.51	122.23
1	g	45	GLY	C-N-CA	5.05	129.51	122.23
1	g	138	ILE	O-C-N	5.05	128.56	123.20
2	3	152	GLU	N-CA-C	-5.05	107.16	113.38
3	I	321	PHE	CB-CG-CD2	-5.05	112.11	120.70
3	J	330	LEU	N-CA-CB	5.05	119.03	110.49
1	G	238	GLU	CB-CG-CD	-5.05	104.01	112.60
1	g	87	VAL	CA-C-N	5.05	127.47	120.29
1	g	87	VAL	C-N-CA	5.05	127.47	120.29
1	B	151	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	198	LEU	O-C-N	5.05	127.91	122.15
2	5	20	LYS	CA-C-O	5.05	125.58	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	44	TYR	CA-CB-CG	-5.05	104.81	113.90
3	H	44	TYR	CB-CA-C	-5.05	100.97	110.67
3	I	119	LEU	CA-C-N	5.05	125.33	119.92
3	I	119	LEU	C-N-CA	5.05	125.33	119.92
3	K	375	PHE	CA-C-O	-5.05	115.20	120.55
3	M	207	VAL	N-CA-C	-5.05	100.84	108.12
1	g	153	SER	CA-C-N	5.05	129.03	122.26
1	g	153	SER	C-N-CA	5.05	129.03	122.26
3	H	153	ILE	N-CA-C	-5.05	105.62	110.72
1	D	158	GLU	N-CA-C	-5.05	101.48	109.76
2	i	147	ALA	O-C-N	5.05	127.95	122.20
2	l	83	ARG	N-CA-C	-5.05	101.07	108.79
1	c	113	ALA	N-CA-C	5.05	116.78	111.28
2	j	63	ALA	CA-C-N	5.05	127.00	120.44
2	j	63	ALA	C-N-CA	5.05	127.00	120.44
1	d	107	ILE	CA-C-O	-5.04	116.53	121.58
1	E	229	LEU	N-CA-C	-5.04	106.29	112.90
1	G	100	ARG	CA-C-N	5.04	127.45	120.29
1	G	100	ARG	C-N-CA	5.04	127.45	120.29
2	k	166	GLU	CA-C-N	5.04	127.04	120.28
2	k	166	GLU	C-N-CA	5.04	127.04	120.28
3	K	67	VAL	O-C-N	5.04	128.65	123.20
1	a	73	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	c	40	ILE	O-C-N	-5.04	117.73	123.18
2	6	75	ASN	CA-C-N	5.04	127.04	120.28
2	6	75	ASN	C-N-CA	5.04	127.04	120.28
3	H	356	THR	O-C-N	5.04	127.26	122.07
3	I	255	THR	CA-CB-CG2	-5.04	101.92	110.50
1	B	178	GLU	CA-C-N	5.04	128.01	120.90
1	B	178	GLU	C-N-CA	5.04	128.01	120.90
1	C	77	ALA	CA-C-O	-5.04	115.56	121.46
1	G	11	ALA	CA-C-N	5.04	128.78	121.52
1	G	11	ALA	C-N-CA	5.04	128.78	121.52
1	G	124	THR	CA-C-N	5.04	127.45	120.29
1	G	124	THR	C-N-CA	5.04	127.45	120.29
1	G	165	GLY	CA-C-O	-5.04	113.91	122.43
3	H	55	VAL	N-CA-C	5.04	115.81	110.72
3	L	13	LEU	O-C-N	-5.04	116.32	122.22
3	J	256	SER	N-CA-C	-5.04	106.30	112.90
1	a	159	TYR	N-CA-C	-5.04	101.75	109.41
1	b	106	PRO	CA-C-O	-5.04	115.26	121.31
1	b	208	ASN	CA-CB-CG	5.04	117.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	84	ASP	CA-C-N	5.04	127.34	120.54
1	d	84	ASP	C-N-CA	5.04	127.34	120.54
1	E	166	MET	N-CA-C	-5.04	105.87	111.36
1	e	187	ASP	CA-C-O	-5.04	115.51	120.70
1	e	216	VAL	CB-CA-C	-5.04	105.49	112.24
1	g	242	GLU	CA-C-N	5.04	127.97	120.31
1	g	242	GLU	C-N-CA	5.04	127.97	120.31
2	k	109	GLN	N-CA-C	-5.04	100.20	108.41
2	k	114	GLY	N-CA-C	-5.04	101.24	113.18
2	n	176	MET	O-C-N	5.04	128.12	122.22
3	I	194	ALA	CB-CA-C	-5.04	102.28	110.85
3	K	250	ARG	CA-C-N	5.04	128.02	120.87
3	K	250	ARG	C-N-CA	5.04	128.02	120.87
3	M	373	LEU	N-CA-CB	5.04	117.62	110.16
1	G	240	ILE	N-CA-C	-5.04	105.63	110.72
1	a	205	VAL	N-CA-C	-5.04	104.30	108.63
1	b	100	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	G	173	GLU	CB-CA-C	-5.04	101.00	110.67
2	4	191	ILE	N-CA-CB	5.04	118.25	111.90
3	I	70	ASP	CA-CB-CG	-5.04	107.56	112.60
3	L	238	ILE	N-CA-C	-5.04	100.40	107.75
3	J	397	PHE	N-CA-C	-5.04	101.03	109.24
1	G	182	ASP	N-CA-C	-5.03	106.73	112.92
2	3	75	ASN	N-CA-CB	5.03	117.61	110.16
2	3	176	MET	N-CA-C	-5.03	107.14	113.28
2	k	165	VAL	O-C-N	5.03	126.75	121.87
3	L	275	PHE	CA-CB-CG	5.03	118.83	113.80
1	G	232	TYR	CB-CG-CD1	-5.03	113.25	120.80
3	I	101	LYS	O-C-N	-5.03	117.98	121.65
3	K	309	VAL	N-CA-CB	5.03	117.42	111.08
3	J	211	PHE	CB-CG-CD1	5.03	129.25	120.70
1	D	185	PHE	O-C-N	5.03	127.25	122.07
1	g	184	SER	N-CA-CB	5.03	118.07	110.42
2	2	212	ARG	NE-CZ-NH1	-5.03	116.47	121.50
2	m	158	GLU	N-CA-C	-5.03	106.73	112.92
2	k	173	TYR	CA-C-N	5.03	127.95	120.31
2	k	173	TYR	C-N-CA	5.03	127.95	120.31
2	6	144	SER	N-CA-C	5.03	117.42	111.33
3	M	271	GLU	N-CA-C	-5.03	105.50	111.69
3	J	152	GLU	CB-CG-CD	-5.03	104.05	112.60
1	B	237	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	78	THR	CA-C-O	-5.03	115.56	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	29	GLU	N-CA-C	-5.03	106.41	112.54
3	K	350	ASP	N-CA-CB	5.03	117.60	110.16
1	a	74	ILE	CA-C-O	5.03	126.29	120.76
1	b	223	GLU	CA-C-N	5.03	128.65	122.37
1	b	223	GLU	C-N-CA	5.03	128.65	122.37
2	m	142	SER	CA-CB-OG	5.03	121.15	111.10
2	4	154	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	5	156	THR	N-CA-C	-5.02	100.33	108.82
2	l	137	ILE	N-CA-CB	5.02	119.52	111.23
1	G	81	LEU	O-C-N	-5.02	116.72	122.95
2	1	77	TYR	CA-C-N	5.02	126.97	120.44
2	1	77	TYR	C-N-CA	5.02	126.97	120.44
2	3	193	GLU	N-CA-C	-5.02	106.02	113.40
2	7	175	ALA	N-CA-CB	5.02	117.50	110.12
3	K	272	LEU	CB-CA-C	-5.02	102.45	110.79
3	J	102	PRO	N-CD-CG	5.02	110.73	103.20
3	J	321	PHE	O-C-N	5.02	127.24	122.07
1	a	130	ARG	CB-CA-C	5.02	116.36	108.63
2	5	128	ILE	CB-CA-C	-5.02	105.00	111.88
3	M	134	GLU	CB-CA-C	-5.02	102.31	109.84
1	B	53	ARG	CG-CD-NE	-5.02	100.96	112.00
1	D	19	GLY	CA-C-O	5.02	124.59	119.02
1	F	223	GLU	CA-C-N	5.02	129.14	122.01
1	F	223	GLU	C-N-CA	5.02	129.14	122.01
2	5	14	THR	N-CA-C	-5.02	101.66	109.24
3	H	77	VAL	O-C-N	-5.02	117.78	123.20
3	I	327	LYS	CA-C-O	-5.02	115.10	120.42
3	J	66	GLY	N-CA-C	-5.02	101.12	110.66
1	A	173	GLU	CA-C-O	5.02	125.87	120.55
1	C	46	VAL	N-CA-CB	5.02	119.59	111.36
2	h	202	GLU	CA-C-N	5.02	127.42	120.29
2	h	202	GLU	C-N-CA	5.02	127.42	120.29
3	H	309	VAL	N-CA-C	-5.02	103.18	108.15
3	I	140	TYR	N-CA-C	-5.02	106.42	112.54
3	K	246	ILE	O-C-N	-5.02	116.30	122.57
3	M	339	LEU	N-CA-C	-5.02	105.70	111.07
1	g	10	ARG	CA-C-N	5.02	130.83	122.20
1	g	10	ARG	C-N-CA	5.02	130.83	122.20
2	n	49	ALA	O-C-N	5.02	129.28	122.96
3	K	97	GLU	CA-C-O	5.02	124.25	119.08
1	C	107	ILE	N-CA-C	5.01	116.85	109.63
1	e	193	LEU	CA-C-N	5.01	127.54	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	193	LEU	C-N-CA	5.01	127.54	120.42
1	f	17	PRO	O-C-N	5.01	129.37	122.35
1	g	178	GLU	N-CA-C	5.01	116.83	111.36
2	j	97	LEU	N-CA-CB	5.01	117.49	110.12
3	J	365	GLU	O-C-N	5.01	128.44	122.27
1	G	81	LEU	CA-C-O	5.01	126.64	120.92
2	j	57	ALA	O-C-N	-5.01	117.15	123.27
2	i	194	ASP	CA-C-N	-5.01	113.65	121.87
2	i	194	ASP	C-N-CA	-5.01	113.65	121.87
2	7	74	ALA	CB-CA-C	-5.01	102.98	110.90
2	7	121	SER	N-CA-CB	5.01	119.33	111.56
3	H	72	LEU	N-CA-C	-5.01	101.93	109.85
3	L	36	PHE	CB-CG-CD1	5.01	129.22	120.70
3	J	224	ARG	CA-C-N	5.01	127.41	120.29
3	J	224	ARG	C-N-CA	5.01	127.41	120.29
2	k	126	ASP	CA-C-N	5.01	125.45	120.04
2	k	126	ASP	C-N-CA	5.01	125.45	120.04
3	L	260	GLU	CA-C-O	-5.01	115.24	120.55
3	J	283	VAL	N-CA-C	-5.01	100.31	107.78
1	e	95	GLU	CA-C-N	5.01	126.95	120.44
1	e	95	GLU	C-N-CA	5.01	126.95	120.44
1	F	105	GLU	CA-C-O	-5.01	115.16	119.72
1	g	151	ASP	O-C-N	5.01	125.75	120.99
2	1	91	ALA	CB-CA-C	-5.01	102.34	110.85
2	1	92	THR	O-C-N	5.01	127.86	122.15
2	5	187	ASP	O-C-N	5.01	129.82	123.11
2	m	49	ALA	N-CA-C	-5.01	101.63	108.24
2	1	105	PRO	CA-C-O	-5.00	115.11	120.97
2	4	186	ILE	N-CA-C	-5.00	101.00	108.46
2	l	184	ASP	O-C-N	-5.00	116.71	122.87
1	D	89	ILE	CB-CA-C	-5.00	104.15	112.26
1	E	21	LEU	N-CA-C	-5.00	100.57	108.73
1	F	106	PRO	CA-C-N	5.00	127.28	120.63
1	F	106	PRO	C-N-CA	5.00	127.28	120.63
2	j	151	LEU	N-CA-CB	5.00	117.47	110.12
2	7	147	ALA	CA-C-N	5.00	127.69	120.38
2	7	147	ALA	C-N-CA	5.00	127.69	120.38
3	M	351	ILE	N-CA-C	-5.00	105.67	110.72
3	J	173	GLU	O-C-N	-5.00	114.83	121.64
3	J	262	GLN	N-CA-C	-5.00	105.83	111.28
1	A	74	ILE	N-CA-C	-5.00	101.05	108.45
2	n	181	ALA	CA-C-O	5.00	125.18	118.38

There are no chirality outliers.

All (280) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	101	TYR	Sidechain
2	1	102	ARG	Sidechain
2	1	170	ARG	Sidechain
2	1	212	ARG	Sidechain
2	1	30	ARG	Sidechain
2	1	77	TYR	Sidechain
2	1	80	ARG	Sidechain
2	1	81	ARG	Sidechain
2	2	139	ALA	Peptide
2	2	211	PHE	Sidechain
2	2	30	ARG	Sidechain
2	2	46	TYR	Sidechain
2	2	51	ARG	Sidechain
2	2	81	ARG	Sidechain
2	3	148	TYR	Sidechain
2	3	36	PHE	Sidechain
2	3	83	ARG	Sidechain
2	4	106	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	148	TYR	Sidechain
2	4	199	TYR	Sidechain
2	4	83	ARG	Sidechain
2	5	132	ILE	Peptide
2	5	148	TYR	Sidechain
2	5	170	ARG	Sidechain
2	5	173	TYR	Sidechain
2	5	30	ARG	Sidechain
2	5	36	PHE	Sidechain
2	6	178	ARG	Sidechain
2	6	211	PHE	Sidechain
2	6	81	ARG	Sidechain
2	7	104	PHE	Sidechain
2	7	106	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	154	ARG	Sidechain
2	7	197	TYR	Sidechain
2	7	51	ARG	Sidechain
2	7	77	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	103	TYR	Sidechain
1	A	123	TYR	Sidechain
1	A	15	PHE	Sidechain
1	A	20	ARG	Sidechain
1	A	65	GLU	Peptide
1	A	91	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	10	ARG	Sidechain
1	B	14	VAL	Mainchain
1	B	179	TYR	Sidechain
1	B	213	TYR	Sidechain
1	B	220	THR	Peptide
1	B	221	PHE	Sidechain
1	B	53	ARG	Sidechain
1	B	66	LYS	Peptide
1	B	86	ARG	Sidechain
1	C	126	TYR	Sidechain
1	C	220	THR	Peptide
1	C	26	TYR	Sidechain
1	C	28	ARG	Sidechain
1	C	53	ARG	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	C	93	ARG	Sidechain
1	D	10	ARG	Sidechain
1	D	103	TYR	Sidechain
1	D	123	TYR	Sidechain
1	D	126	TYR	Sidechain
1	D	132	PHE	Sidechain
1	D	15	PHE	Sidechain
1	D	180	ARG	Sidechain
1	D	185	PHE	Sidechain
1	D	213	TYR	Sidechain
1	D	220	THR	Peptide
1	D	33	ARG	Sidechain
1	D	8	TYR	Sidechain
1	E	148	TYR	Sidechain
1	E	175	PHE	Sidechain
1	E	179	TYR	Sidechain
1	E	215	LYS	Peptide
1	E	220	THR	Peptide
1	E	8	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	103	TYR	Sidechain
1	F	126	TYR	Sidechain
1	F	130	ARG	Sidechain
1	F	14	VAL	Peptide
1	F	159	TYR	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	86	ARG	Sidechain
1	G	10	ARG	Sidechain
1	G	103	TYR	Sidechain
1	G	126	TYR	Sidechain
1	G	220	THR	Peptide
1	G	239	ARG	Sidechain
1	G	35	ALA	Peptide
1	G	5	GLN	Peptide
3	H	128	TYR	Sidechain
3	H	140	TYR	Sidechain
3	H	186	THR	Peptide
3	H	203	PHE	Sidechain
3	H	207	VAL	Peptide
3	H	215	TYR	Sidechain
3	H	24	ARG	Sidechain
3	H	259	ARG	Sidechain
3	H	28	ARG	Sidechain
3	H	289	ARG	Sidechain
3	H	364	ARG	Sidechain
3	H	385	LYS	Peptide
3	H	386	THR	Peptide
3	H	387	THR	Peptide
3	I	128	TYR	Sidechain
3	I	200	ARG	Sidechain
3	I	201	ALA	Peptide
3	I	21	TYR	Sidechain
3	I	221	ARG	Sidechain
3	I	258	ASP	Mainchain
3	I	269	LEU	Peptide
3	I	277	PRO	Peptide
3	I	29	ARG	Sidechain
3	I	361	PHE	Sidechain
3	I	387	THR	Peptide
3	I	41	ARG	Sidechain
3	I	50	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	J	181	TYR	Sidechain
3	J	20	TYR	Sidechain
3	J	215	TYR	Sidechain
3	J	245	ALA	Mainchain
3	J	263	ARG	Sidechain
3	J	29	ARG	Sidechain
3	J	302	ARG	Sidechain
3	J	385	LYS	Peptide
3	J	44	TYR	Sidechain
3	J	57	ARG	Sidechain
3	J	76	ARG	Sidechain
3	J	87	PHE	Sidechain
3	J	94	TYR	Sidechain
3	K	167	PHE	Sidechain
3	K	181	TYR	Sidechain
3	K	20	TYR	Sidechain
3	K	214	LYS	Peptide
3	K	215	TYR	Peptide,Sidechain
3	K	24	ARG	Sidechain
3	K	254	ASP	Peptide
3	K	371	THR	Peptide
3	K	52	ARG	Sidechain
3	L	118	VAL	Peptide
3	L	163	LYS	Mainchain
3	L	211	PHE	Sidechain
3	L	215	TYR	Peptide
3	L	236	SER	Peptide
3	L	24	ARG	Sidechain
3	L	240	ILE	Peptide
3	L	254	ASP	Peptide
3	L	259	ARG	Sidechain
3	L	263	ARG	Sidechain
3	L	276	ASP	Peptide
3	L	28	ARG	Sidechain
3	L	29	ARG	Sidechain
3	L	311	LEU	Peptide
3	L	367	ARG	Sidechain
3	L	386	THR	Peptide
3	L	387	THR	Peptide
3	L	44	TYR	Sidechain
3	L	46	ARG	Sidechain
3	L	50	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	L	57	ARG	Sidechain
3	L	76	ARG	Sidechain
3	L	87	PHE	Sidechain
3	M	128	TYR	Sidechain
3	M	154	ARG	Sidechain
3	M	181	TYR	Peptide,Sidechain
3	M	200	ARG	Sidechain
3	M	24	ARG	Sidechain
3	M	249	ARG	Sidechain
3	M	250	ARG	Sidechain
3	M	254	ASP	Peptide
3	M	259	ARG	Sidechain
3	M	269	LEU	Peptide
3	M	302	ARG	Sidechain
3	M	303	PHE	Peptide
3	M	305	ARG	Sidechain
3	M	385	LYS	Peptide
3	M	386	THR	Peptide
3	M	44	TYR	Sidechain
3	M	46	ARG	Sidechain
1	a	10	ARG	Sidechain
1	a	130	ARG	Sidechain
1	a	179	TYR	Sidechain
1	a	213	TYR	Sidechain
1	a	220	THR	Peptide
1	a	239	ARG	Sidechain
1	a	68	TYR	Sidechain
1	b	126	TYR	Sidechain
1	b	130	ARG	Sidechain
1	b	213	TYR	Sidechain
1	b	22	PHE	Sidechain
1	b	220	THR	Peptide
1	b	239	ARG	Sidechain
1	b	33	ARG	Sidechain
1	b	86	ARG	Sidechain
1	c	126	TYR	Sidechain
1	c	148	TYR	Sidechain
1	c	159	TYR	Sidechain
1	c	68	TYR	Sidechain
1	c	73	HIS	Sidechain
1	c	86	ARG	Sidechain
1	d	123	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	d	33	ARG	Sidechain
1	e	123	TYR	Sidechain
1	e	15	PHE	Sidechain
1	e	159	TYR	Sidechain
1	e	179	TYR	Sidechain
1	e	180	ARG	Sidechain
1	e	220	THR	Peptide
1	e	241	ARG	Sidechain
1	e	86	ARG	Sidechain
1	f	103	TYR	Sidechain
1	f	119	PHE	Sidechain
1	f	123	TYR	Sidechain
1	f	159	TYR	Sidechain
1	f	213	TYR	Sidechain
1	f	220	THR	Peptide
1	g	126	TYR	Sidechain
1	g	159	TYR	Sidechain
1	g	220	THR	Peptide
1	g	221	PHE	Sidechain
1	g	232	TYR	Sidechain
1	g	239	ARG	Sidechain
1	g	26	TYR	Sidechain
1	g	86	ARG	Sidechain
2	h	104	PHE	Sidechain
2	h	106	TYR	Sidechain
2	h	123	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	173	TYR	Sidechain
2	h	197	TYR	Sidechain
2	h	46	TYR	Sidechain
2	h	81	ARG	Sidechain
2	i	106	TYR	Sidechain
2	i	139	ALA	Peptide
2	i	199	TYR	Sidechain
2	i	81	ARG	Sidechain
2	i	88	ARG	Sidechain
2	j	102	ARG	Sidechain
2	j	106	TYR	Sidechain
2	j	148	TYR	Sidechain
2	j	173	TYR	Sidechain
2	j	46	TYR	Sidechain
2	k	102	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	k	106	TYR	Sidechain
2	k	123	TYR	Sidechain
2	k	148	TYR	Sidechain
2	k	155	PHE	Sidechain
2	k	173	TYR	Sidechain
2	k	197	TYR	Sidechain
2	k	199	TYR	Sidechain
2	k	212	ARG	Sidechain
2	k	46	TYR	Sidechain
2	l	101	TYR	Sidechain
2	l	148	TYR	Sidechain
2	l	173	TYR	Sidechain
2	l	196	PHE	Sidechain
2	m	106	TYR	Sidechain
2	m	148	TYR	Sidechain
2	m	170	ARG	Sidechain
2	m	196	PHE	Sidechain
2	m	30	ARG	Sidechain
2	m	80	ARG	Sidechain
2	n	103	TYR	Sidechain
2	n	123	TYR	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	155	PHE	Sidechain
2	n	178	ARG	Sidechain
2	n	199	TYR	Sidechain
2	n	68	ARG	Sidechain
2	n	81	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1941	4	0
1	B	1907	0	1941	3	0
1	C	1907	0	1941	5	0
1	D	1907	0	1941	3	0
1	E	1907	0	1941	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1907	0	1941	8	0
1	G	1907	0	1941	8	0
1	a	1866	0	1908	4	0
1	b	1866	0	1908	9	0
1	c	1866	0	1908	6	0
1	d	1866	0	1908	9	0
1	e	1866	0	1908	2	0
1	f	1866	0	1908	12	0
1	g	1866	0	1908	6	0
2	1	1553	0	1580	4	0
2	2	1553	0	1580	9	0
2	3	1553	0	1580	3	0
2	4	1553	0	1580	4	0
2	5	1553	0	1580	30	0
2	6	1553	0	1580	10	0
2	7	1553	0	1580	6	0
2	h	1553	0	1580	8	0
2	i	1553	0	1580	3	0
2	j	1553	0	1580	3	0
2	k	1553	0	1580	4	0
2	l	1553	0	1580	30	0
2	m	1553	0	1580	5	0
2	n	1553	0	1580	6	0
3	H	3100	0	3220	32	0
3	I	3100	0	3220	31	0
3	J	3100	0	3220	49	0
3	K	3100	0	3220	20	0
3	L	3100	0	3220	37	0
3	M	3100	0	3220	15	0
4	H	31	0	12	2	0
4	I	31	0	12	0	0
4	L	31	0	12	0	0
4	M	31	0	12	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	J	27	0	11	11	0
All	All	66909	0	68442	355	0

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

All (355) 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:l:211:PHE:CE1	2:l:211:PHE:CD1	1.98	1.49
2:l:211:PHE:CE1	2:l:211:PHE:CZ	2.02	1.47
2:5:211:PHE:CZ	2:5:211:PHE:CE2	2.02	1.47
2:5:211:PHE:CE2	2:5:211:PHE:CD2	2.02	1.47
2:5:211:PHE:CZ	2:5:211:PHE:CE1	2.01	1.46
2:l:211:PHE:CE2	2:l:211:PHE:CD2	2.01	1.46
2:5:211:PHE:CE1	2:5:211:PHE:CD1	2.04	1.45
2:l:211:PHE:CZ	2:l:211:PHE:CE2	2.04	1.44
2:l:211:PHE:CD1	2:l:211:PHE:CG	2.08	1.40
2:5:211:PHE:CD1	2:5:211:PHE:CG	2.09	1.38
2:l:211:PHE:CD2	2:l:211:PHE:CG	2.13	1.36
2:5:211:PHE:CD2	2:5:211:PHE:CG	2.16	1.33
2:l:170:ARG:CZ	2:l:170:ARG:NH1	2.11	1.14
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.10	1.13
2:l:170:ARG:CZ	2:l:211:PHE:CE2	2.34	1.11
2:l:170:ARG:CZ	2:l:211:PHE:CD1	2.33	1.10
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.36	1.09
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.34	1.09
2:l:170:ARG:NH1	2:l:211:PHE:CD1	2.21	1.09
2:l:170:ARG:CZ	2:l:211:PHE:CG	2.38	1.07
2:l:170:ARG:NH1	2:l:211:PHE:CD2	2.21	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.21	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CZ	2.23	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.23	1.07
2:l:170:ARG:NH1	2:l:211:PHE:CG	2.22	1.07
2:l:170:ARG:NH1	2:l:211:PHE:CE2	2.23	1.06
2:l:170:ARG:NH1	2:l:211:PHE:CE1	2.22	1.06
2:l:170:ARG:CZ	2:l:211:PHE:CD2	2.39	1.05
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.38	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.25	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.24	1.05
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.41	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.41	1.03
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.26	1.03
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.42	1.03
2:l:170:ARG:NH1	2:l:211:PHE:CZ	2.26	1.03
2:l:170:ARG:CZ	2:l:211:PHE:CE1	2.43	1.01
2:l:170:ARG:CZ	2:l:211:PHE:CZ	2.43	1.00
3:I:212:VAL:CG1	3:J:216:ILE:HG22	1.92	1.00
3:I:212:VAL:HG12	3:J:216:ILE:HG22	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:ILE:HG13	6:J:401:ADP:C6	2.00	0.95
3:J:143:ILE:HG13	6:J:401:ADP:N6	1.84	0.93
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.44	0.85
3:I:212:VAL:CG1	3:J:216:ILE:CG2	2.55	0.85
3:J:389:ILE:HG12	3:J:391:ASP:H	1.43	0.84
2:l:170:ARG:NE	2:l:211:PHE:CZ	2.46	0.83
2:l:170:ARG:NE	2:l:211:PHE:CE1	2.47	0.83
3:J:320:ILE:HG22	3:J:351:ILE:HG21	1.62	0.82
3:H:363:ILE:CG2	3:I:172:ILE:HD11	2.10	0.82
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.48	0.82
3:J:143:ILE:HG13	6:J:401:ADP:N1	1.95	0.81
3:J:320:ILE:CG2	3:J:351:ILE:HG21	2.10	0.81
3:I:212:VAL:HG11	3:J:216:ILE:CG2	2.10	0.81
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.50	0.80
1:D:141:VAL:HG11	1:D:216:VAL:HA	1.64	0.78
3:I:398:VAL:HG22	3:I:398:VAL:OXT	1.83	0.78
2:l:170:ARG:NH2	2:l:211:PHE:CG	2.52	0.77
3:H:363:ILE:HG23	3:I:172:ILE:HD11	1.66	0.76
3:H:153:ILE:HG21	3:H:195:VAL:HG21	1.68	0.76
2:l:170:ARG:NH2	2:l:211:PHE:CD2	2.54	0.75
3:L:236:SER:HA	3:L:237:ILE:HB	1.67	0.74
3:L:236:SER:C	3:L:237:ILE:HG12	2.14	0.72
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.57	0.72
3:J:143:ILE:HG13	6:J:401:ADP:HN62	1.51	0.72
3:H:208:GLY:O	3:H:246:ILE:HD12	1.90	0.72
3:H:153:ILE:CG2	3:H:195:VAL:HG21	2.21	0.70
3:I:398:VAL:OXT	3:I:398:VAL:CG2	2.38	0.70
3:J:143:ILE:CG1	6:J:401:ADP:N6	2.55	0.69
1:f:237:ASN:HD22	1:f:240:ILE:HD12	1.60	0.67
3:L:236:SER:HA	3:L:237:ILE:CB	2.25	0.67
3:J:143:ILE:CG1	6:J:401:ADP:C6	2.76	0.66
3:J:389:ILE:CD1	3:J:391:ASP:O	2.44	0.65
3:L:311:LEU:HD23	3:L:311:LEU:H	1.61	0.65
3:J:389:ILE:HG12	3:J:391:ASP:O	1.96	0.64
2:6:138:VAL:HG22	2:6:139:ALA:H	1.61	0.64
1:b:71:ASP:OD2	1:b:73:HIS:CE1	2.50	0.64
3:L:236:SER:CA	3:L:237:ILE:HG12	2.28	0.63
3:J:230:ALA:HB1	3:J:238:ILE:HD11	1.81	0.63
3:H:153:ILE:HD11	3:H:180:LEU:HD21	1.81	0.62
3:K:342:ILE:CG2	3:K:379:ILE:HG21	2.29	0.62
2:j:14:THR:HB	2:j:111:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:240:ILE:HG22	1:d:244:LEU:HD12	1.82	0.62
3:H:153:ILE:HG12	3:H:178:VAL:HG11	1.82	0.62
3:H:142:ASP:OD1	4:H:401:ATP:C2	2.53	0.61
3:J:398:VAL:HG22	3:J:398:VAL:OXT	1.99	0.61
3:M:320:ILE:HG22	3:M:351:ILE:HG21	1.82	0.61
3:M:342:ILE:HG21	3:M:379:ILE:HG21	1.83	0.60
3:L:236:SER:HA	3:L:237:ILE:CG1	2.32	0.60
3:H:208:GLY:O	3:H:246:ILE:CD1	2.49	0.60
3:L:290:ILE:C	3:L:290:ILE:HD12	2.26	0.60
3:H:398:VAL:HG22	3:H:398:VAL:OXT	2.02	0.59
3:J:143:ILE:CD1	6:J:401:ADP:N6	2.66	0.58
3:K:342:ILE:HG22	3:K:379:ILE:HG21	1.85	0.58
3:H:178:VAL:HG13	3:H:307:ILE:HD12	1.84	0.58
3:L:202:THR:O	3:L:237:ILE:HG21	2.04	0.57
1:c:164:ILE:HG22	1:c:168:ARG:HH21	1.69	0.57
3:J:283:VAL:HA	3:J:284:ILE:HB	1.86	0.57
3:L:398:VAL:HG22	3:L:398:VAL:OXT	2.05	0.57
1:C:70:ILE:HG21	1:C:112:LEU:HD21	1.87	0.57
1:c:21:LEU:HD12	1:c:21:LEU:H	1.70	0.57
3:L:342:ILE:HG21	3:L:379:ILE:HG21	1.85	0.56
3:H:363:ILE:HG21	3:I:172:ILE:HD11	1.87	0.56
3:J:389:ILE:HG12	3:J:391:ASP:N	2.19	0.56
2:i:76:LEU:HG	2:i:80:ARG:HE	1.70	0.56
2:l:137:ILE:HD12	2:l:152:GLU:HA	1.87	0.56
3:L:287:THR:HG21	3:L:290:ILE:HG22	1.86	0.56
2:m:115:ILE:C	2:m:115:ILE:HD12	2.31	0.55
3:H:142:ASP:CG	4:H:401:ATP:C2	2.85	0.55
3:J:320:ILE:HG22	3:J:351:ILE:CG2	2.35	0.55
2:l:66:LEU:HD21	2:l:98:LEU:HD21	1.88	0.55
3:H:359:GLY:CA	3:I:172:ILE:HG12	2.36	0.55
3:K:181:TYR:CE2	3:K:306:ILE:HD12	2.42	0.55
2:2:150:VAL:HG11	2:2:171:ALA:HA	1.87	0.55
3:L:181:TYR:CE1	3:L:290:ILE:HG13	2.42	0.55
3:H:216:ILE:HD12	3:H:260:GLU:HG2	1.87	0.54
2:k:32:THR:HG22	2:k:37:ILE:HG22	1.89	0.54
1:A:65:GLU:H	1:A:66:LYS:HA	1.71	0.54
3:K:359:GLY:HA3	3:L:172:ILE:HG21	1.88	0.54
3:L:236:SER:HA	3:L:237:ILE:HG12	1.90	0.54
1:F:11:ALA:O	1:F:14:VAL:HG22	2.07	0.54
3:J:320:ILE:HG21	3:J:351:ILE:HG21	1.89	0.54
1:g:185:PHE:CZ	1:g:215:LYS:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:208:GLY:O	3:J:246:ILE:HD12	2.07	0.53
3:I:64:LEU:HD11	3:I:83:THR:HG23	1.90	0.53
3:K:320:ILE:HG22	3:K:351:ILE:HG21	1.90	0.53
3:J:389:ILE:CG1	3:J:391:ASP:O	2.57	0.53
1:B:49:ILE:HD13	1:B:193:LEU:HD12	1.91	0.53
1:G:81:LEU:HD12	1:G:81:LEU:H	1.74	0.53
3:J:143:ILE:CG1	6:J:401:ADP:N1	2.71	0.53
3:H:398:VAL:OXT	3:H:398:VAL:CG2	2.57	0.53
3:J:389:ILE:O	3:J:389:ILE:HG23	2.07	0.52
3:H:178:VAL:CG1	3:H:307:ILE:HD12	2.40	0.52
3:L:146:LEU:H	3:L:147:ASP:HA	1.74	0.52
3:J:320:ILE:CG2	3:J:351:ILE:CG2	2.87	0.52
1:b:190:VAL:O	1:b:194:VAL:HG23	2.10	0.52
3:L:215:TYR:HA	3:L:216:ILE:HG13	1.91	0.52
3:J:398:VAL:OXT	3:J:398:VAL:CG2	2.57	0.52
1:C:189:MET:HE3	1:C:211:VAL:HG11	1.91	0.52
2:7:137:ILE:HD11	2:7:155:PHE:CD1	2.45	0.52
1:b:99:ASN:HD21	2:j:81:ARG:HH22	1.57	0.52
1:a:109:VAL:HG13	1:a:138:ILE:HG22	1.91	0.51
2:6:138:VAL:HG22	2:6:139:ALA:N	2.24	0.51
3:L:318:ILE:HG12	3:L:337:LYS:HA	1.92	0.51
2:3:126:ASP:HB3	2:3:127:PRO:HD2	1.93	0.51
2:m:68:ARG:H	2:m:68:ARG:HD3	1.76	0.51
3:H:363:ILE:HG21	3:I:172:ILE:CD1	2.39	0.51
3:K:172:ILE:HD12	3:J:359:GLY:C	2.36	0.51
1:g:38:ILE:HG12	1:g:196:MET:HE3	1.91	0.50
2:5:91:ALA:HA	2:5:112:ILE:HD12	1.93	0.50
2:l:68:ARG:HH22	2:m:131:ALA:H	1.59	0.50
3:L:167:PHE:CD2	3:L:172:ILE:HD11	2.46	0.50
1:E:20:ARG:HH12	3:M:389:ILE:HG22	1.77	0.50
2:h:45:ILE:HG21	2:h:198:GLN:HE21	1.77	0.50
3:I:391:ASP:CG	3:I:392:LEU:H	2.19	0.50
2:1:52:MET:HE1	2:1:90:ILE:HG13	1.94	0.50
3:L:389:ILE:H	3:L:390:PRO:HD2	1.75	0.50
3:I:176:LYS:HB2	3:I:302:ARG:HA	1.93	0.50
2:6:95:SER:HB3	2:6:130:GLY:H	1.77	0.49
3:J:143:ILE:CD1	6:J:401:ADP:C6	2.94	0.49
3:H:196:ALA:HB2	3:H:203:PHE:CE1	2.47	0.49
3:L:292:ILE:HG21	3:M:250:ARG:HG3	1.93	0.49
3:K:172:ILE:HD12	3:J:360:MET:N	2.27	0.49
2:5:135:LYS:H	2:5:135:LYS:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:359:GLY:HA3	3:I:172:ILE:HG12	1.95	0.49
3:M:299:ARG:HH12	3:M:302:ARG:HG2	1.77	0.49
3:J:216:ILE:HG23	3:J:263:ARG:NH2	2.28	0.49
3:I:359:GLY:HA3	3:J:172:ILE:HG21	1.95	0.49
1:c:113:ALA:HB1	1:c:156:LEU:HD11	1.94	0.49
2:6:186:ILE:HG23	2:6:204:VAL:HG11	1.93	0.49
3:J:238:ILE:HD13	3:J:281:VAL:CG1	2.43	0.49
3:K:172:ILE:HD11	3:J:356:THR:O	2.13	0.48
3:K:398:VAL:OXT	3:K:398:VAL:HG22	2.13	0.48
3:M:297:ILE:HG13	3:M:303:PHE:CE1	2.47	0.48
1:g:214:VAL:HA	1:g:221:PHE:H	1.77	0.48
3:J:389:ILE:HD13	3:J:391:ASP:O	2.12	0.48
3:I:324:HIS:CD2	3:I:352:LYS:HA	2.49	0.48
3:K:216:ILE:C	3:K:216:ILE:HD12	2.38	0.48
1:D:208:ASN:HD22	1:D:209:ILE:HG23	1.78	0.48
2:n:115:ILE:HD12	2:n:191:ILE:HG22	1.95	0.48
1:E:68:TYR:CD2	1:E:89:ILE:HD13	2.49	0.48
3:L:257:GLY:O	3:L:261:VAL:HG23	2.14	0.48
1:a:104:ASP:OD2	2:i:92:THR:HG21	2.13	0.47
3:L:166:LEU:O	3:L:170:VAL:HG23	2.13	0.47
2:h:20:LYS:HB3	2:h:158:GLU:HA	1.96	0.47
2:4:61:GLY:HA2	2:4:64:GLN:HE21	1.80	0.47
2:6:162:ASP:O	2:6:165:VAL:HG22	2.15	0.47
1:b:20:ARG:HH21	1:b:25:GLU:HA	1.80	0.47
1:f:189:MET:HE2	1:f:232:TYR:CD2	2.49	0.47
1:G:93:ARG:HH11	2:7:80:ARG:HD2	1.80	0.47
1:f:20:ARG:HH21	1:f:24:VAL:HG12	1.78	0.47
2:4:12:THR:HG21	2:4:58:GLY:H	1.80	0.47
3:L:181:TYR:CZ	3:L:290:ILE:HG13	2.49	0.47
3:H:206:VAL:CG1	3:H:240:ILE:HG12	2.45	0.47
3:I:153:ILE:HG12	3:I:178:VAL:HG11	1.97	0.47
3:J:324:HIS:HD1	3:J:351:ILE:HG22	1.80	0.47
1:E:204:LEU:HD13	1:E:209:ILE:HG21	1.97	0.47
2:7:165:VAL:O	2:7:169:VAL:HG23	2.15	0.47
3:H:206:VAL:HG22	3:H:207:VAL:H	1.78	0.47
1:a:164:ILE:HG22	1:a:168:ARG:HH21	1.80	0.46
2:2:15:VAL:HB	2:2:151:LEU:HD11	1.96	0.46
3:K:342:ILE:HG21	3:K:379:ILE:HG21	1.97	0.46
3:M:230:ALA:HB2	3:M:238:ILE:HD11	1.97	0.46
3:I:211:PHE:HB3	3:I:264:THR:HG21	1.97	0.46
3:H:359:GLY:C	3:I:172:ILE:HG12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:211:VAL:HG21	1:f:229:LEU:HD21	1.98	0.46
2:3:14:THR:HG22	2:3:27:THR:HG22	1.98	0.46
3:M:109:ASN:HB2	3:M:116:VAL:HG11	1.97	0.46
2:5:86:THR:HG23	2:5:89:ALA:H	1.81	0.46
3:K:321:PHE:CZ	3:K:339:LEU:HD13	2.51	0.46
1:F:97:GLN:HE21	2:6:76:LEU:HD13	1.82	0.45
1:g:63:THR:O	1:g:63:THR:HG22	2.16	0.45
2:h:108:VAL:H	2:h:127:PRO:HG3	1.81	0.45
3:M:23:LEU:O	3:M:27:TYR:CD1	2.68	0.45
1:B:197:GLY:HA3	1:B:240:ILE:HD13	1.98	0.45
1:d:205:VAL:HG23	1:d:207:GLU:H	1.81	0.45
1:a:90:ASP:HB3	2:h:80:ARG:HH12	1.82	0.45
3:M:320:ILE:HD13	3:M:348:GLY:HA2	1.97	0.45
1:A:53:ARG:HH22	1:A:205:VAL:H	1.65	0.45
3:H:216:ILE:HD12	3:H:260:GLU:CG	2.47	0.45
2:h:102:ARG:HH21	2:h:128:ILE:HG13	1.81	0.45
1:G:174:PHE:CD2	1:G:195:ALA:HB2	2.52	0.45
3:H:238:ILE:HG22	3:H:240:ILE:HG13	1.99	0.45
1:F:117:CYS:SG	1:F:150:THR:HG22	2.57	0.45
1:F:124:THR:HG22	1:G:130:ARG:HH21	1.82	0.45
1:f:28:ARG:O	1:f:31:VAL:HG22	2.17	0.45
3:H:46:ARG:HD2	3:H:49:ARG:HH21	1.81	0.45
1:b:11:ALA:HB1	1:b:127:GLY:HA3	1.99	0.44
1:C:88:LEU:HD11	1:C:116:ILE:HG23	1.98	0.44
2:h:72:ILE:HD13	2:h:75:ASN:HD22	1.82	0.44
2:i:13:THR:HB	2:i:143:GLY:HA3	1.99	0.44
2:k:136:ASP:CG	2:k:137:ILE:H	2.25	0.44
3:I:212:VAL:CG1	3:J:216:ILE:HG21	2.46	0.44
3:L:342:ILE:CG2	3:L:379:ILE:HG21	2.47	0.44
1:b:73:HIS:HA	1:b:221:PHE:H	1.82	0.44
1:d:156:LEU:HD12	1:d:156:LEU:HA	1.71	0.44
2:2:212:ARG:HA	2:2:212:ARG:HH11	1.82	0.44
3:J:259:ARG:HH11	3:J:262:GLN:HE22	1.63	0.44
2:3:81:ARG:HE	2:3:83:ARG:HE	1.65	0.44
3:H:216:ILE:CD1	3:H:260:GLU:HG2	2.47	0.44
3:L:287:THR:CG2	3:L:290:ILE:CG2	2.96	0.44
1:d:81:LEU:H	1:d:81:LEU:HD22	1.82	0.44
2:1:12:THR:HA	2:1:28:GLU:CD	2.43	0.44
2:6:86:THR:HG23	2:6:89:ALA:H	1.81	0.44
3:I:351:ILE:HD13	3:I:354:ILE:HD12	2.00	0.44
3:J:283:VAL:CA	3:J:284:ILE:HB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:24:ARG:HE	3:J:23:LEU:HD13	1.83	0.44
1:b:215:LYS:HG3	1:b:217:ASP:H	1.83	0.44
2:m:86:THR:HG23	2:m:89:ALA:H	1.83	0.44
3:L:236:SER:CA	3:L:237:ILE:CB	2.93	0.44
2:1:131:ALA:H	2:7:64:GLN:HE21	1.66	0.44
2:5:24:VAL:HG11	2:5:165:VAL:HA	2.00	0.44
3:H:281:VAL:HG12	3:H:283:VAL:HG23	1.99	0.44
3:K:128:TYR:HB3	3:L:250:ARG:HH12	1.83	0.44
2:j:49:ALA:HB3	2:j:52:MET:HB2	2.00	0.43
3:J:143:ILE:HD11	6:J:401:ADP:N6	2.33	0.43
1:G:157:LEU:HD23	1:G:157:LEU:HA	1.91	0.43
2:m:45:ILE:HG12	2:m:189:VAL:HG21	1.99	0.43
3:H:105:ARG:HH21	3:H:123:LYS:HE3	1.81	0.43
3:J:230:ALA:CB	3:J:238:ILE:HD11	2.46	0.43
2:h:13:THR:HA	2:h:141:GLY:HA3	2.00	0.43
3:K:230:ALA:CB	3:K:238:ILE:HD11	2.48	0.43
3:L:44:TYR:CE1	3:M:44:TYR:HB3	2.53	0.43
2:h:132:ILE:HG12	2:n:64:GLN:HE22	1.82	0.43
3:L:181:TYR:CE1	3:L:290:ILE:CG1	3.00	0.43
2:2:109:GLN:HG2	2:2:127:PRO:HB3	2.01	0.43
3:I:153:ILE:HG22	3:I:195:VAL:HG21	2.01	0.43
2:5:208:LEU:H	2:5:208:LEU:HG	1.72	0.43
3:J:163:LYS:HZ3	3:J:165:GLU:HB3	1.84	0.43
1:G:80:GLY:O	3:L:398:VAL:O	2.37	0.43
3:J:299:ARG:HH12	3:J:302:ARG:HG3	1.82	0.43
1:F:151:ASP:HB2	1:F:155:ALA:HB3	2.01	0.43
1:f:189:MET:HE2	1:f:232:TYR:CG	2.54	0.43
2:l:135:LYS:HB2	2:l:135:LYS:NZ	2.34	0.43
1:c:13:THR:HG22	1:c:13:THR:O	2.19	0.43
1:g:73:HIS:CD2	1:g:74:ILE:HG13	2.53	0.43
2:4:86:THR:HG23	2:4:89:ALA:H	1.84	0.43
1:f:123:TYR:CD2	1:f:129:VAL:HG21	2.54	0.42
3:I:240:ILE:HD12	3:I:283:VAL:CG1	2.48	0.42
3:K:247:ALA:CB	3:K:293:LEU:HD22	2.48	0.42
1:b:215:LYS:HB3	1:b:218:ASP:OD1	2.19	0.42
3:K:247:ALA:HB1	3:K:293:LEU:HD22	2.01	0.42
1:b:81:LEU:HD12	1:b:81:LEU:HA	1.89	0.42
1:f:134:VAL:HG22	1:f:135:SER:N	2.33	0.42
2:2:29:LYS:H	2:2:186:ILE:HG22	1.85	0.42
3:H:320:ILE:HG22	3:H:351:ILE:HG21	2.01	0.42
3:I:360:MET:HA	3:I:363:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:53:ARG:HE	1:d:61:ALA:HB3	1.85	0.42
1:E:43:LYS:H	1:E:43:LYS:HD3	1.84	0.42
1:f:61:ALA:HA	1:f:64:ILE:HG22	2.01	0.42
2:6:125:ILE:N	2:6:125:ILE:HD12	2.34	0.42
3:L:199:THR:HG21	3:L:237:ILE:HD11	2.01	0.42
3:L:214:LYS:HG2	3:L:215:TYR:CD2	2.55	0.42
2:l:137:ILE:HG22	2:l:148:TYR:CD1	2.55	0.42
2:n:176:MET:HE2	2:n:183:GLY:HA2	2.02	0.42
3:I:151:GLU:HG2	3:I:154:ARG:HH21	1.84	0.42
1:e:189:MET:SD	1:e:232:TYR:CD2	3.13	0.42
1:G:237:ASN:HD22	1:G:240:ILE:HD12	1.84	0.42
1:g:88:LEU:HD11	1:g:116:ILE:HG23	2.01	0.42
2:7:17:LEU:HD11	2:7:164:ALA:HB1	2.02	0.42
1:C:159:TYR:CE2	1:D:59:LEU:HG	2.54	0.42
2:6:22:GLY:HA2	2:6:115:ILE:HD11	2.02	0.41
2:n:70:ILE:HD13	2:n:70:ILE:HA	1.95	0.41
3:I:87:PHE:CE1	3:I:113:LEU:HB3	2.55	0.41
3:I:342:ILE:HG21	3:I:379:ILE:HG21	2.02	0.41
1:C:52:LYS:HD2	1:C:61:ALA:O	2.19	0.41
1:f:189:MET:O	1:f:193:LEU:HD13	2.19	0.41
2:n:130:GLY:O	2:n:131:ALA:HB2	2.20	0.41
3:H:216:ILE:HD13	3:I:216:ILE:CD1	2.50	0.41
3:M:217:GLY:H	3:M:263:ARG:CZ	2.32	0.41
1:d:109:VAL:HG13	1:d:138:ILE:HG22	2.02	0.41
3:L:157:VAL:HG11	3:L:195:VAL:HG11	2.02	0.41
3:L:236:SER:CA	3:L:237:ILE:HB	2.43	0.41
3:M:320:ILE:CG2	3:M:351:ILE:HG21	2.50	0.41
1:A:108:THR:HG22	1:A:110:LYS:H	1.86	0.41
2:5:64:GLN:HG2	2:6:131:ALA:H	1.85	0.41
3:J:143:ILE:CG1	6:J:401:ADP:HN62	2.24	0.41
2:2:131:ALA:C	2:2:132:ILE:HG13	2.45	0.41
2:5:13:THR:HA	2:5:141:GLY:HA3	2.03	0.41
3:I:238:ILE:HG22	3:I:240:ILE:HG13	2.01	0.41
3:L:287:THR:HG21	3:L:290:ILE:CG2	2.51	0.41
1:d:97:GLN:HG3	2:k:76:LEU:HD13	2.01	0.41
1:F:186:ASP:O	1:F:190:VAL:HG23	2.20	0.41
2:l:66:LEU:CD2	2:l:98:LEU:HD21	2.50	0.41
3:J:95:ILE:HA	3:J:99:GLU:HG3	2.01	0.41
2:2:74:ALA:HA	2:2:90:ILE:HD11	2.03	0.41
2:k:213:LYS:HA	2:k:213:LYS:HD2	1.83	0.41
2:n:46:TYR:CD2	2:n:54:MET:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:36:THR:HB	1:d:167:GLY:H	1.86	0.41
2:1:40:LYS:HG3	2:2:137:ILE:CD1	2.51	0.41
2:2:52:MET:HE1	2:2:85:PRO:HB2	2.02	0.41
3:L:398:VAL:OXT	3:L:398:VAL:CG2	2.64	0.41
3:J:238:ILE:HD13	3:J:281:VAL:HG13	2.02	0.41
1:f:34:GLY:HA3	1:f:80:GLY:H	1.86	0.41
3:I:225:GLU:HA	3:I:228:GLN:HG2	2.02	0.41
3:M:297:ILE:HG13	3:M:303:PHE:HE1	1.85	0.41
3:J:389:ILE:O	3:J:389:ILE:CG2	2.69	0.41
1:B:90:ASP:HA	1:B:93:ARG:HD2	2.02	0.40
1:c:10:ARG:HB3	1:d:12:ILE:HG22	2.02	0.40
3:K:52:ARG:O	3:K:56:GLU:HG2	2.21	0.40
1:F:48:LEU:HD23	1:F:67:ILE:HG23	2.03	0.40
2:4:12:THR:CG2	2:4:58:GLY:H	2.34	0.40
2:l:136:ASP:C	2:l:137:ILE:HG12	2.46	0.40
3:L:181:TYR:CZ	3:L:290:ILE:CG1	3.04	0.40
1:A:24:VAL:HG11	1:A:153:SER:HB2	2.03	0.40
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.98	0.40
1:e:38:ILE:HD12	1:e:196:MET:SD	2.61	0.40
1:f:185:PHE:CE2	1:f:215:LYS:HE2	2.56	0.40
1:G:110:LYS:O	1:G:114:LYS:HG3	2.22	0.40
3:K:376:THR:HA	3:K:379:ILE:HD12	2.03	0.40
1:c:232:TYR:CD1	1:c:235:ARG:NH1	2.89	0.40
3:M:317:ARG:CZ	3:M:344:GLU:HA	2.51	0.40
1:F:24:VAL:O	1:F:27:ALA:HB3	2.22	0.40
2:7:14:THR:HG22	2:7:27:THR:HA	2.04	0.40
3:H:206:VAL:HG12	3:H:240:ILE:HG12	2.03	0.40
3:K:376:THR:O	3:K:379:ILE:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/242 (99%)	225 (94%)	12 (5%)	3 (1%)	9	42
1	B	240/242 (99%)	224 (93%)	10 (4%)	6 (2%)	4	26
1	C	240/242 (99%)	226 (94%)	11 (5%)	3 (1%)	9	42
1	D	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	5	30
1	E	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	30	67
1	F	240/242 (99%)	229 (95%)	8 (3%)	3 (1%)	9	42
1	G	240/242 (99%)	224 (93%)	13 (5%)	3 (1%)	9	42
1	a	235/242 (97%)	220 (94%)	8 (3%)	7 (3%)	3	23
1	b	235/242 (97%)	218 (93%)	13 (6%)	4 (2%)	7	36
1	c	235/242 (97%)	220 (94%)	14 (6%)	1 (0%)	30	67
1	d	235/242 (97%)	225 (96%)	5 (2%)	5 (2%)	5	30
1	e	235/242 (97%)	219 (93%)	11 (5%)	5 (2%)	5	30
1	f	235/242 (97%)	225 (96%)	9 (4%)	1 (0%)	30	67
1	g	235/242 (97%)	220 (94%)	10 (4%)	5 (2%)	5	30
2	1	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	8	40
2	2	200/202 (99%)	174 (87%)	18 (9%)	8 (4%)	2	18
2	3	200/202 (99%)	181 (90%)	17 (8%)	2 (1%)	12	48
2	4	200/202 (99%)	187 (94%)	11 (6%)	2 (1%)	12	48
2	5	200/202 (99%)	188 (94%)	6 (3%)	6 (3%)	3	23
2	6	200/202 (99%)	183 (92%)	9 (4%)	8 (4%)	2	18
2	7	200/202 (99%)	185 (92%)	12 (6%)	3 (2%)	8	40
2	h	200/202 (99%)	175 (88%)	16 (8%)	9 (4%)	2	17
2	i	200/202 (99%)	186 (93%)	11 (6%)	3 (2%)	8	40
2	j	200/202 (99%)	183 (92%)	12 (6%)	5 (2%)	4	26
2	k	200/202 (99%)	180 (90%)	16 (8%)	4 (2%)	6	31
2	l	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	6	31
2	m	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	24	63
2	n	200/202 (99%)	183 (92%)	11 (6%)	6 (3%)	3	23
3	H	388/390 (100%)	340 (88%)	32 (8%)	16 (4%)	2	18
3	I	388/390 (100%)	348 (90%)	25 (6%)	15 (4%)	2	19
3	J	388/390 (100%)	346 (89%)	31 (8%)	11 (3%)	4	24
3	K	388/390 (100%)	353 (91%)	27 (7%)	8 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	388/390 (100%)	344 (89%)	27 (7%)	17 (4%)	2	17
3	M	388/390 (100%)	341 (88%)	28 (7%)	19 (5%)	1	16
All	All	8453/8556 (99%)	7770 (92%)	481 (6%)	202 (2%)	7	27

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	a	54	VAL
1	B	64	ILE
1	C	67	ILE
1	D	65	GLU
1	d	221	PHE
1	G	54	VAL
2	1	212	ARG
2	h	85	PRO
2	h	128	ILE
2	h	140	THR
2	2	41	ALA
2	2	139	ALA
2	6	40	LYS
2	6	139	ALA
2	n	131	ALA
3	H	190	LEU
3	H	191	LEU
3	H	280	ASP
3	I	269	LEU
3	I	270	ALA
3	I	388	PRO
3	K	212	VAL
3	L	119	LEU
3	L	237	ILE
3	L	248	ALA
3	L	255	THR
3	L	333	ASP
3	M	74	ASP
3	M	244	ASP
3	M	270	ALA
3	M	282	LYS
3	M	292	ILE
3	J	282	LYS

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Mol	Chain	Res	Type
3	J	386	THR
1	A	143	GLU
1	a	34	GLY
1	a	73	HIS
1	a	161	ALA
1	b	54	VAL
1	b	57	LYS
1	C	9	ASP
1	C	221	PHE
1	c	15	PHE
1	D	9	ASP
1	D	161	ALA
1	d	143	GLU
1	E	221	PHE
1	e	161	ALA
1	F	64	ILE
1	f	12	ILE
1	G	143	GLU
1	G	221	PHE
1	g	143	GLU
2	1	136	ASP
2	h	35	ASN
2	h	139	ALA
2	h	210	LYS
2	2	30	ARG
2	2	140	THR
2	2	182	SER
2	3	139	ALA
2	j	136	ASP
2	4	140	THR
2	5	191	ILE
2	5	193	GLU
2	5	212	ARG
2	l	212	ARG
2	6	41	ALA
2	6	102	ARG
2	n	132	ILE
3	H	113	LEU
3	H	304	ASP
3	I	123	LYS
3	I	242	GLU
3	I	246	ILE

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Mol	Chain	Res	Type
3	K	244	ASP
3	L	122	SER
3	L	163	LYS
3	L	202	THR
3	L	242	GLU
3	L	296	ALA
3	M	212	VAL
3	M	221	ARG
3	M	255	THR
3	M	269	LEU
3	M	310	PRO
3	J	273	ASP
3	J	290	ILE
1	A	9	ASP
1	a	143	GLU
1	B	65	GLU
1	B	143	GLU
1	b	66	LYS
1	D	56	SER
1	d	161	ALA
1	e	72	GLU
1	e	179	TYR
1	F	9	ASP
1	F	221	PHE
1	g	217	ASP
1	g	218	ASP
2	h	183	GLY
2	2	83	ARG
2	2	106	TYR
2	2	212	ARG
2	i	210	LYS
2	j	21	ASP
2	j	41	ALA
2	j	185	GLY
2	4	136	ASP
2	k	155	PHE
2	5	133	GLU
2	l	137	ILE
2	6	193	GLU
2	7	34	GLY
2	7	133	GLU
2	n	139	ALA

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Mol	Chain	Res	Type
3	H	129	GLY
3	H	139	SER
3	H	175	PRO
3	H	273	ASP
3	H	282	LYS
3	H	333	ASP
3	I	212	VAL
3	K	330	LEU
3	K	332	GLU
3	L	280	ASP
3	L	366	GLU
3	L	387	THR
3	M	146	LEU
3	M	202	THR
3	M	273	ASP
3	M	330	LEU
1	a	13	THR
1	B	15	PHE
1	B	221	PHE
1	b	73	HIS
1	d	56	SER
1	e	14	VAL
1	e	36	THR
1	g	73	HIS
1	g	221	PHE
2	i	41	ALA
2	i	44	LYS
2	l	30	ARG
2	6	20	LYS
2	6	136	ASP
2	6	140	THR
2	n	30	ARG
3	I	134	GLU
3	I	393	LYS
3	K	175	PRO
3	K	235	PRO
3	L	85	PRO
3	L	135	LYS
3	L	304	ASP
3	L	389	ILE
3	J	133	GLU
3	J	242	GLU

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Mol	Chain	Res	Type
3	J	284	ILE
3	J	387	THR
1	a	221	PHE
2	h	191	ILE
2	h	193	GLU
2	3	181	ALA
2	j	40	LYS
2	k	140	THR
2	m	200	SER
2	n	137	ILE
3	H	125	PRO
3	H	344	GLU
3	I	85	PRO
3	I	200	ARG
3	I	256	SER
3	I	303	PHE
3	M	246	ILE
3	M	312	PRO
3	M	332	GLU
3	J	330	LEU
3	J	366	GLU
3	J	390	PRO
1	B	36	THR
2	k	183	GLY
2	5	83	ARG
2	5	200	SER
2	l	193	GLU
2	7	136	ASP
3	H	136	PRO
3	K	310	PRO
3	M	174	PRO
3	M	257	GLY
3	H	292	ILE
3	I	132	VAL
2	1	183	GLY
1	d	54	VAL
3	K	125	PRO
2	k	200	SER
3	H	310	PRO
1	D	64	ILE
2	n	129	GLY
3	I	136	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%)	197 (97%)	6 (3%)	36	57
1	B	203/203 (100%)	193 (95%)	10 (5%)	22	43
1	C	203/203 (100%)	195 (96%)	8 (4%)	28	49
1	D	203/203 (100%)	194 (96%)	9 (4%)	25	47
1	E	203/203 (100%)	192 (95%)	11 (5%)	20	41
1	F	203/203 (100%)	193 (95%)	10 (5%)	22	43
1	G	203/203 (100%)	194 (96%)	9 (4%)	25	47
1	a	199/203 (98%)	191 (96%)	8 (4%)	28	49
1	b	199/203 (98%)	189 (95%)	10 (5%)	22	43
1	c	199/203 (98%)	191 (96%)	8 (4%)	28	49
1	d	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	e	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	f	199/203 (98%)	193 (97%)	6 (3%)	36	57
1	g	199/203 (98%)	192 (96%)	7 (4%)	32	53
2	1	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	2	164/164 (100%)	154 (94%)	10 (6%)	17	38
2	3	164/164 (100%)	161 (98%)	3 (2%)	51	68
2	4	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	5	164/164 (100%)	157 (96%)	7 (4%)	26	47
2	6	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	7	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	h	164/164 (100%)	155 (94%)	9 (6%)	19	41
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%)	151 (92%)	13 (8%)	11	32
2	l	164/164 (100%)	156 (95%)	8 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	m	164/164 (100%)	162 (99%)	2 (1%)	63	75
2	n	164/164 (100%)	156 (95%)	8 (5%)	22	43
3	H	338/338 (100%)	322 (95%)	16 (5%)	23	45
3	I	338/338 (100%)	322 (95%)	16 (5%)	23	45
3	J	338/338 (100%)	327 (97%)	11 (3%)	33	55
3	K	338/338 (100%)	330 (98%)	8 (2%)	43	64
3	L	338/338 (100%)	327 (97%)	11 (3%)	33	55
3	M	338/338 (100%)	326 (96%)	12 (4%)	31	52
All	All	7138/7166 (100%)	6842 (96%)	296 (4%)	28	49

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	41	LYS
1	A	86	ARG
1	A	121	GLN
1	A	144	VAL
1	A	169	ASN
1	a	13	THR
1	a	33	ARG
1	a	56	SER
1	a	145	PRO
1	a	208	ASN
1	a	209	ILE
1	a	219	ARG
1	a	234	GLU
1	B	6	MET
1	B	46	VAL
1	B	75	CYS
1	B	102	THR
1	B	121	GLN
1	B	134	VAL
1	B	142	ASP
1	B	152	PRO
1	B	190	VAL
1	B	209	ILE
1	b	15	PHE
1	b	24	VAL

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Mol	Chain	Res	Type
1	b	31	VAL
1	b	63	THR
1	b	67	ILE
1	b	82	VAL
1	b	102	THR
1	b	121	GLN
1	b	164	ILE
1	b	235	ARG
1	C	36	THR
1	C	67	ILE
1	C	69	LYS
1	C	129	VAL
1	C	164	ILE
1	C	206	PRO
1	C	208	ASN
1	C	224	VAL
1	c	14	VAL
1	c	16	SER
1	c	62	ASP
1	c	71	ASP
1	c	81	LEU
1	c	109	VAL
1	c	198	LEU
1	c	213	TYR
1	D	38	ILE
1	D	99	ASN
1	D	102	THR
1	D	121	GLN
1	D	147	LEU
1	D	162	THR
1	D	208	ASN
1	D	216	VAL
1	D	226	PRO
1	d	14	VAL
1	d	40	ILE
1	d	81	LEU
1	d	116	ILE
1	d	134	VAL
1	d	169	ASN
1	d	182	ASP
1	d	200	ILE
1	d	234	GLU

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Mol	Chain	Res	Type
1	E	9	ASP
1	E	14	VAL
1	E	40	ILE
1	E	43	LYS
1	E	89	ILE
1	E	98	ILE
1	E	121	GLN
1	E	130	ARG
1	E	145	PRO
1	E	156	LEU
1	E	178	GLU
1	e	40	ILE
1	e	73	HIS
1	e	98	ILE
1	e	121	GLN
1	e	129	VAL
1	e	162	THR
1	e	208	ASN
1	e	216	VAL
1	e	226	PRO
1	F	28	ARG
1	F	54	VAL
1	F	59	LEU
1	F	87	VAL
1	F	104	ASP
1	F	121	GLN
1	F	129	VAL
1	F	142	ASP
1	F	153	SER
1	F	182	ASP
1	f	13	THR
1	f	40	ILE
1	f	70	ILE
1	f	98	ILE
1	f	129	VAL
1	f	218	ASP
1	G	5	GLN
1	G	9	ASP
1	G	40	ILE
1	G	57	LYS
1	G	59	LEU
1	G	87	VAL

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Mol	Chain	Res	Type
1	G	121	GLN
1	G	172	THR
1	G	209	ILE
1	g	46	VAL
1	g	59	LEU
1	g	86	ARG
1	g	126	TYR
1	g	157	LEU
1	g	209	ILE
1	g	224	VAL
2	1	12	THR
2	1	23	VAL
2	1	27	THR
2	1	28	GLU
2	1	45	ILE
2	1	64	GLN
2	1	101	TYR
2	1	120	LYS
2	h	13	THR
2	h	52	MET
2	h	137	ILE
2	h	156	THR
2	h	161	VAL
2	h	195	GLU
2	h	201	PRO
2	h	205	GLU
2	h	210	LYS
2	2	14	THR
2	2	27	THR
2	2	45	ILE
2	2	60	VAL
2	2	71	LYS
2	2	72	ILE
2	2	84	LYS
2	2	110	LEU
2	2	137	ILE
2	2	188	VAL
2	i	17	LEU
2	i	44	LYS
2	i	45	ILE
2	i	72	ILE
2	i	122	ILE

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Mol	Chain	Res	Type
2	i	137	ILE
2	i	140	THR
2	i	150	VAL
2	i	186	ILE
2	3	17	LEU
2	3	206	GLN
2	3	213	LYS
2	j	14	THR
2	j	115	ILE
2	j	121	SER
2	j	122	ILE
2	j	186	ILE
2	j	205	GLU
2	4	69	ILE
2	4	123	TYR
2	4	132	ILE
2	4	146	THR
2	4	156	THR
2	4	188	VAL
2	k	14	THR
2	k	15	VAL
2	k	19	CYS
2	k	33	MET
2	k	69	ILE
2	k	116	ASP
2	k	120	LYS
2	k	125	ILE
2	k	146	THR
2	k	156	THR
2	k	169	VAL
2	k	170	ARG
2	k	188	VAL
2	5	45	ILE
2	5	135	LYS
2	5	136	ASP
2	5	161	VAL
2	5	190	LYS
2	5	204	VAL
2	5	205	GLU
2	l	21	ASP
2	l	27	THR
2	l	30	ARG

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Mol	Chain	Res	Type
2	l	72	ILE
2	l	136	ASP
2	l	186	ILE
2	l	191	ILE
2	l	201	PRO
2	6	45	ILE
2	6	72	ILE
2	6	101	TYR
2	6	142	SER
2	m	51	ARG
2	m	186	ILE
2	7	28	GLU
2	7	45	ILE
2	7	60	VAL
2	7	64	GLN
2	7	85	PRO
2	7	110	LEU
2	7	132	ILE
2	7	177	LYS
2	7	201	PRO
2	n	20	LYS
2	n	35	ASN
2	n	45	ILE
2	n	70	ILE
2	n	87	VAL
2	n	100	SER
2	n	136	ASP
2	n	170	ARG
3	H	62	PRO
3	H	73	GLU
3	H	78	VAL
3	H	136	PRO
3	H	143	ILE
3	H	165	GLU
3	H	175	PRO
3	H	190	LEU
3	H	207	VAL
3	H	210	GLU
3	H	227	PHE
3	H	250	ARG
3	H	265	MET
3	H	272	LEU

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Mol	Chain	Res	Type
3	H	295	PRO
3	H	330	LEU
3	I	37	ILE
3	I	74	ASP
3	I	88	VAL
3	I	106	VAL
3	I	148	VAL
3	I	159	LEU
3	I	200	ARG
3	I	255	THR
3	I	259	ARG
3	I	273	ASP
3	I	282	LYS
3	I	293	LEU
3	I	298	LEU
3	I	352	LYS
3	I	387	THR
3	I	398	VAL
3	K	83	THR
3	K	92	SER
3	K	116	VAL
3	K	260	GLU
3	K	280	ASP
3	K	327	LYS
3	K	332	GLU
3	K	370	VAL
3	L	55	VAL
3	L	79	VAL
3	L	85	PRO
3	L	116	VAL
3	L	125	PRO
3	L	214	LYS
3	L	235	PRO
3	L	295	PRO
3	L	304	ASP
3	L	311	LEU
3	L	330	LEU
3	M	32	ASP
3	M	42	ILE
3	M	88	VAL
3	M	106	VAL
3	M	122	SER

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Mol	Chain	Res	Type
3	M	137	GLU
3	M	149	GLN
3	M	179	LEU
3	M	226	VAL
3	M	250	ARG
3	M	332	GLU
3	M	369	LYS
3	J	15	LYS
3	J	110	GLN
3	J	120	PRO
3	J	140	TYR
3	J	280	ASP
3	J	283	VAL
3	J	288	ASN
3	J	291	ASP
3	J	352	LYS
3	J	390	PRO
3	J	393	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	f	23	GLN
1	f	121	GLN
1	f	208	ASN
1	f	237	ASN
1	G	122	GLN
1	G	125	GLN
1	G	208	ASN
1	G	237	ASN
1	g	97	GLN
1	g	208	ASN
2	1	75	ASN
2	1	99	ASN
2	h	75	ASN
2	h	198	GLN
2	2	35	ASN
2	2	99	ASN
2	i	96	ASN
2	i	99	ASN
2	i	109	GLN
2	3	64	GLN
2	3	75	ASN
2	3	96	ASN
2	3	99	ASN
2	4	64	GLN
2	4	99	ASN
2	k	64	GLN
2	k	99	ASN
2	k	109	GLN
2	5	206	GLN
2	l	109	GLN
2	6	75	ASN
2	6	99	ASN
2	6	198	GLN
2	m	64	GLN
2	m	99	ASN
2	7	64	GLN
2	n	35	ASN
2	n	96	ASN
2	n	198	GLN
3	H	149	GLN
3	H	197	ASN
3	H	198	GLN

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Mol	Chain	Res	Type
3	H	228	GLN
3	H	267	GLN
3	I	96	ASN
3	I	109	ASN
3	I	111	GLN
3	I	198	GLN
3	I	319	GLN
3	K	109	ASN
3	K	110	GLN
3	K	111	GLN
3	K	149	GLN
3	K	198	GLN
3	K	252	ASN
3	K	267	GLN
3	L	96	ASN
3	M	110	GLN
3	M	111	GLN
3	M	149	GLN
3	J	252	ASN
3	J	262	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	L	401	5	32,33,33	4.00	9 (28%)	48,52,52	1.54	3 (6%)
4	ATP	I	401	5	32,33,33	4.14	7 (21%)	48,52,52	1.74	12 (25%)
6	ADP	J	401	5	28,29,29	1.76	4 (14%)	43,45,45	1.41	5 (11%)
4	ATP	M	401	5	32,33,33	3.60	4 (12%)	48,52,52	1.43	8 (16%)
4	ATP	H	401	5	32,33,33	4.15	5 (15%)	48,52,52	1.41	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	L	401	5	-	11/22/38/38	0/3/3/3
4	ATP	I	401	5	-	5/22/38/38	0/3/3/3
6	ADP	J	401	5	-	6/16/32/32	0/3/3/3
4	ATP	M	401	5	-	5/22/38/38	0/3/3/3
4	ATP	H	401	5	-	2/22/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	ATP	PB-O3A	15.91	1.76	1.59
4	M	401	ATP	PB-O3B	15.81	1.76	1.59
4	L	401	ATP	PB-O3A	15.09	1.75	1.59
4	I	401	ATP	PA-O3A	14.94	1.75	1.59
4	H	401	ATP	PB-O3B	14.11	1.74	1.59
4	I	401	ATP	PB-O3B	12.90	1.73	1.59
4	L	401	ATP	PA-O3A	11.62	1.72	1.59
4	M	401	ATP	PB-O3A	10.99	1.71	1.59
4	I	401	ATP	PB-O3A	10.58	1.70	1.59
4	L	401	ATP	PB-O3B	9.10	1.69	1.59
4	H	401	ATP	PA-O3A	7.54	1.67	1.59
6	J	401	ADP	PA-O3A	6.99	1.67	1.59
4	L	401	ATP	C6-N6	3.47	1.43	1.34
4	H	401	ATP	C2-N3	3.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	401	ATP	C1'-N9	2.88	1.54	1.46
6	J	401	ADP	C5-C6	-2.88	1.33	1.41
4	M	401	ATP	C2-N3	2.74	1.38	1.33
6	J	401	ADP	O2'-C2'	-2.70	1.36	1.43
4	H	401	ATP	C8-N9	-2.65	1.33	1.37
4	I	401	ATP	C4-N9	2.58	1.43	1.37
4	L	401	ATP	C8-N9	-2.55	1.33	1.37
4	L	401	ATP	C5-C4	-2.48	1.34	1.39
4	I	401	ATP	O2'-C2'	-2.46	1.36	1.43
4	M	401	ATP	C6-N6	2.42	1.40	1.34
4	I	401	ATP	C6-N6	2.34	1.40	1.34
4	L	401	ATP	C2-N1	2.26	1.38	1.33
4	L	401	ATP	C5-C6	2.23	1.47	1.41
6	J	401	ADP	PA-O2A	-2.12	1.45	1.55
4	I	401	ATP	C2'-C1'	-2.09	1.46	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	401	ATP	N6-C6-N1	5.80	131.29	118.38
4	H	401	ATP	C6-C5-C4	4.68	123.57	117.18
4	I	401	ATP	C1'-N9-C8	4.46	136.99	127.09
4	I	401	ATP	N6-C6-N1	4.03	127.36	118.38
4	L	401	ATP	C5-C6-N6	-3.72	114.07	123.29
4	M	401	ATP	C6-C5-C4	3.49	121.95	117.18
4	H	401	ATP	O4'-C1'-N9	3.30	114.43	108.09
4	M	401	ATP	C1'-N9-C8	3.20	134.21	127.09
6	J	401	ADP	O5'-C5'-C4'	3.19	119.86	108.99
6	J	401	ADP	N3-C4-N9	3.11	132.46	127.17
4	I	401	ATP	C4-N9-C1'	-3.07	119.45	126.63
6	J	401	ADP	C5-C4-N9	-3.04	102.50	105.81
4	I	401	ATP	O5'-C5'-C4'	3.02	119.29	108.99
4	I	401	ATP	C6-C5-N7	-2.95	126.40	132.09
4	I	401	ATP	N3-C2-N1	2.94	133.03	128.58
4	H	401	ATP	C5-C4-N3	-2.80	122.86	126.72
4	I	401	ATP	C5-C6-N6	-2.76	116.46	123.29
4	M	401	ATP	O4'-C1'-N9	2.74	113.36	108.09
4	H	401	ATP	C4-C5-N7	-2.66	107.54	110.58
6	J	401	ADP	C4-N9-C8	2.65	108.52	105.74
4	I	401	ATP	O3'-C3'-C2'	2.57	120.05	111.82
6	J	401	ADP	C1'-N9-C8	-2.48	121.59	127.09
4	M	401	ATP	C5'-C4'-C3'	2.47	124.10	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	ATP	C5-C4-N3	-2.46	123.33	126.72
4	I	401	ATP	C5'-C4'-C3'	2.45	124.05	115.21
4	M	401	ATP	C4-N9-C8	-2.43	103.19	105.74
4	I	401	ATP	C2-N1-C6	-2.27	115.00	118.73
4	L	401	ATP	C5'-C4'-C3'	-2.18	107.38	115.21
4	M	401	ATP	O3G-PG-O2G	2.17	115.95	107.80
4	H	401	ATP	C5-N7-C8	2.14	106.81	103.45
4	M	401	ATP	O5'-C5'-C4'	2.14	116.27	108.99
4	I	401	ATP	C4-N9-C8	-2.11	103.52	105.74
4	I	401	ATP	C4-C5-N7	2.04	112.92	110.58
4	H	401	ATP	O3G-PG-O1G	2.02	118.71	110.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	401	ATP	C5'-O5'-PA-O2A
4	H	401	ATP	C5'-O5'-PA-O3A
4	I	401	ATP	C5'-O5'-PA-O1A
4	I	401	ATP	C5'-O5'-PA-O3A
4	L	401	ATP	PB-O3B-PG-O2G
4	L	401	ATP	C5'-O5'-PA-O2A
4	M	401	ATP	C5'-O5'-PA-O1A
4	M	401	ATP	C5'-O5'-PA-O2A
4	M	401	ATP	C5'-O5'-PA-O3A
6	J	401	ADP	PA-O3A-PB-O2B
6	J	401	ADP	C5'-O5'-PA-O1A
6	J	401	ADP	C5'-O5'-PA-O2A
6	J	401	ADP	C5'-O5'-PA-O3A
4	I	401	ATP	C4'-C5'-O5'-PA
4	M	401	ATP	C4'-C5'-O5'-PA
4	L	401	ATP	PB-O3B-PG-O3G
4	L	401	ATP	C3'-C4'-C5'-O5'
4	L	401	ATP	PG-O3B-PB-O2B
4	L	401	ATP	C5'-O5'-PA-O1A
4	L	401	ATP	C5'-O5'-PA-O3A
4	L	401	ATP	C4'-C5'-O5'-PA
6	J	401	ADP	C4'-C5'-O5'-PA
4	L	401	ATP	PG-O3B-PB-O1B
4	M	401	ATP	PG-O3B-PB-O2B
4	L	401	ATP	O4'-C4'-C5'-O5'
6	J	401	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
4	I	401	ATP	PA-O3A-PB-O1B
4	I	401	ATP	PA-O3A-PB-O2B
4	L	401	ATP	PB-O3B-PG-O1G

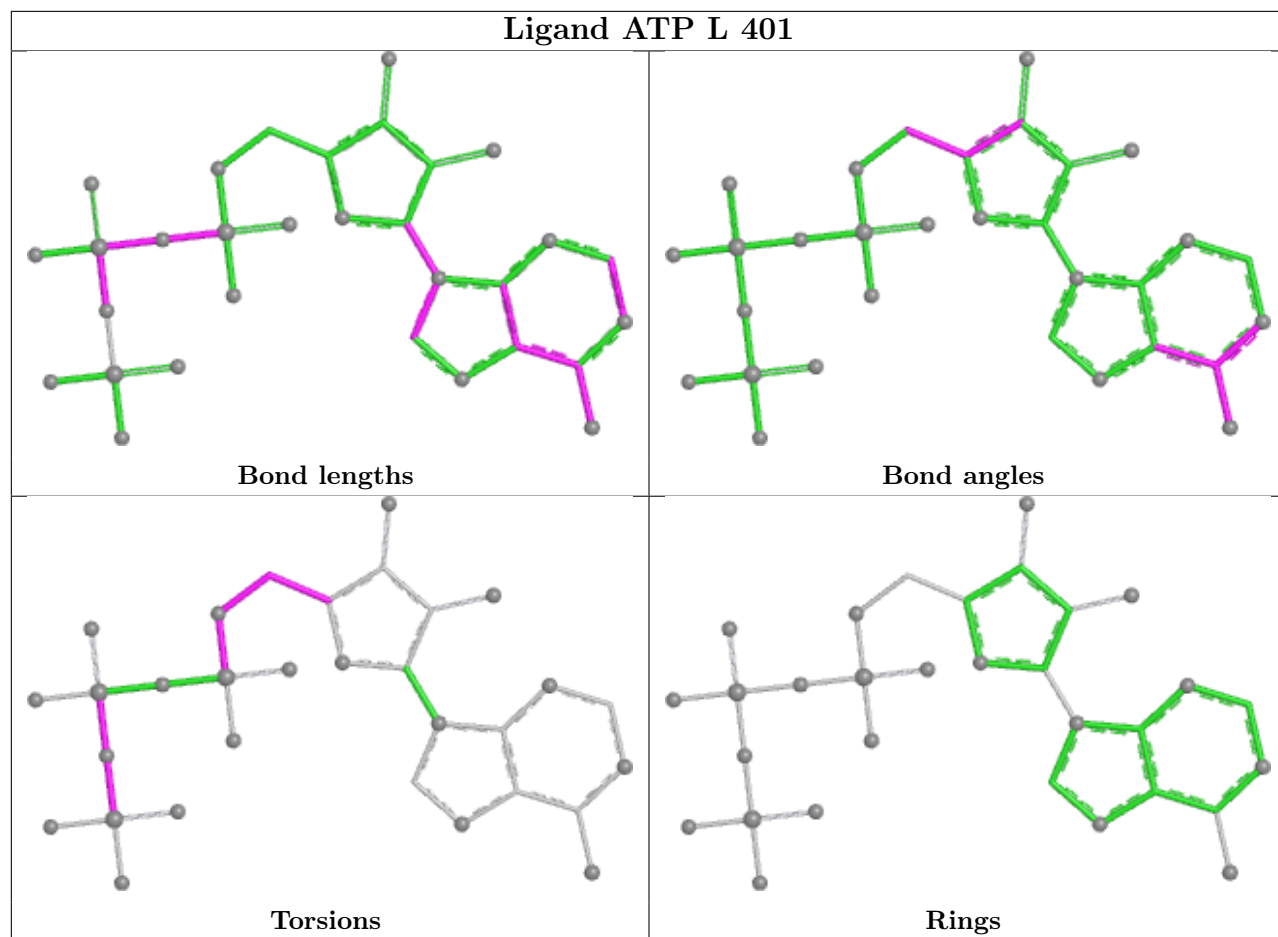
There are no ring outliers.

2 monomers are involved in 13 short contacts:

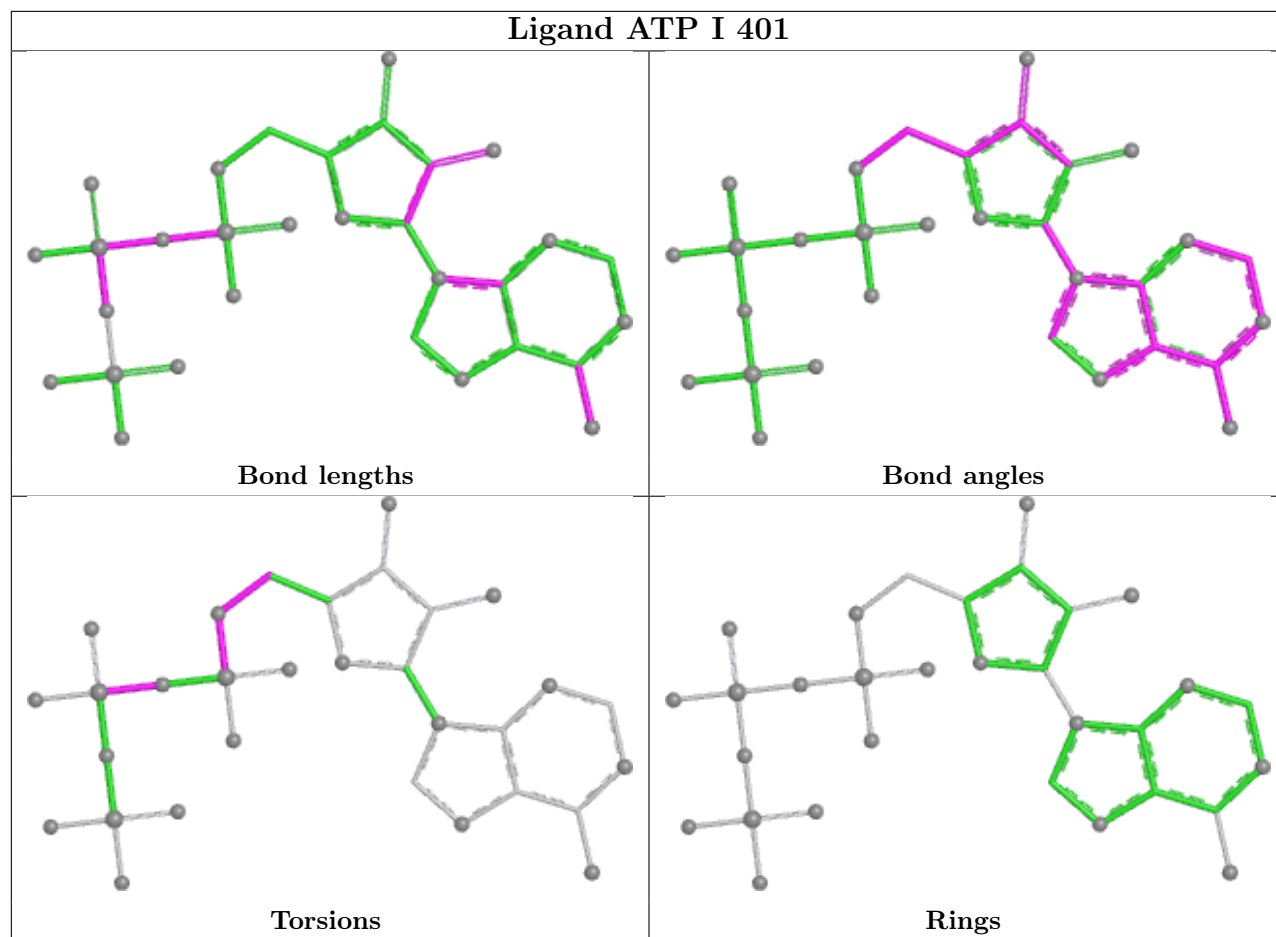
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	401	ADP	11	0
4	H	401	ATP	2	0

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.

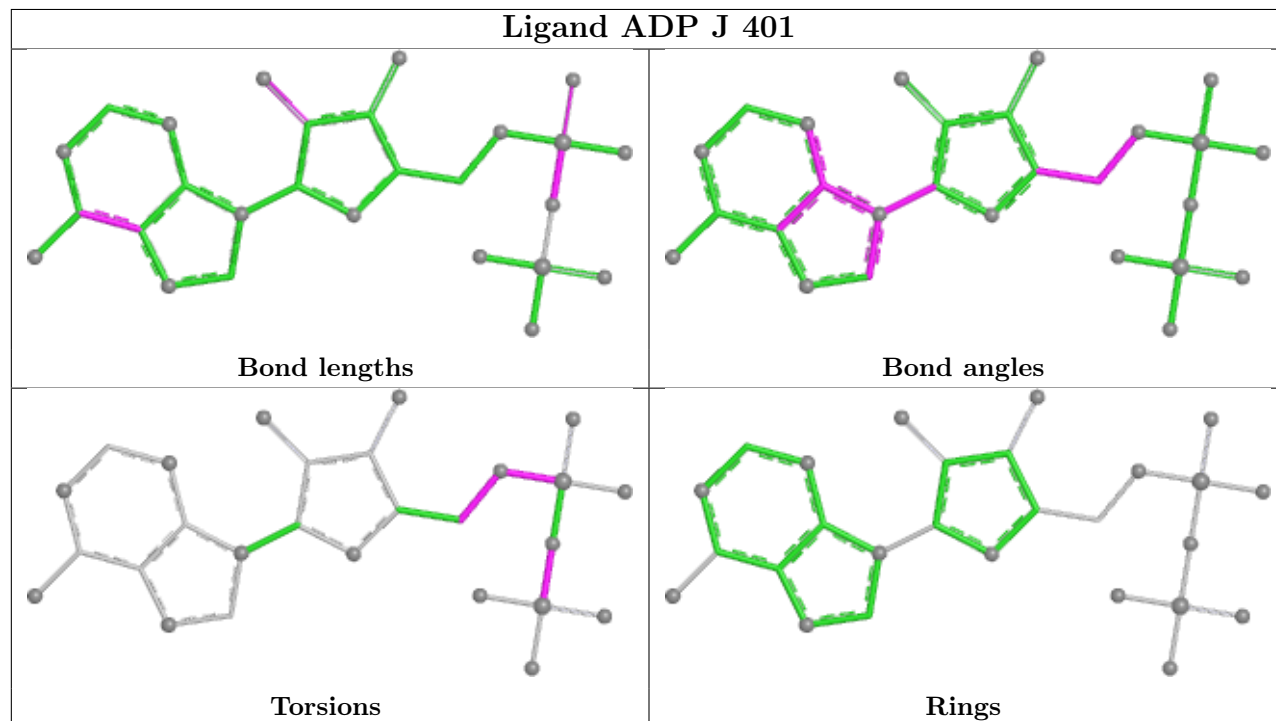
Ligand ATP L 401

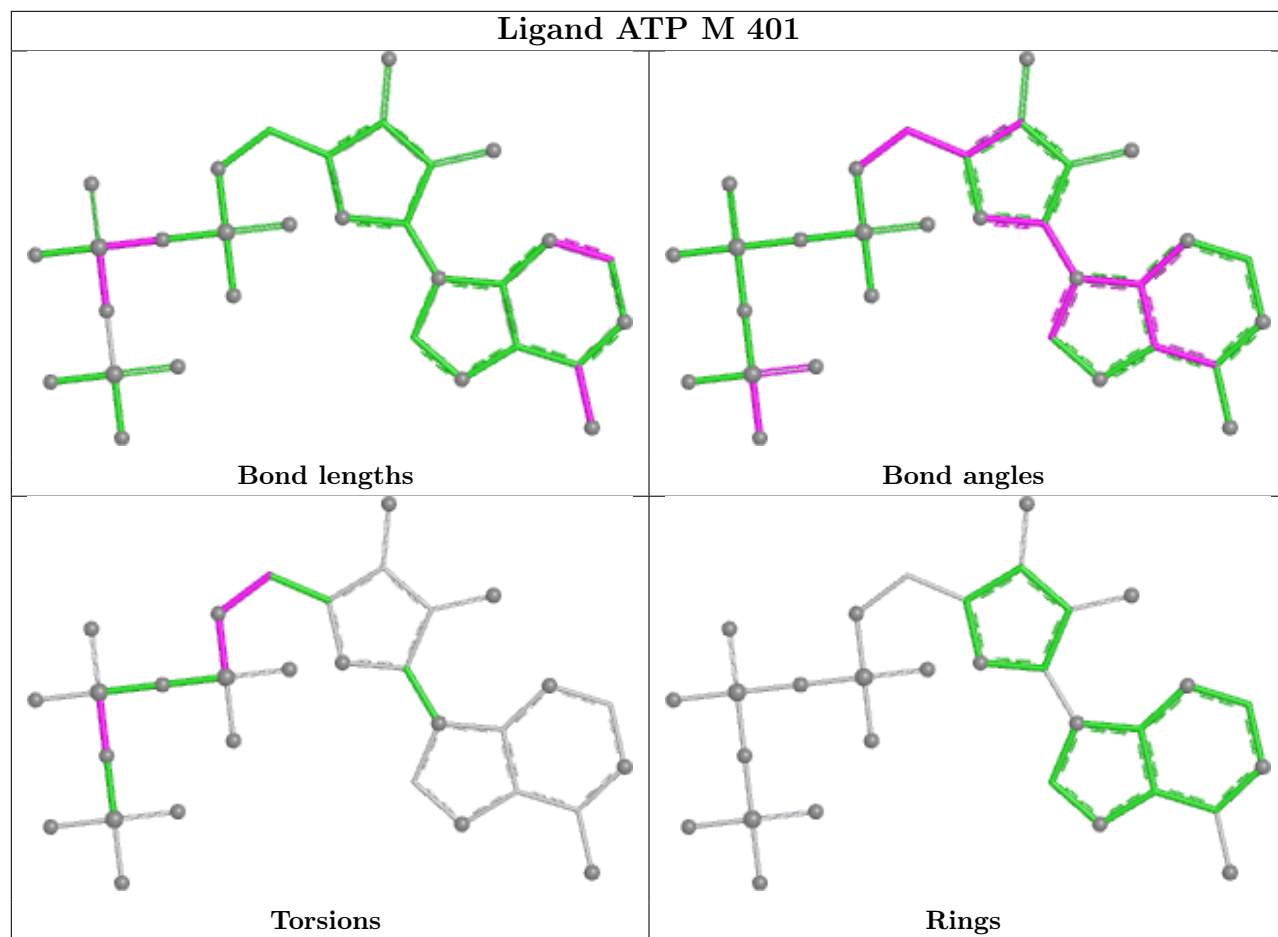


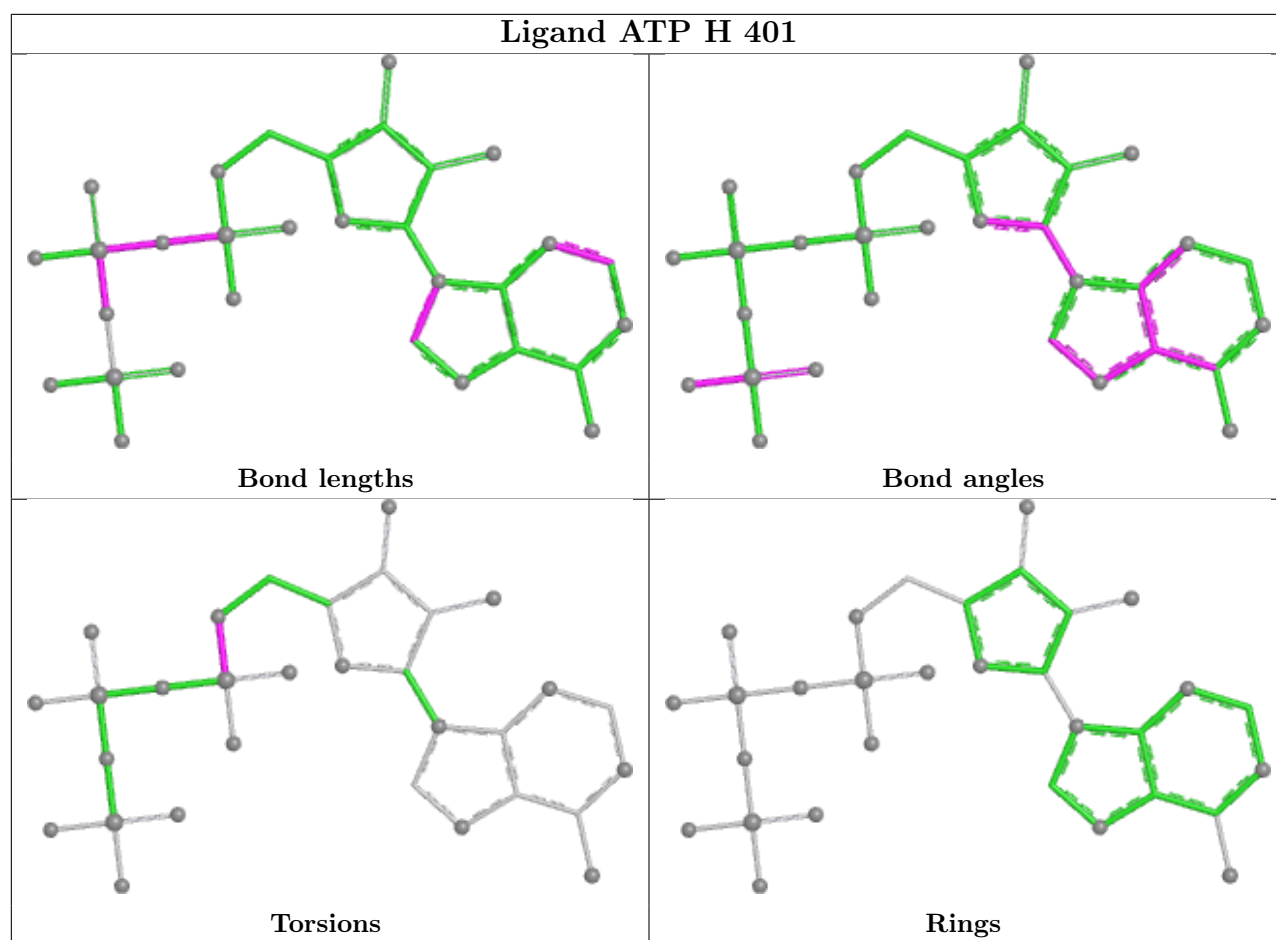
Ligand ATP I 401



Ligand ADP J 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-0215. These allow visual inspection of the internal detail of the map and identification of artifacts.

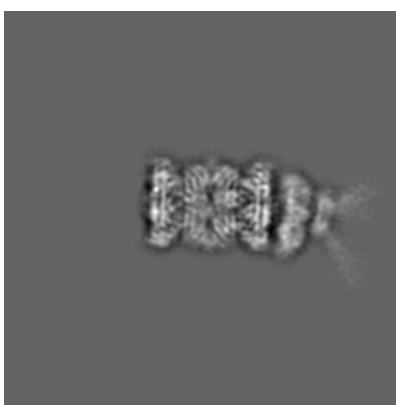
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

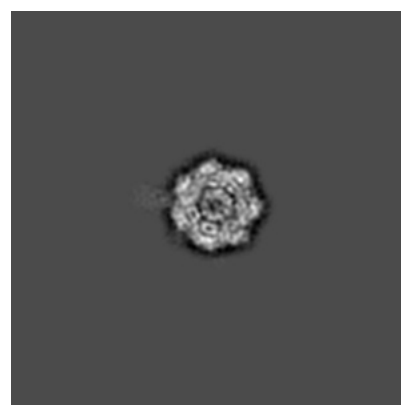
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

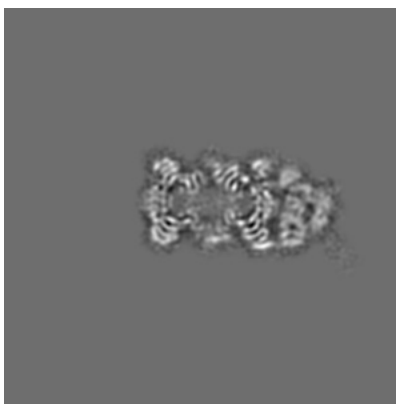
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 179



Y Index: 187

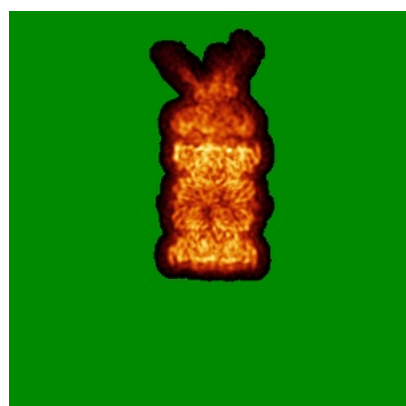


Z Index: 251

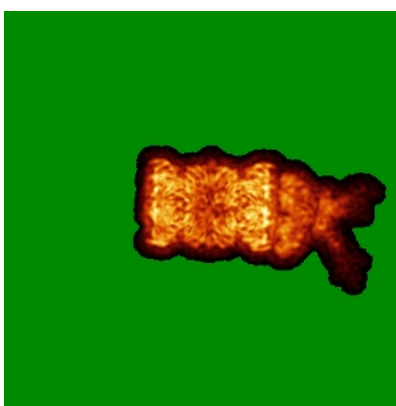
The images above show the largest variance slices of the map in three orthogonal directions.

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

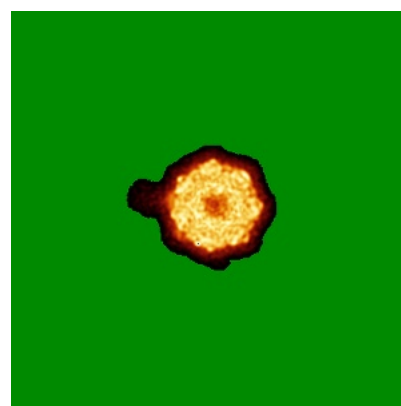
6.4.1 Primary map



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 0.00655. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

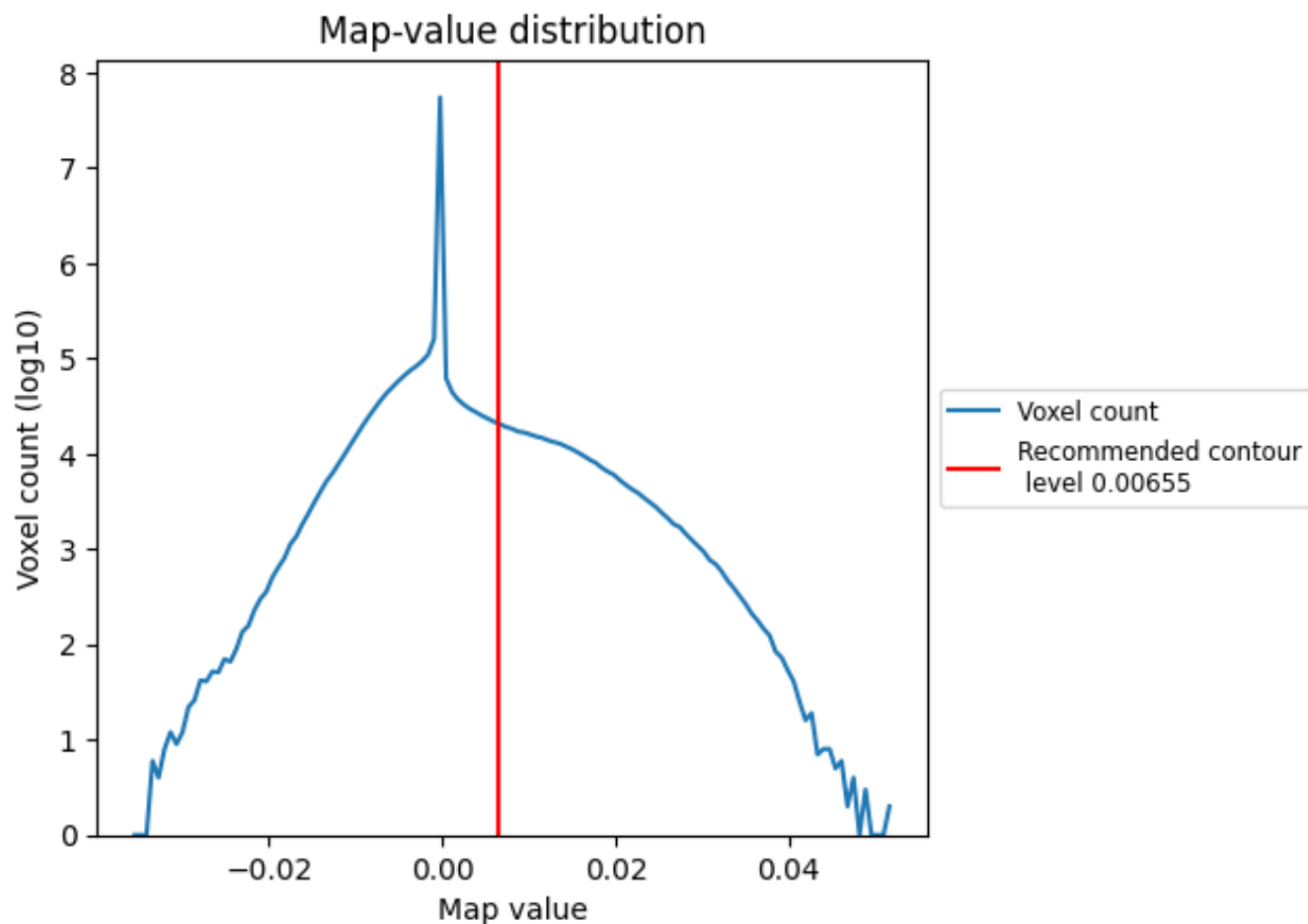
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

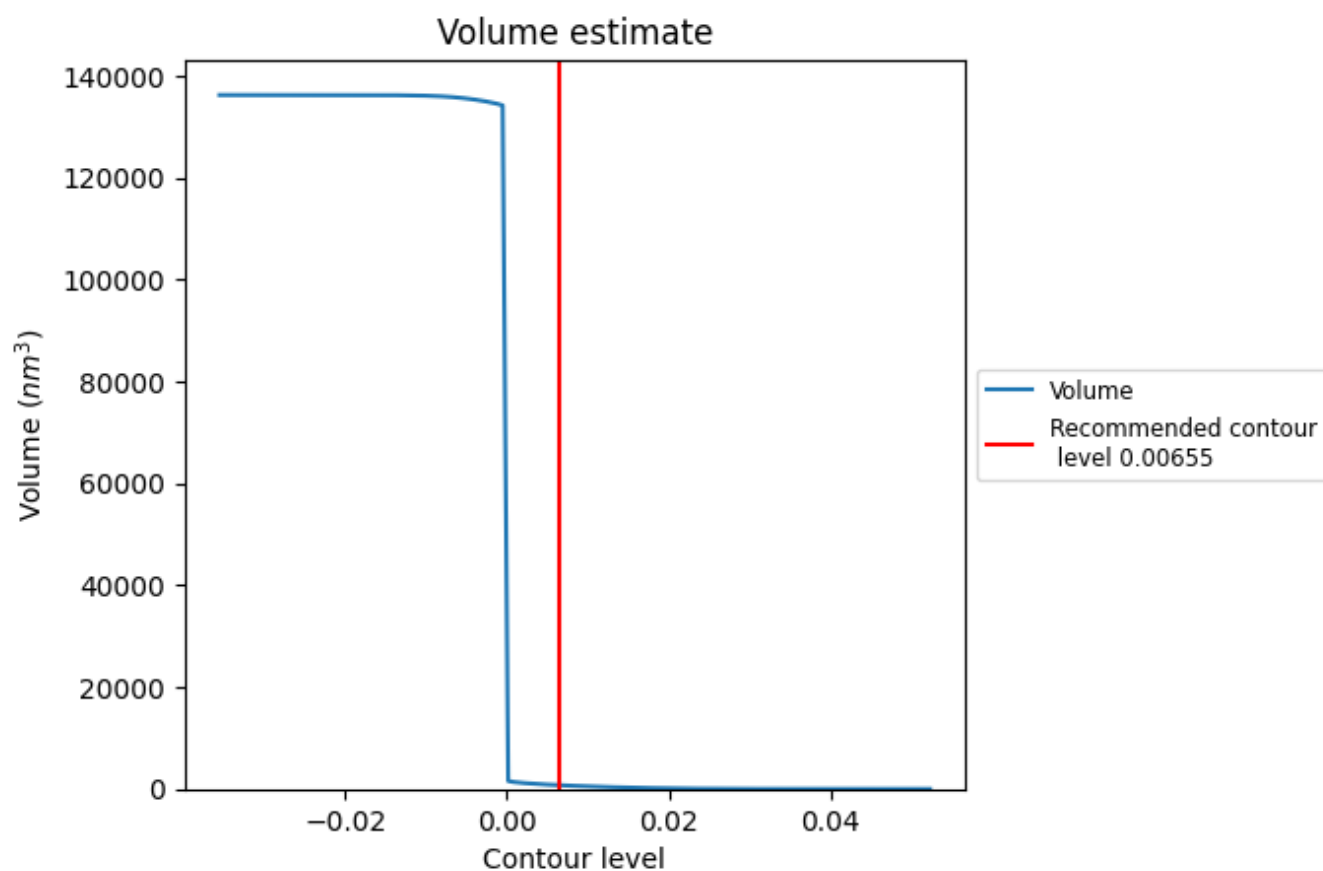
This section contains the results of statistical analysis of the map.

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.

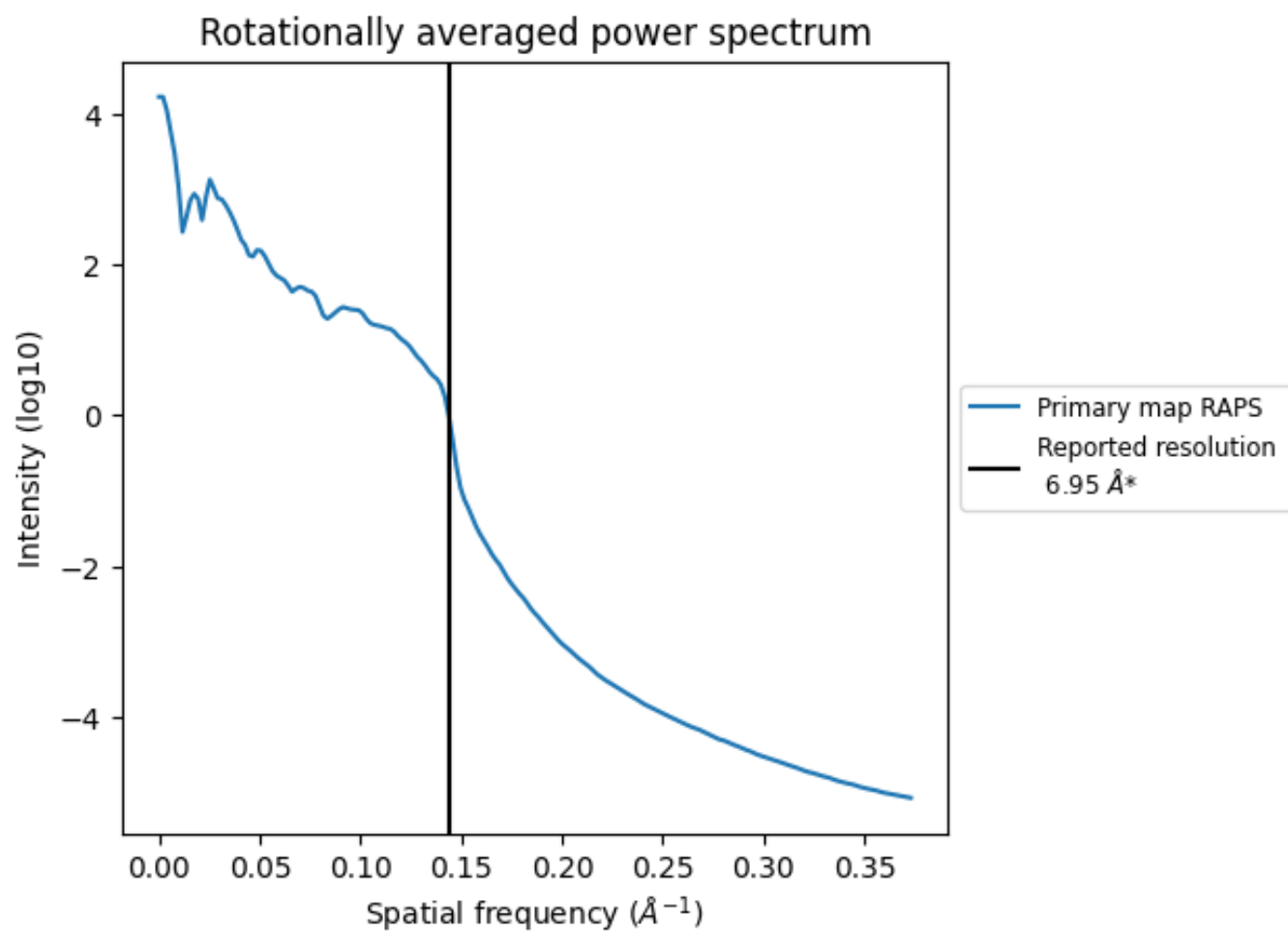
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 736 nm^3 ; this corresponds to an approximate mass of 665 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 0.144 Å⁻¹

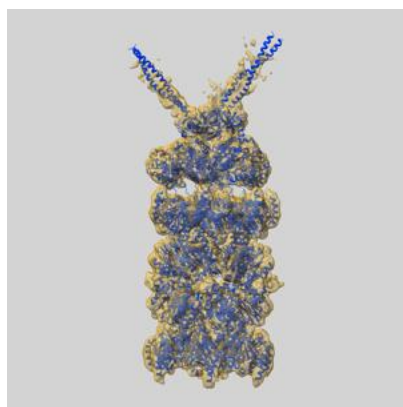
8 Fourier-Shell correlation ⓘ

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

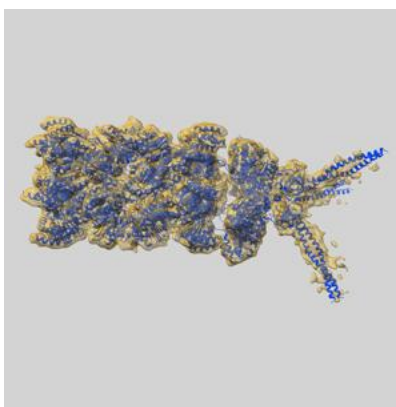
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0215 and PDB model 6HEC. Per-residue inclusion information can be found in section 3 on page 9.

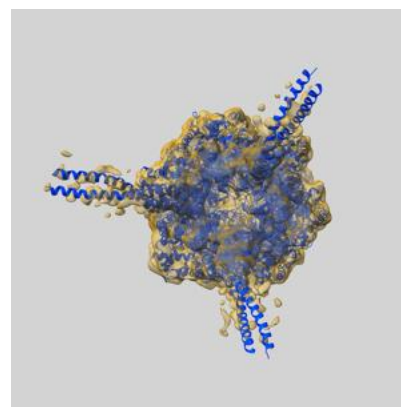
9.1 Map-model overlay [i](#)



X



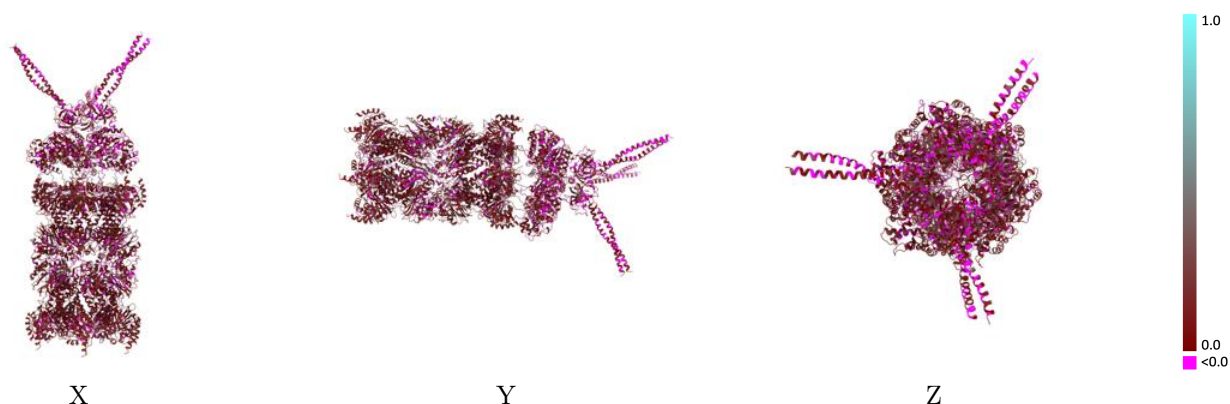
Y



Z

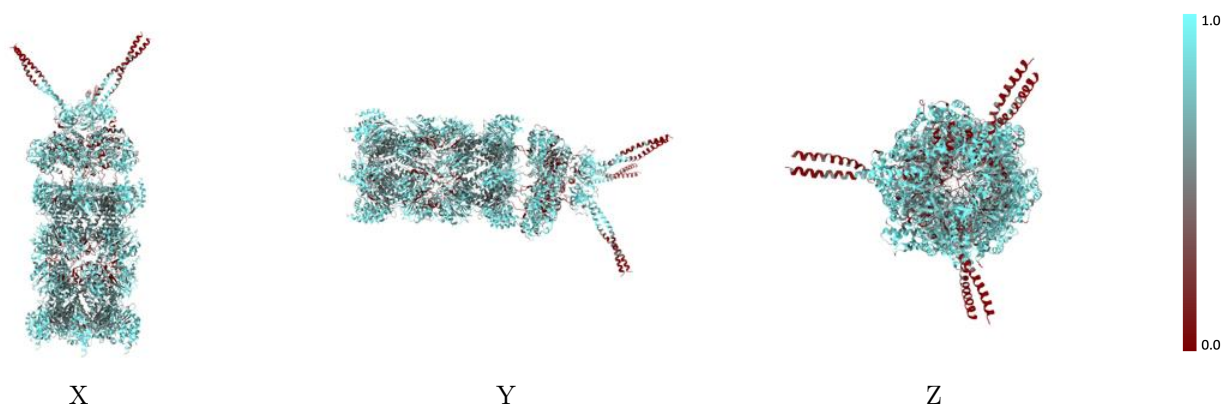
The images above show the 3D surface view of the map at the recommended contour level 0.00655 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



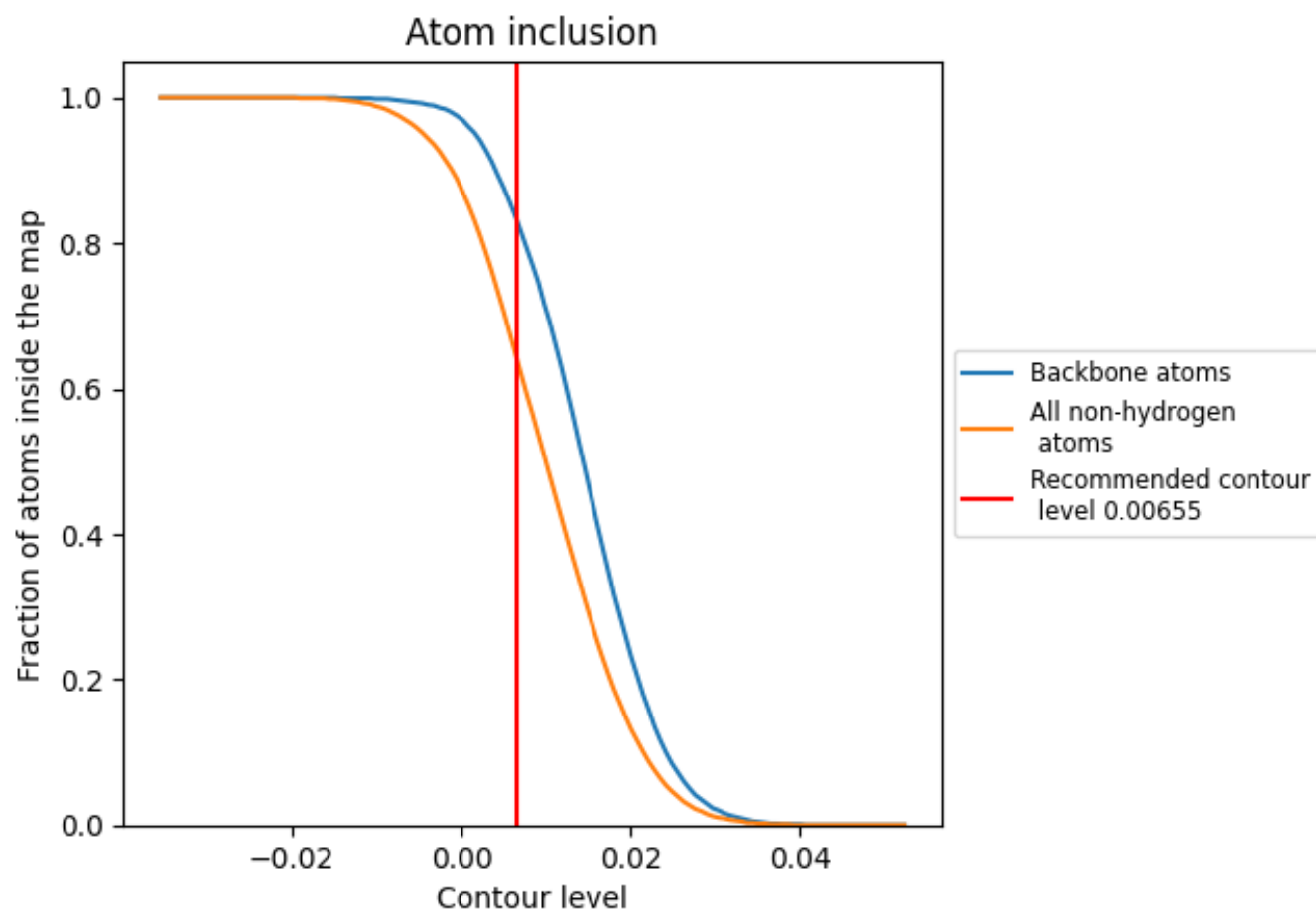
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00655).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00655) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.1140
1	 0.6100	 0.1150
2	 0.6200	 0.1230
3	 0.6260	 0.1250
4	 0.6350	 0.1280
5	 0.6270	 0.1240
6	 0.6250	 0.1230
7	 0.6230	 0.1150
A	 0.7060	 0.1270
B	 0.6940	 0.1350
C	 0.6950	 0.1370
D	 0.7000	 0.1310
E	 0.6950	 0.1300
F	 0.7060	 0.1350
G	 0.6990	 0.1310
H	 0.6010	 0.0920
I	 0.6060	 0.0940
J	 0.6190	 0.0900
K	 0.6010	 0.0900
L	 0.5270	 0.0790
M	 0.5950	 0.0840
a	 0.6960	 0.1320
b	 0.6960	 0.1250
c	 0.6830	 0.1210
d	 0.6810	 0.1180
e	 0.7050	 0.1300
f	 0.6730	 0.1150
g	 0.6800	 0.1250
h	 0.6240	 0.1120
i	 0.6180	 0.1160
j	 0.6230	 0.1230
k	 0.6160	 0.1120
l	 0.6120	 0.1180
m	 0.6120	 0.1070
n	 0.6210	 0.1130

