Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:24 AM UTC

PDB ID	:	6HED / pdb_00006hed
EMDB ID	:	EMD-0216
Title	:	PAN-proteasome in state 5
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:

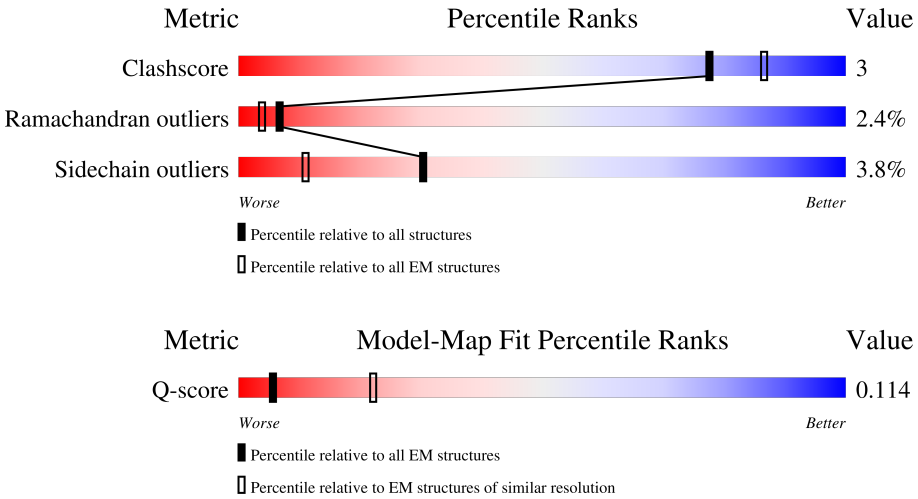
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 <=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	7% 43% 50% 6% •
1	B	242	6% 45% 45% 10%
1	C	242	7% 44% 49% 6% •
1	D	242	9% 44% 46% 10%

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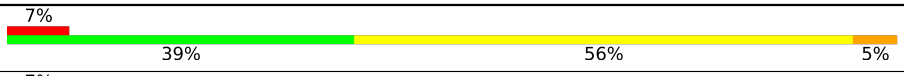
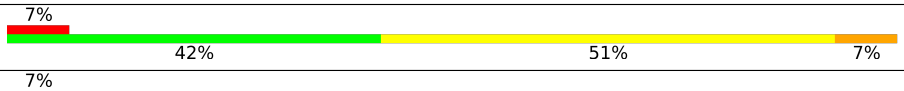
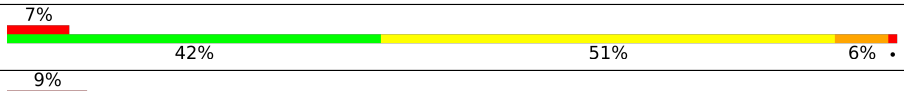
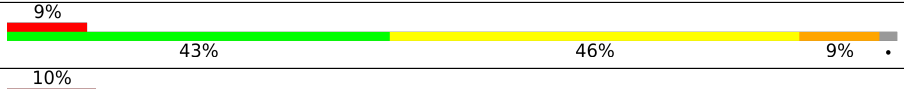
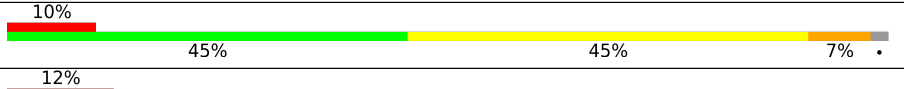
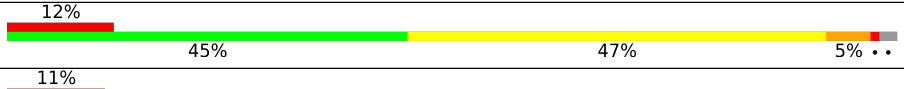
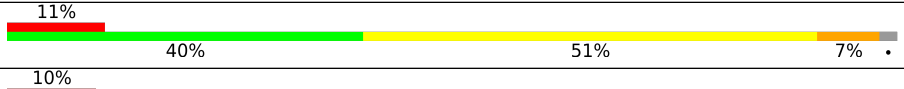
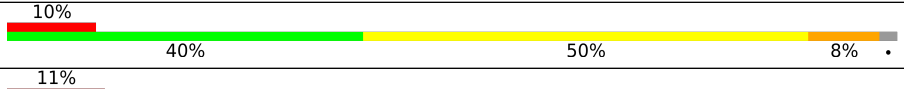
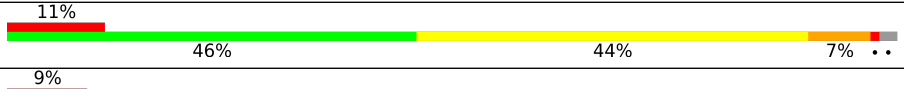
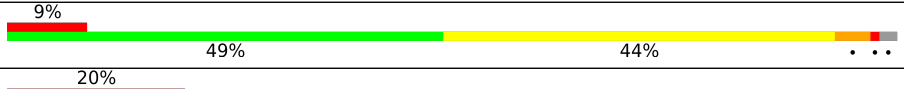
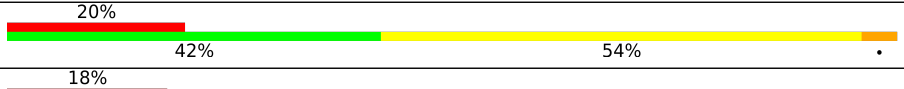
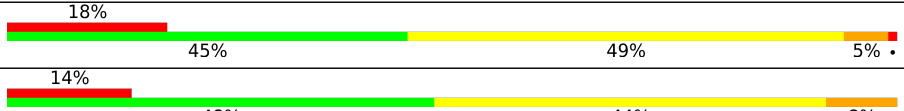
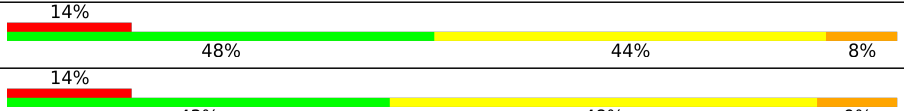
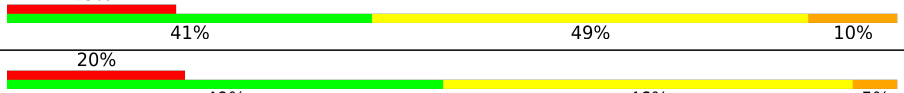
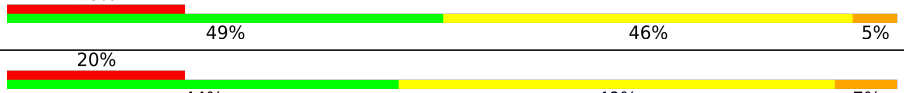
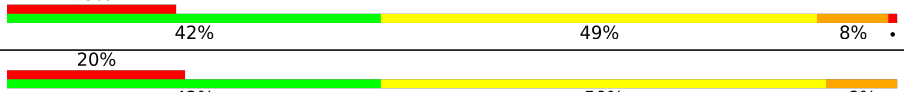
Mol	Chain	Length	Quality of chain
1	E	242	
1	F	242	
1	G	242	
1	a	242	
1	b	242	
1	c	242	
1	d	242	
1	e	242	
1	f	242	
1	g	242	
2	1	202	
2	2	202	
2	3	202	
2	4	202	
2	5	202	
2	6	202	
2	7	202	
2	h	202	
2	i	202	
2	j	202	
2	k	202	
2	l	202	
2	m	202	
2	n	202	
3	H	390	

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Mol	Chain	Length	Quality of chain
3	I	390	26% 39% 51% 9%
3	J	390	33% 40% 51% 8%
3	K	390	31% 38% 50% 11%
3	L	390	32% 39% 50% 10%
3	M	390	28% 42% 47% 11%

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	I	401	-	-	X	-

2 Entry composition

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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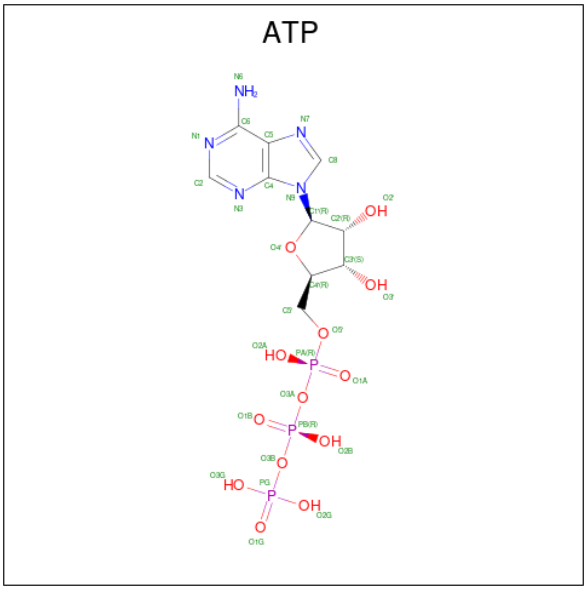
Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	i	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	j	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	4	202	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: $C_{10}H_{16}N_5O_{13}P_3$).

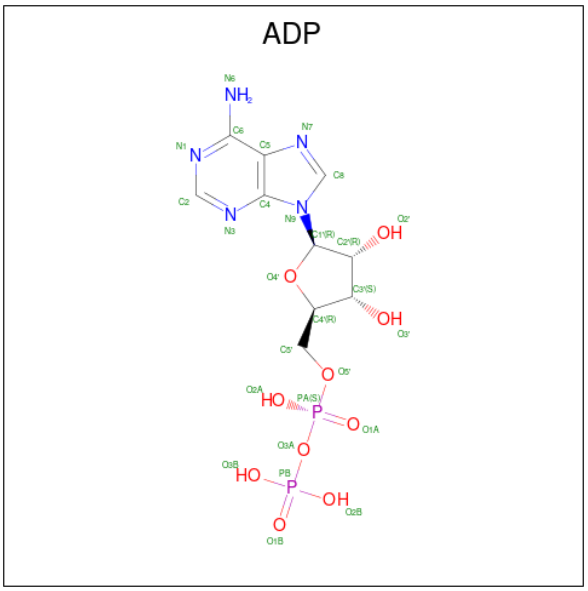


Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	K	1	Total	Mg	0
			1	1	
5	L	1	Total	Mg	0
			1	1	
5	M	1	Total	Mg	0
			1	1	

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

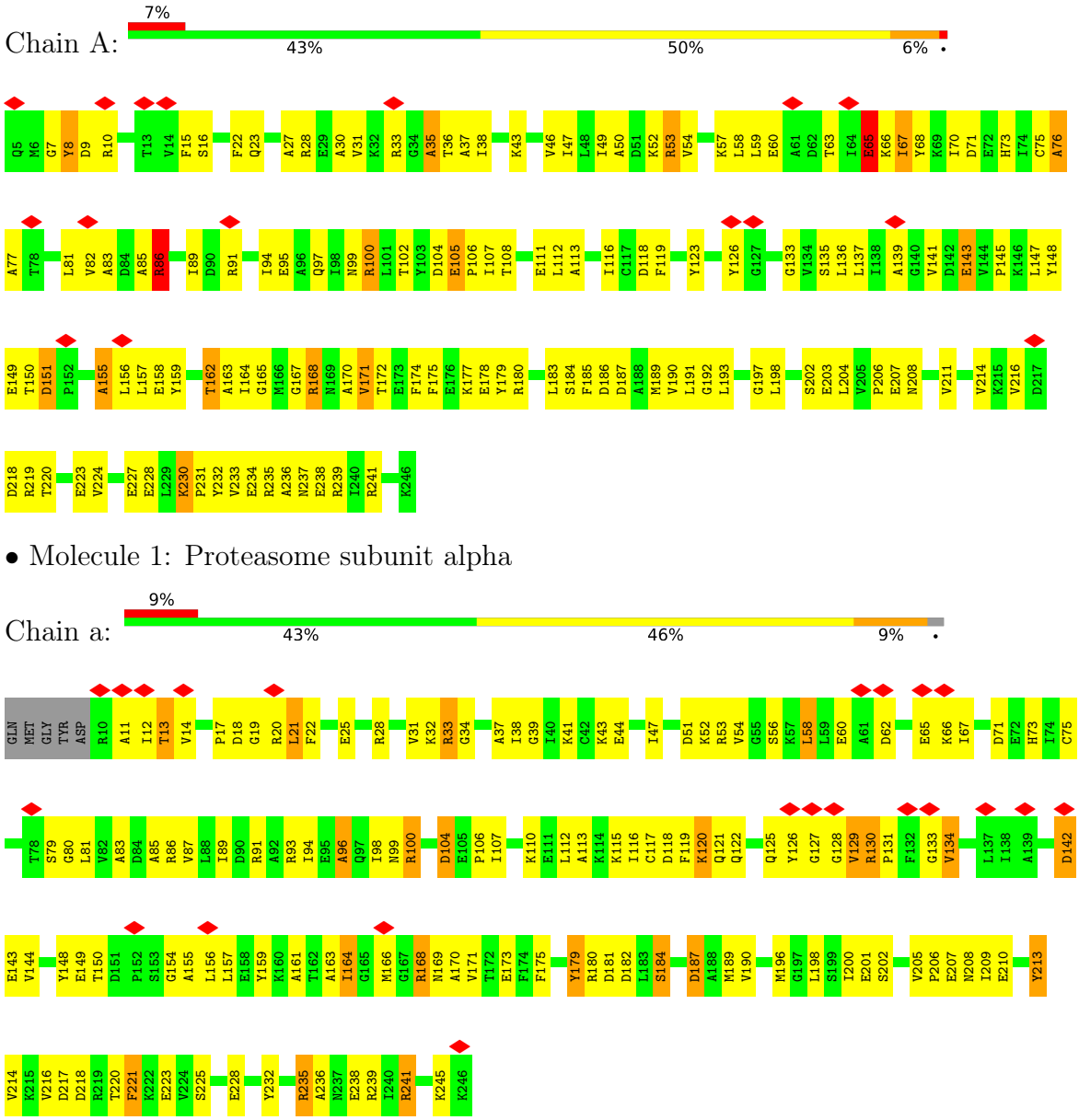


Mol	Chain	Residues	Atoms					AltConf
6	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

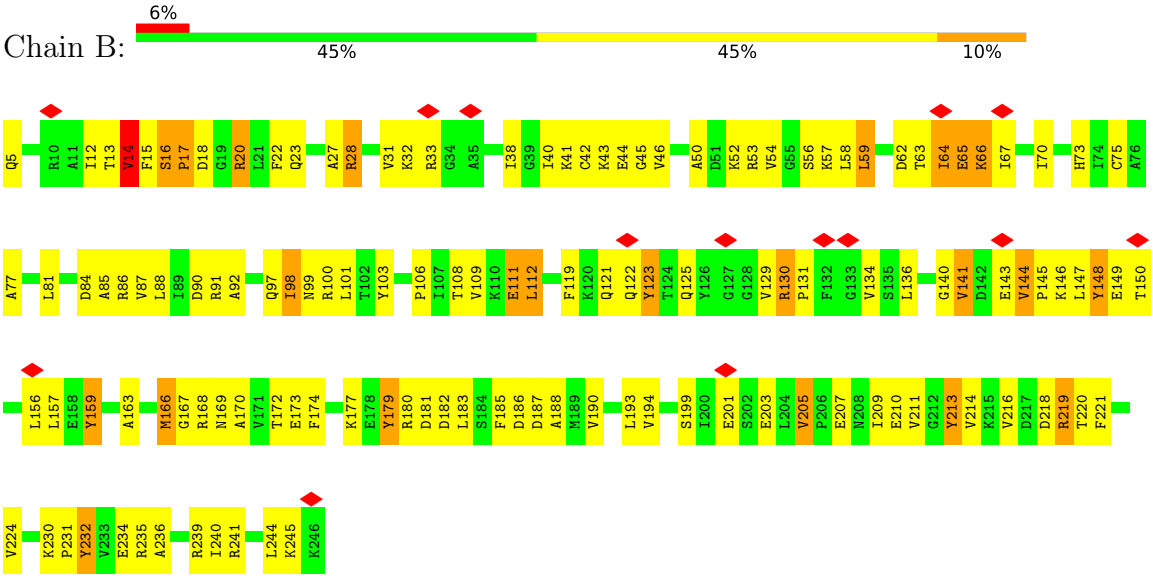
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

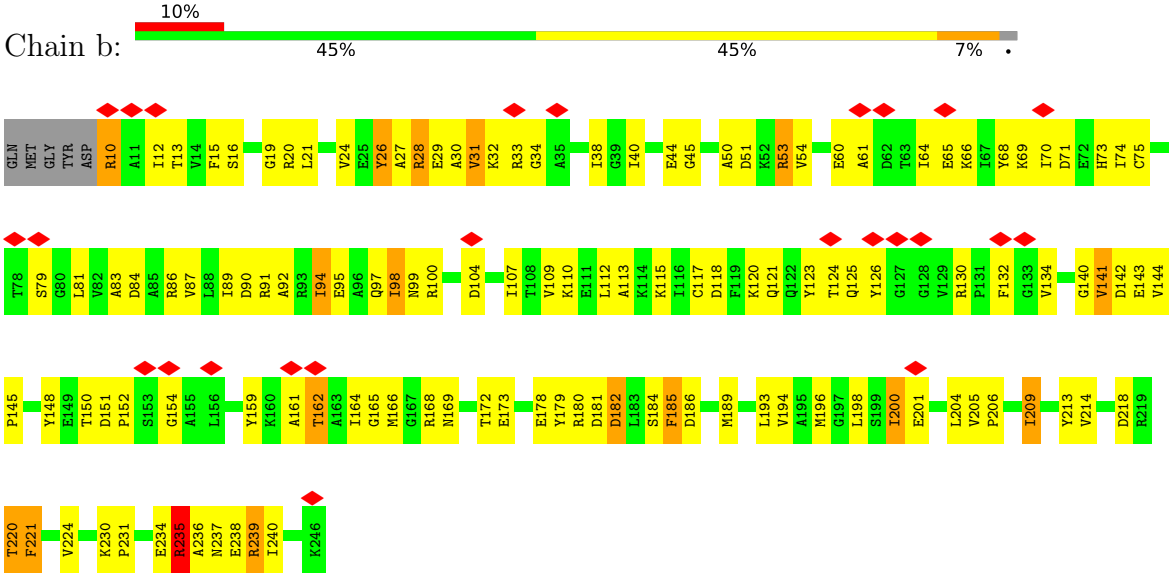
• Molecule 1: Proteasome subunit alpha

Chain B:



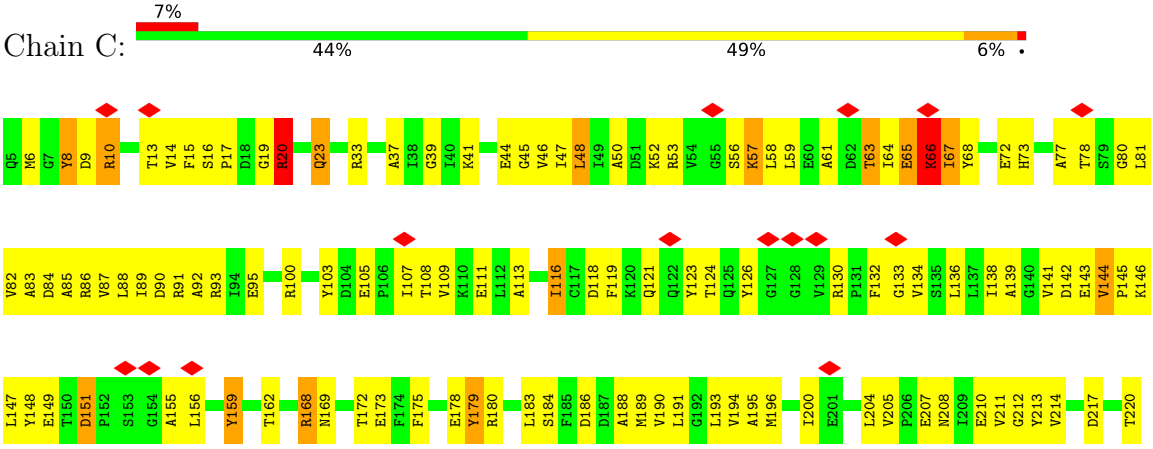
• Molecule 1: Proteasome subunit alpha

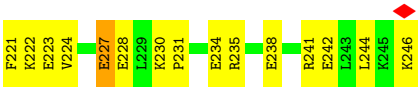
Chain b:



• Molecule 1: Proteasome subunit alpha

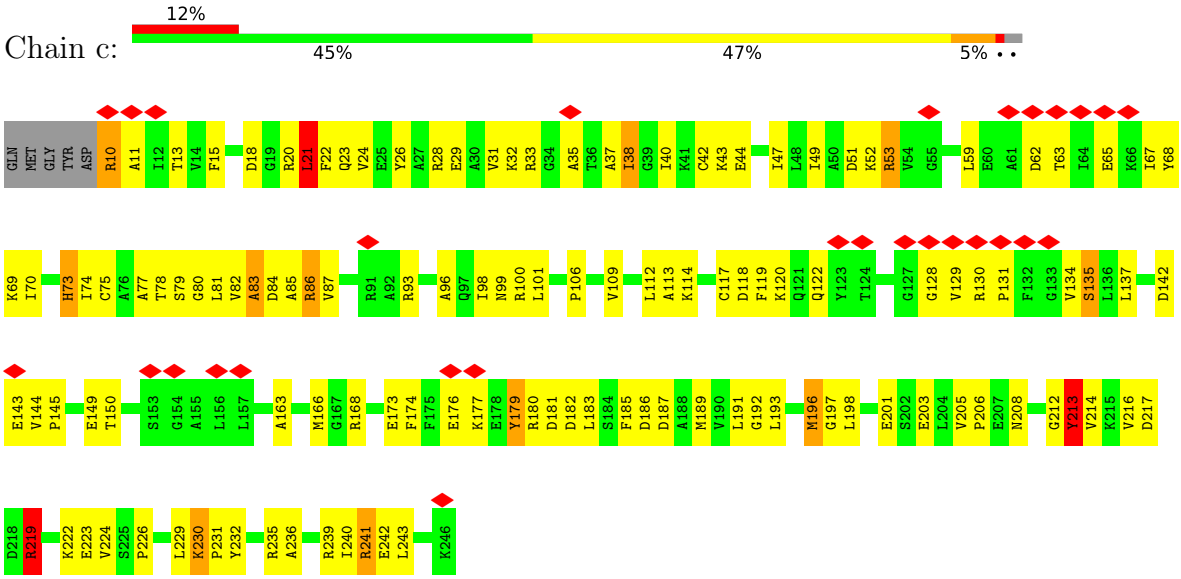
Chain C:





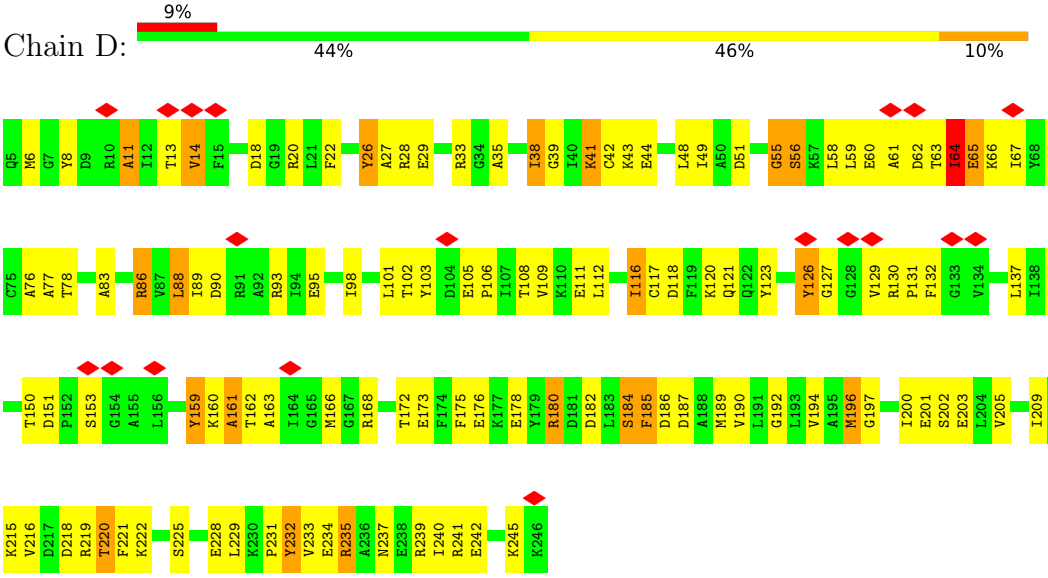
• Molecule 1: Proteasome subunit alpha

Chain c:



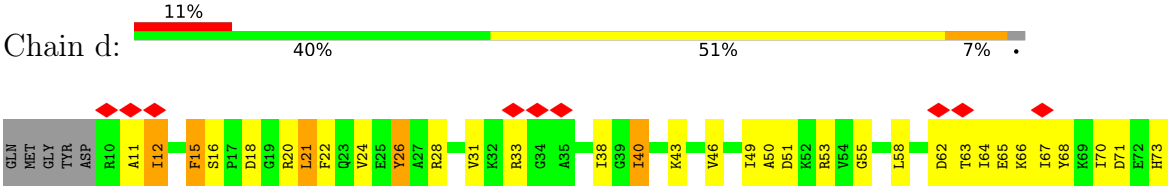
• Molecule 1: Proteasome subunit alpha

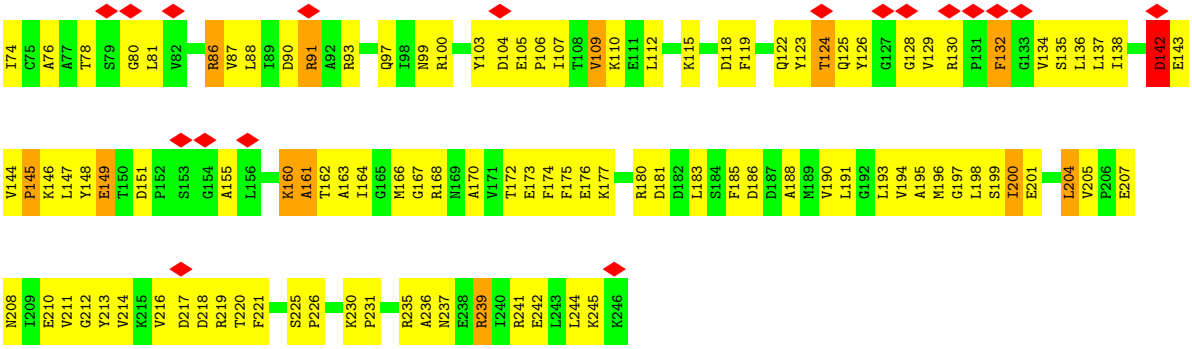
Chain D:



• Molecule 1: Proteasome subunit alpha

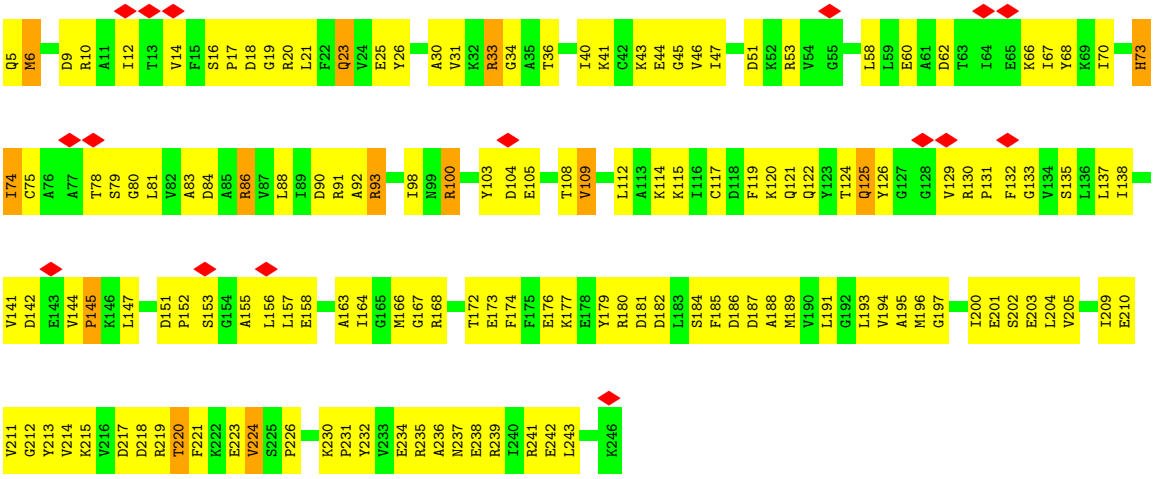
Chain d:





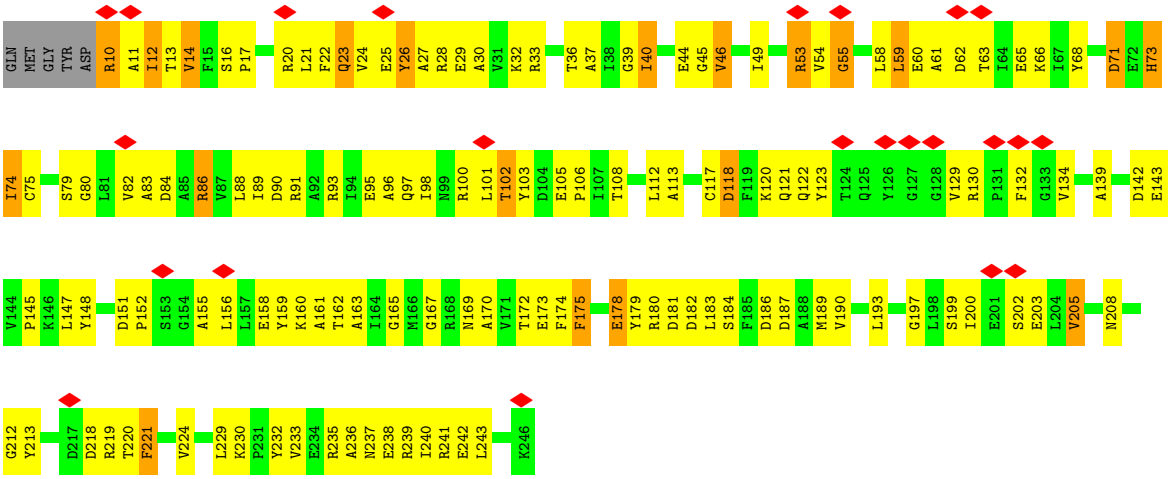
• Molecule 1: Proteasome subunit alpha

Chain E:



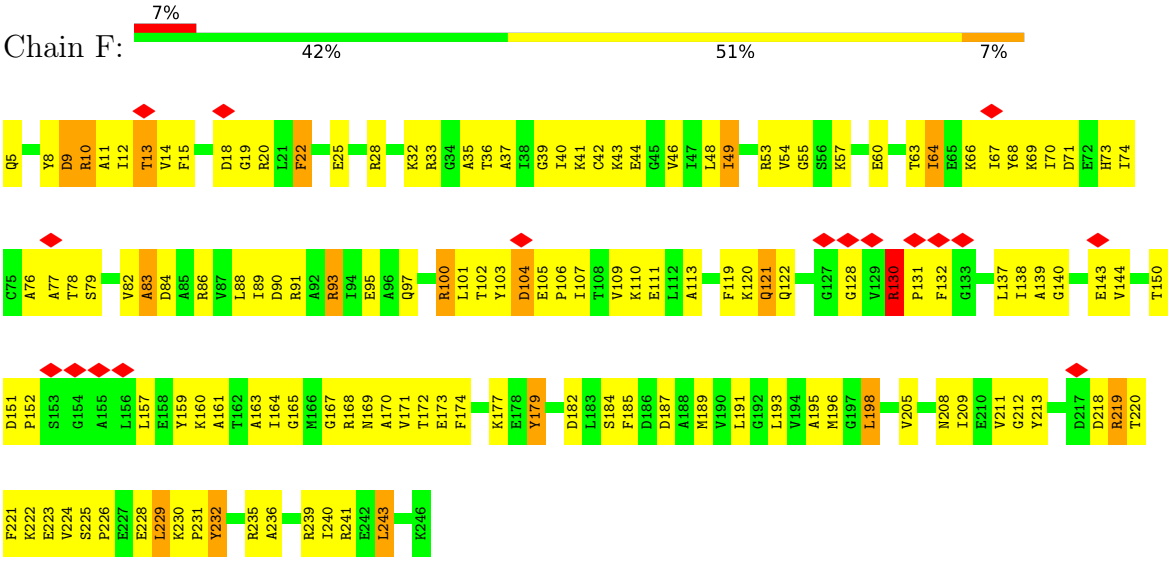
• Molecule 1: Proteasome subunit alpha

Chain e:



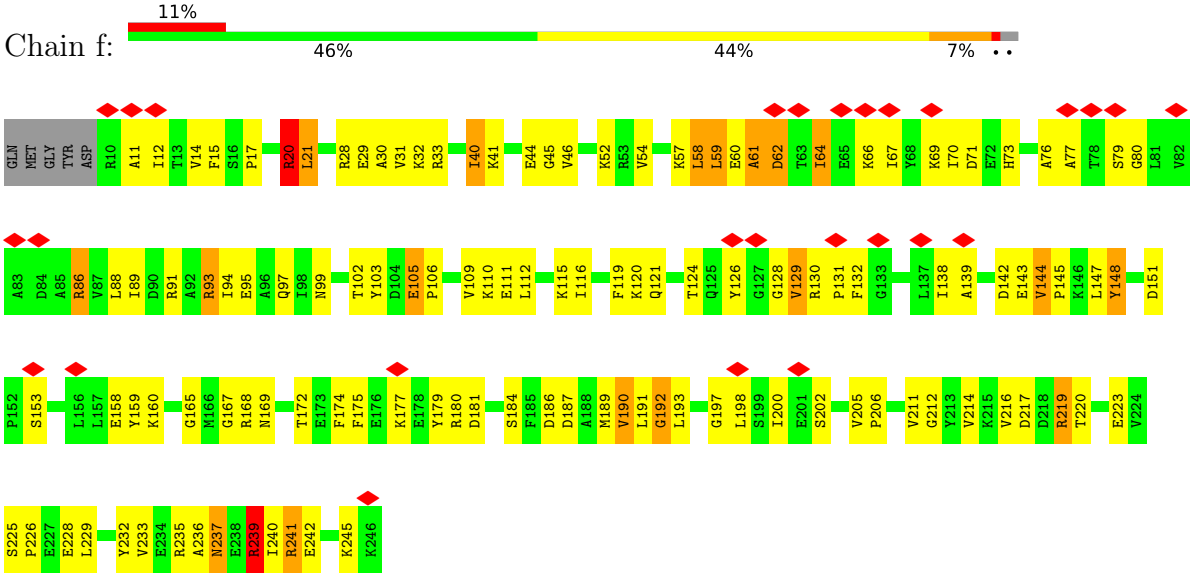
• Molecule 1: Proteasome subunit alpha

Chain F:



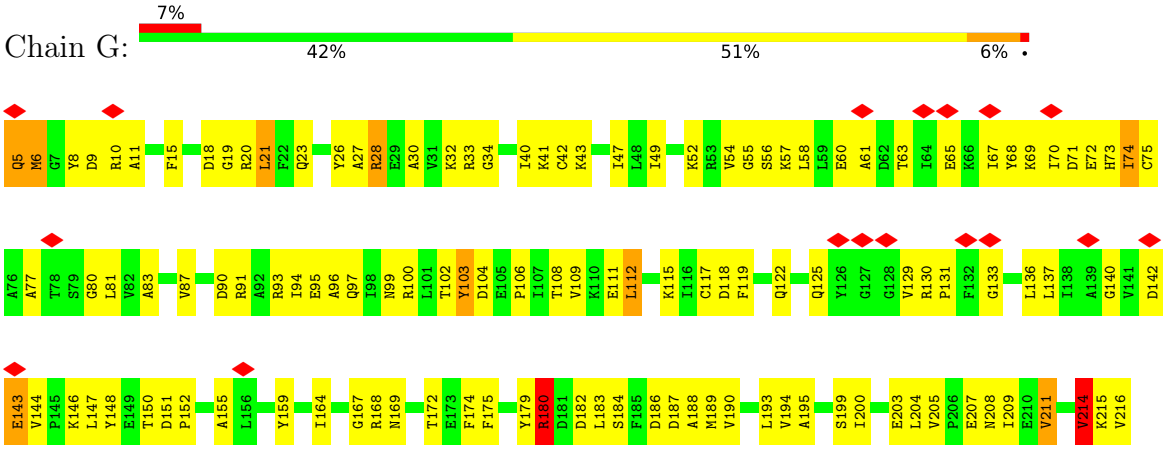
• Molecule 1: Proteasome subunit alpha

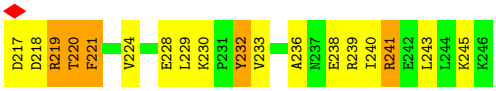
Chain f:



• Molecule 1: Proteasome subunit alpha

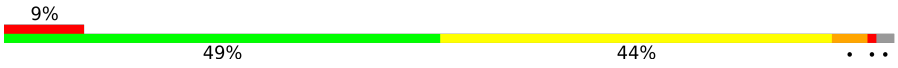
Chain G:

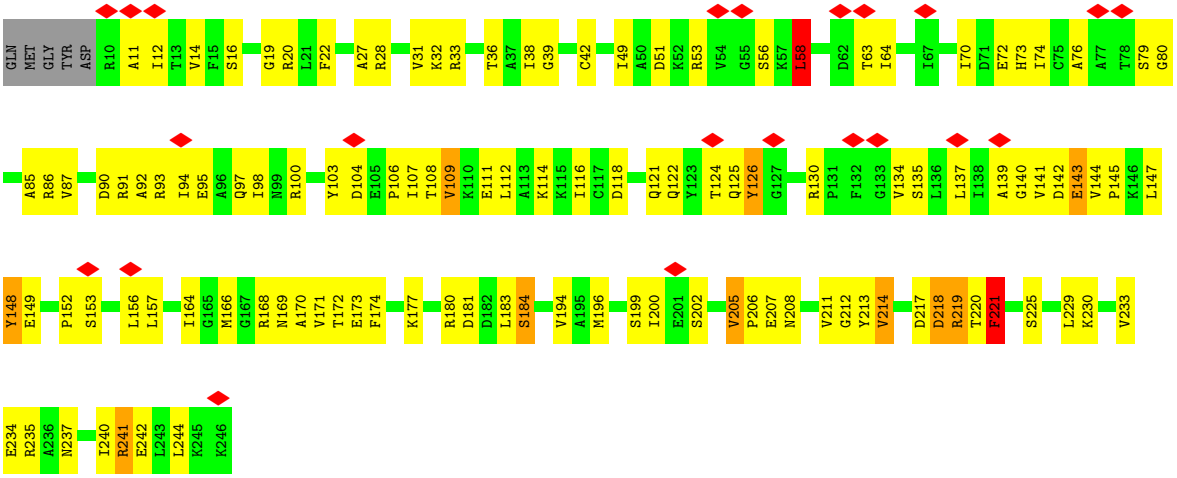




• Molecule 1: Proteasome subunit alpha

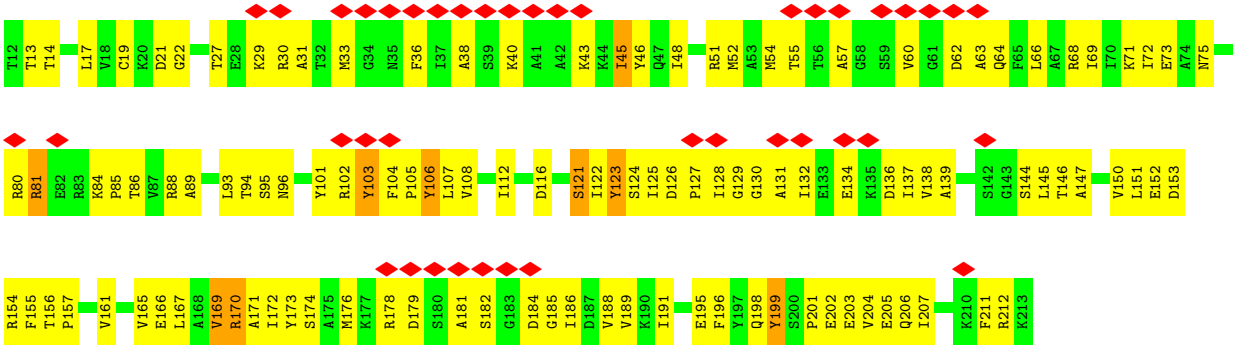
Chain g:





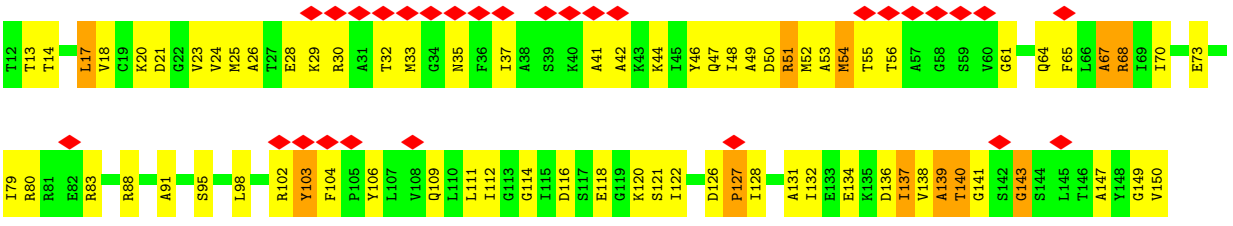
• Molecule 2: Proteasome subunit beta

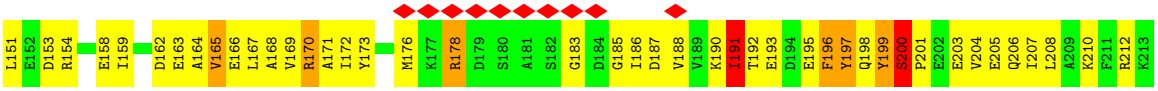
Chain 1:



• Molecule 2: Proteasome subunit beta

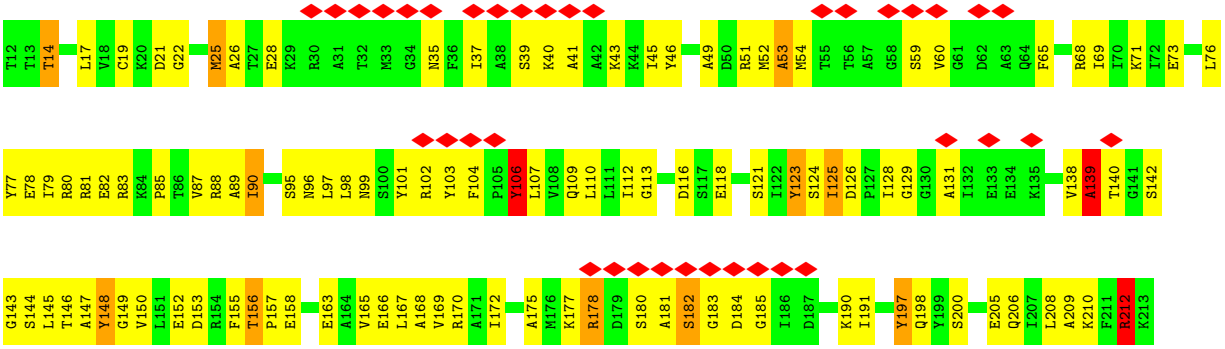
Chain h:





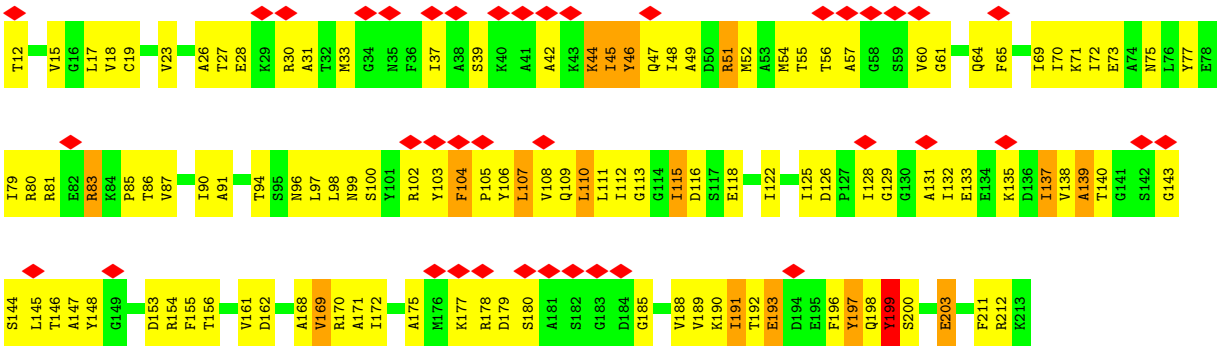
• Molecule 2: Proteasome subunit beta

Chain 2:



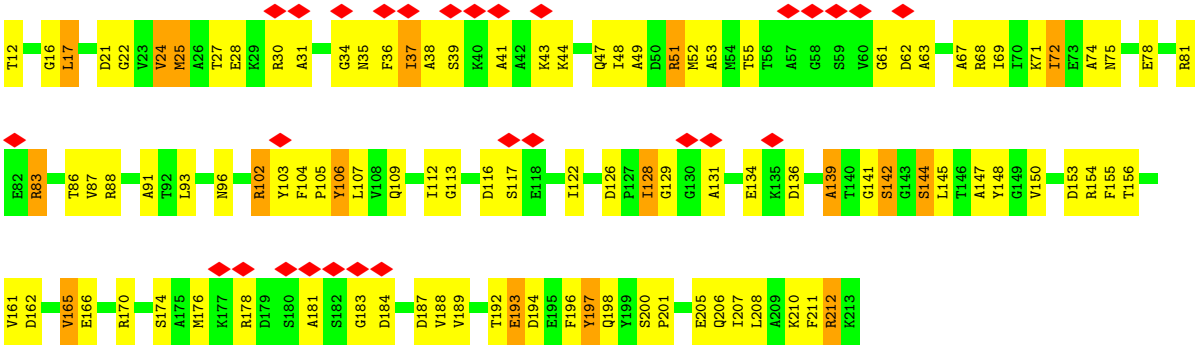
• Molecule 2: Proteasome subunit beta

Chain i:



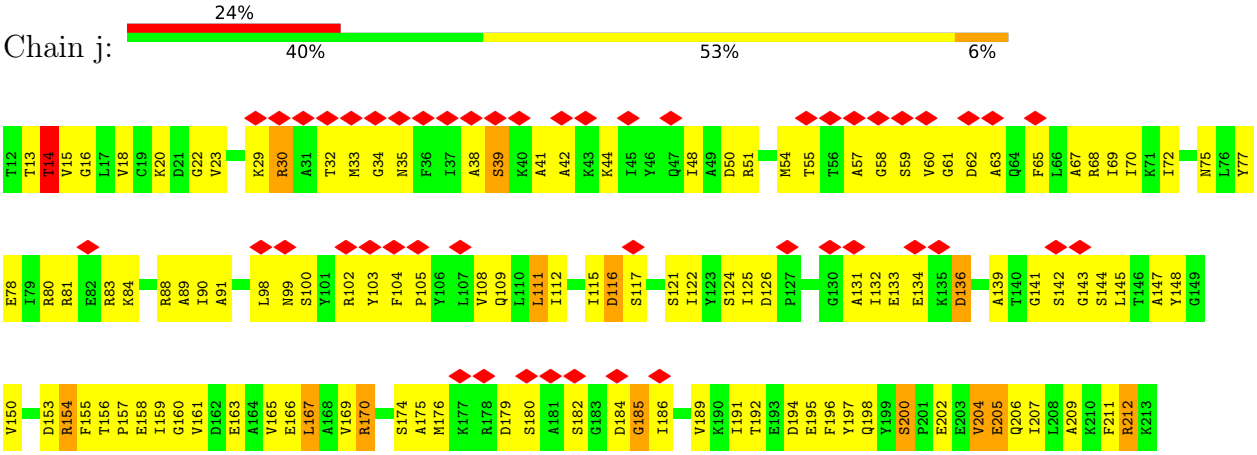
• Molecule 2: Proteasome subunit beta

Chain 3:



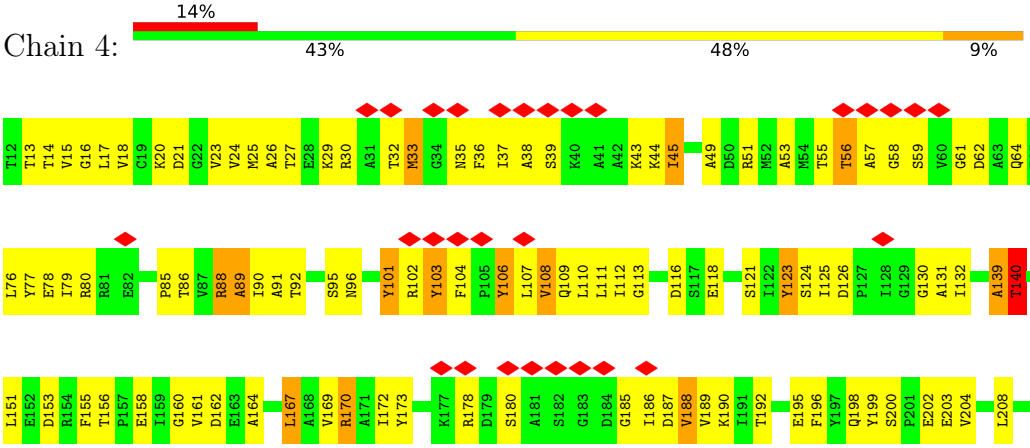
• Molecule 2: Proteasome subunit beta

Chain j:



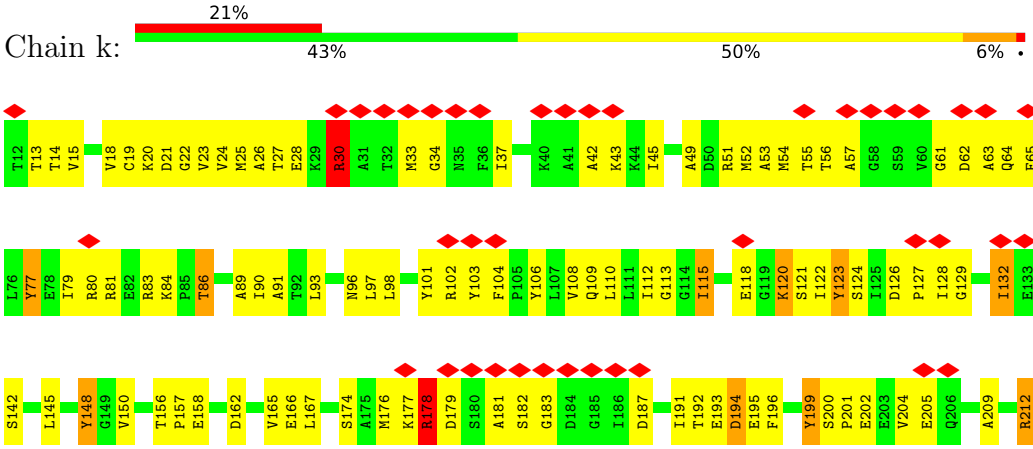
• Molecule 2: Proteasome subunit beta

Chain 4:



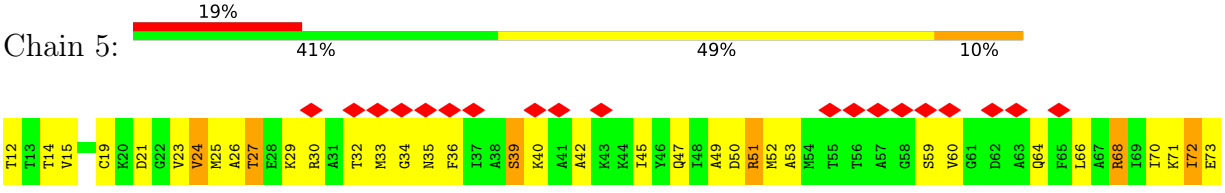
• Molecule 2: Proteasome subunit beta

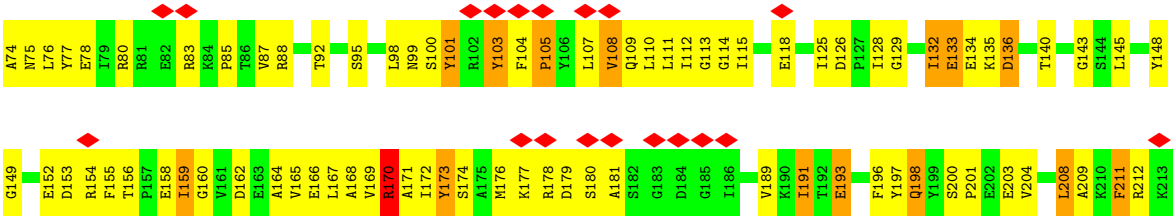
Chain k:



• Molecule 2: Proteasome subunit beta

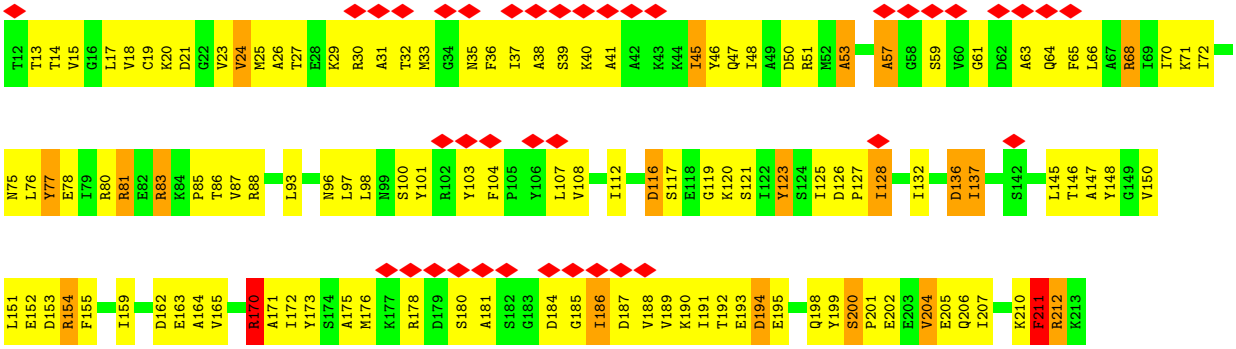
Chain 5:





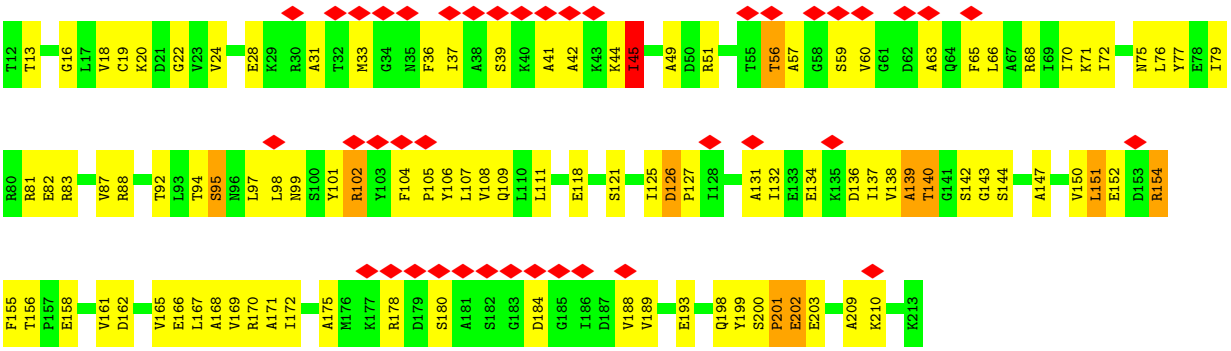
• Molecule 2: Proteasome subunit beta

Chain l:



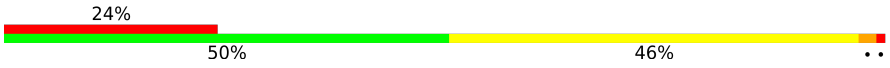
• Molecule 2: Proteasome subunit beta

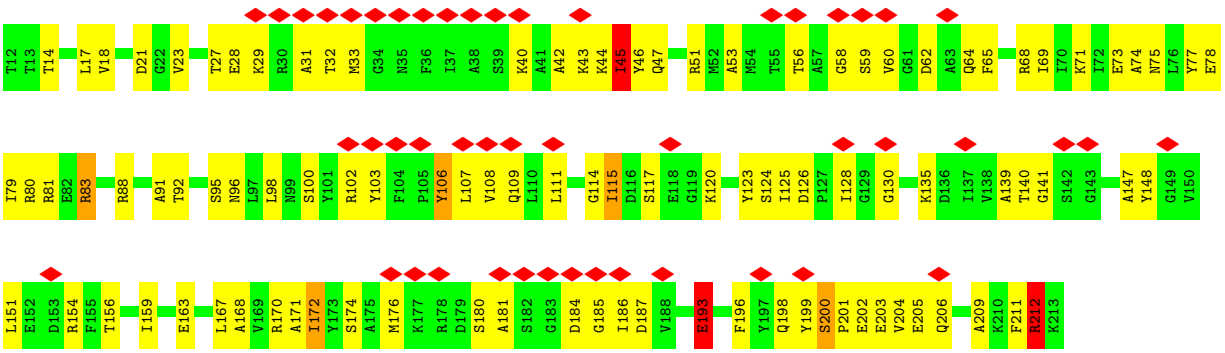
Chain 6:



• Molecule 2: Proteasome subunit beta

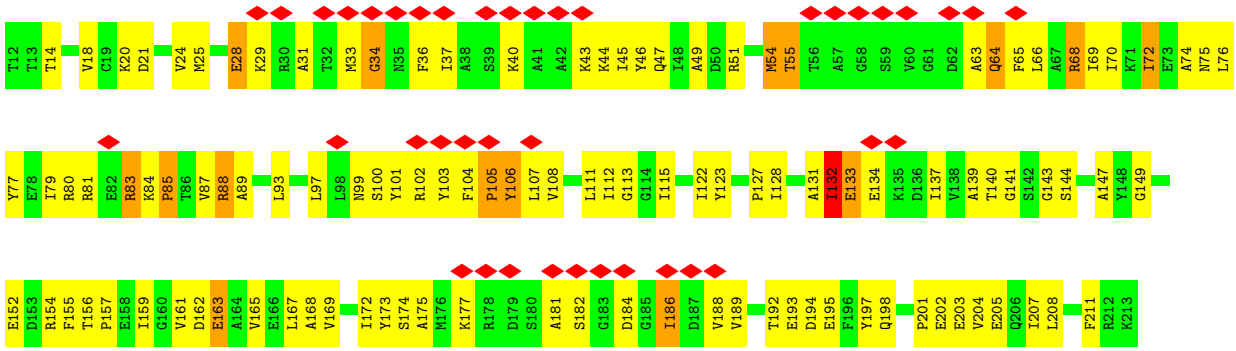
Chain m:





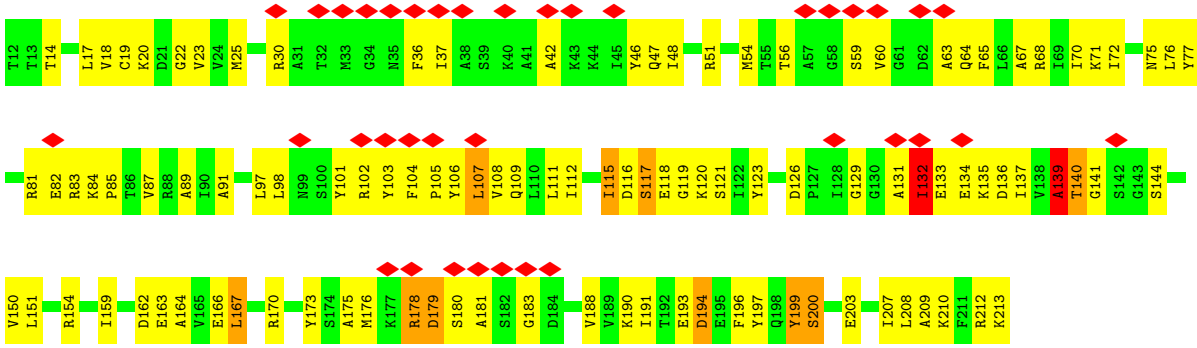
• Molecule 2: Proteasome subunit beta

Chain 7:



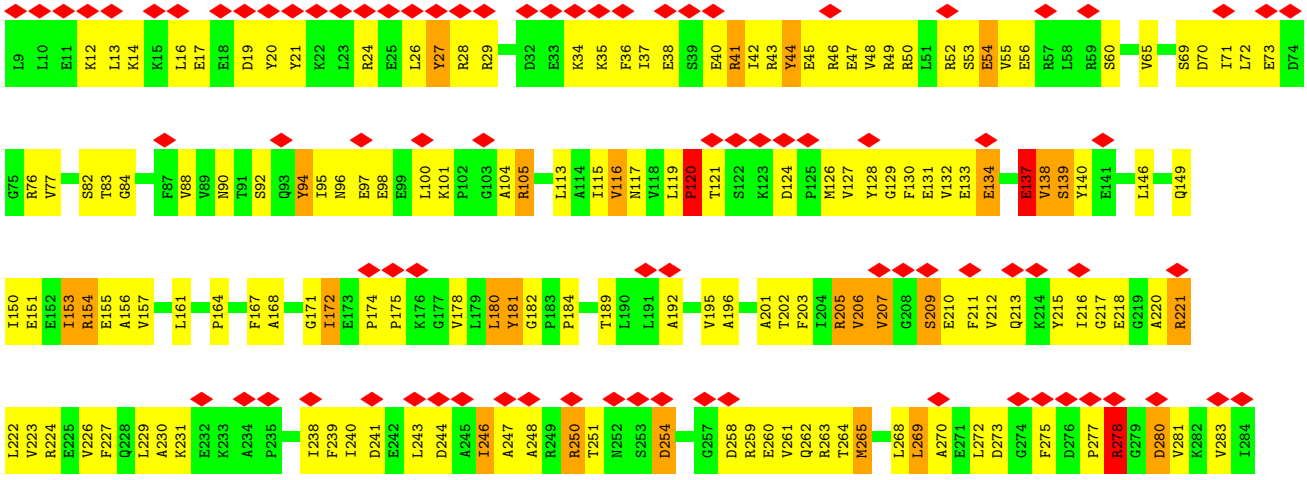
• Molecule 2: Proteasome subunit beta

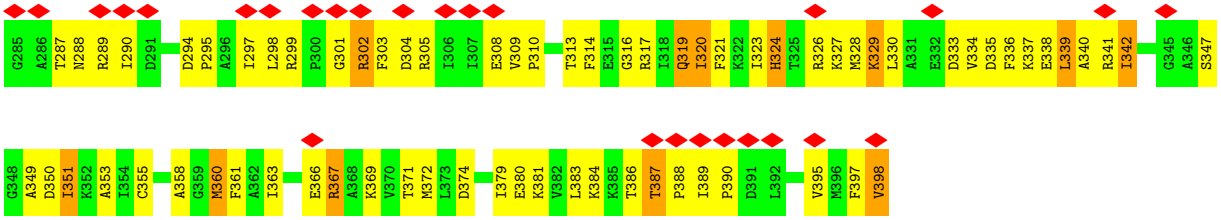
Chain n:



• Molecule 3: Proteasome-activating nucleotidase

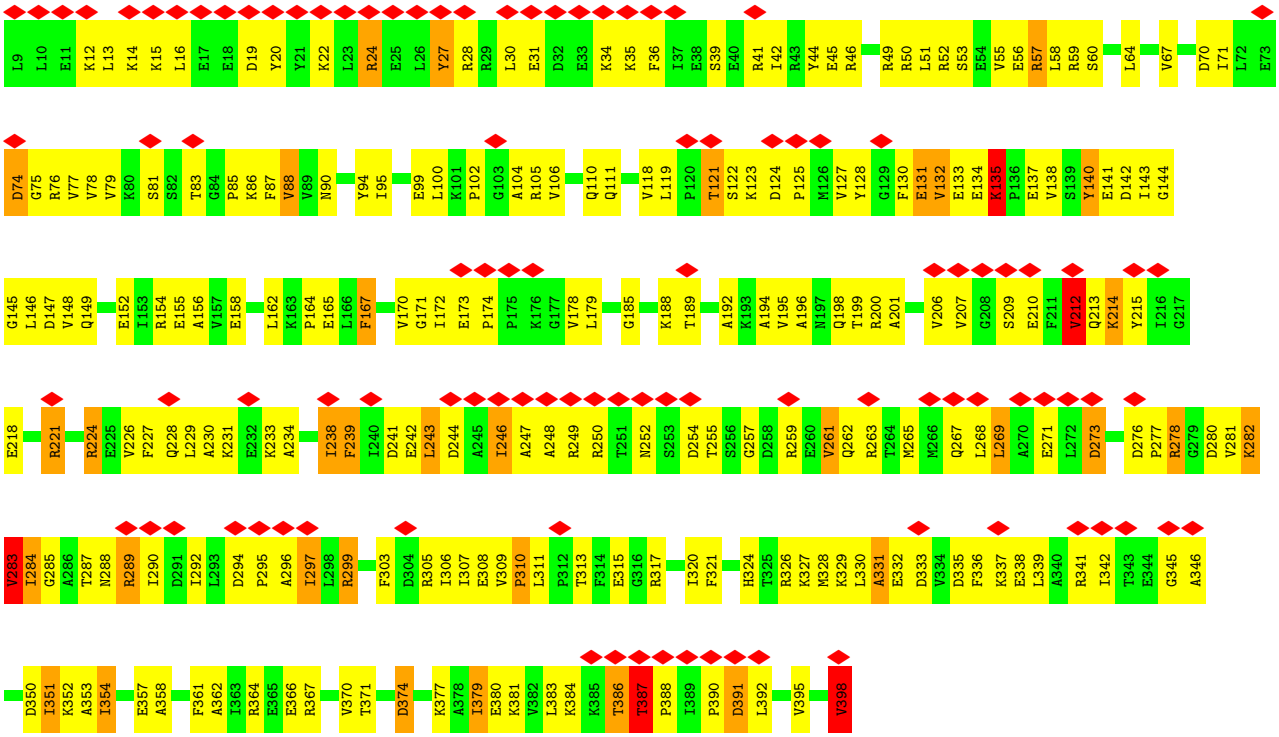
Chain H:





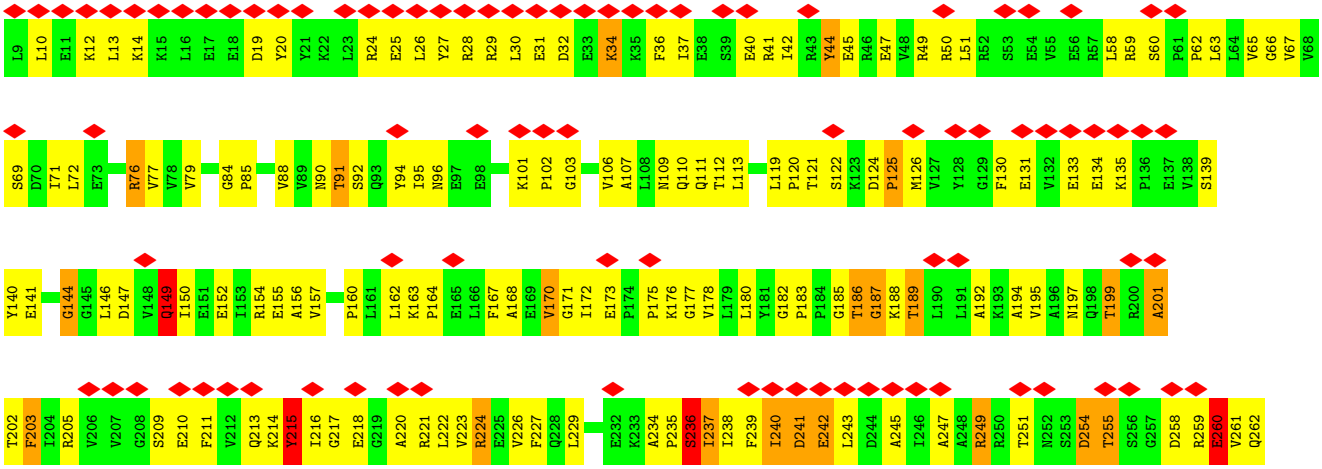
• Molecule 3: Proteasome-activating nucleotidase

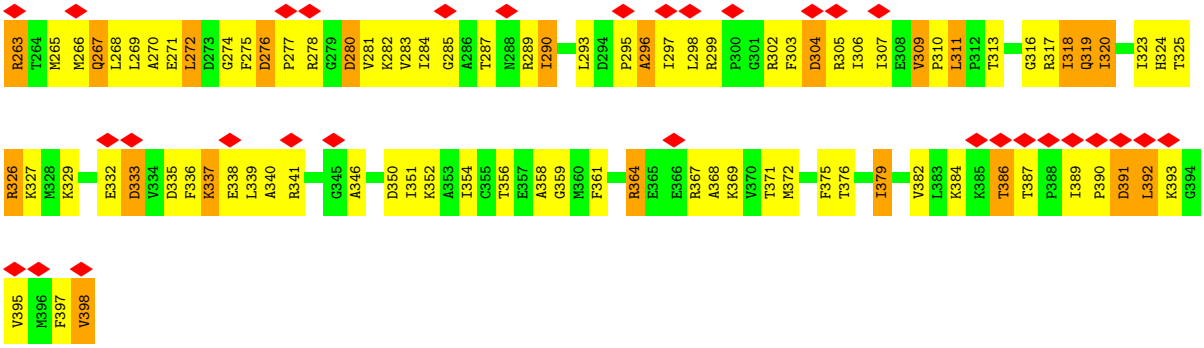
Chain I:



• Molecule 3: Proteasome-activating nucleotidase

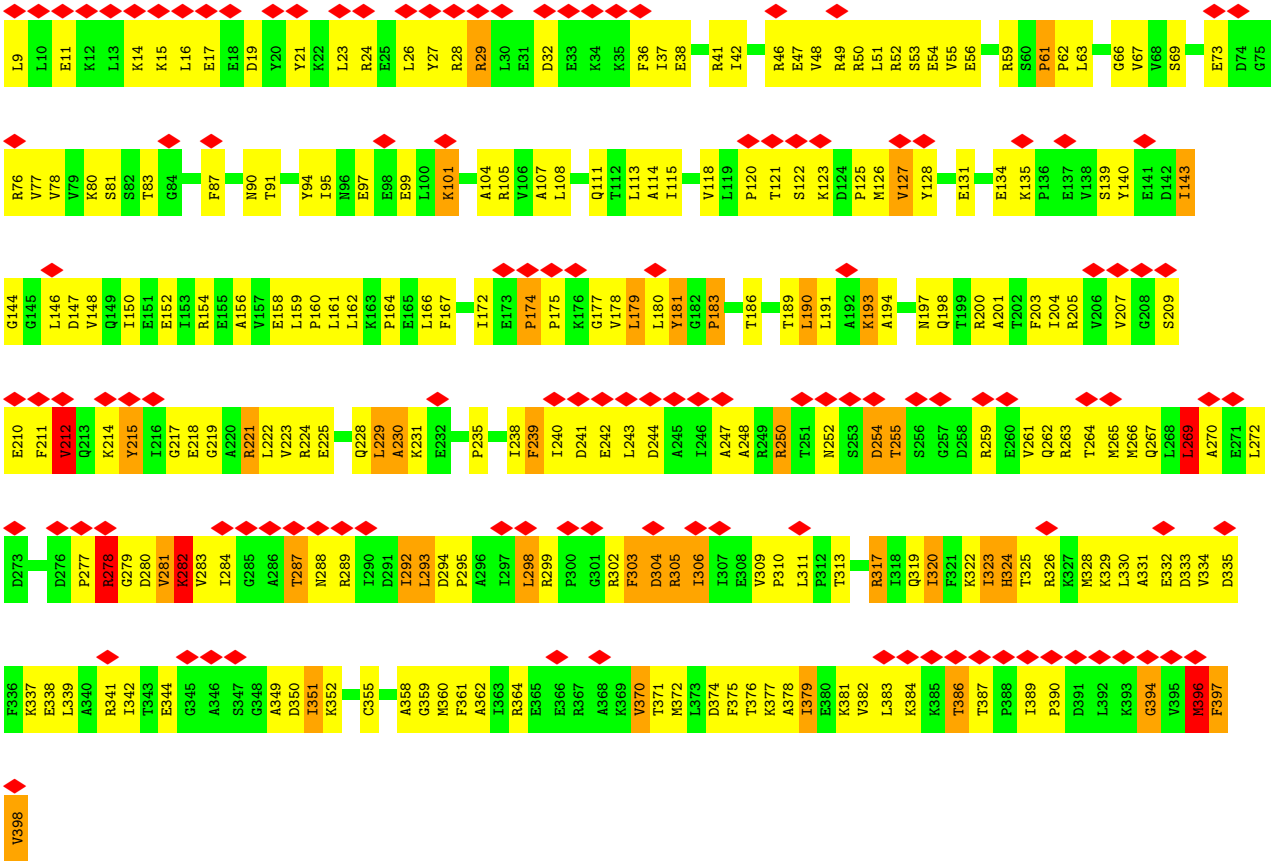
Chain K:





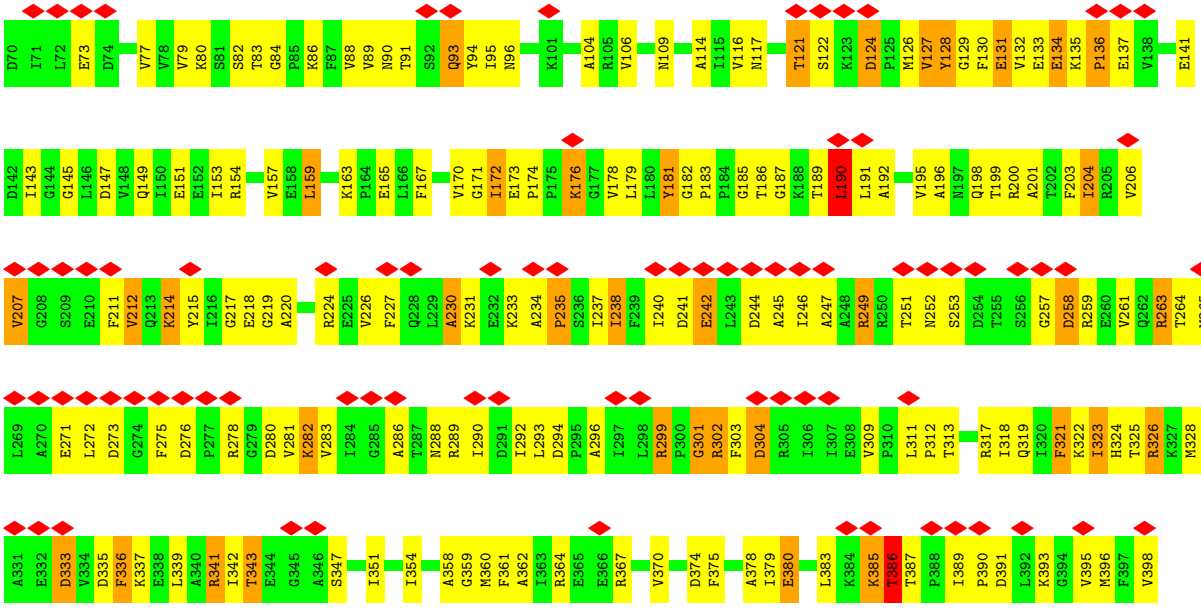
• Molecule 3: Proteasome-activating nucleotidase

Chain L:

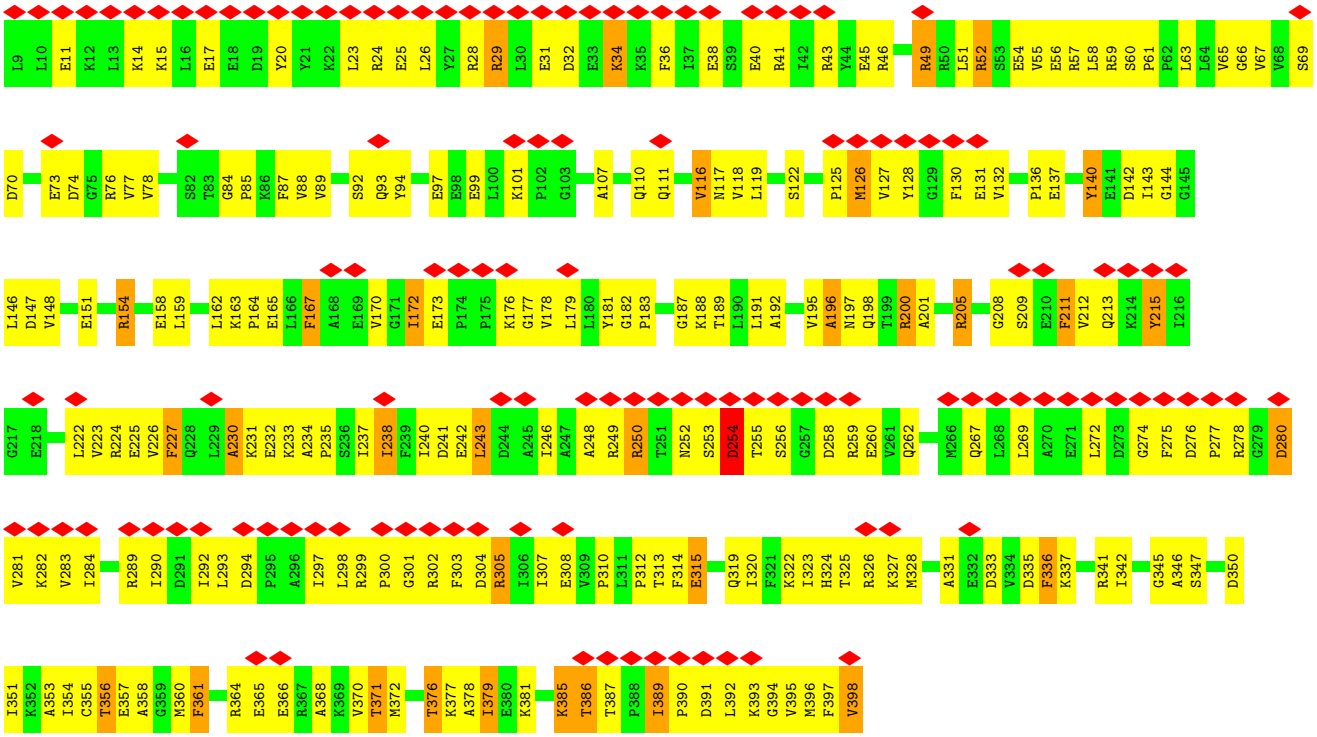


• Molecule 3: Proteasome-activating nucleotidase

Chain M:



• Molecule 3: Proteasome-activating nucleotidase



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.051	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0068	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	2.26	77/1934 (4.0%)	2.41	115/2605 (4.4%)
1	B	2.28	74/1934 (3.8%)	2.43	132/2605 (5.1%)
1	C	2.35	82/1934 (4.2%)	2.40	122/2605 (4.7%)
1	D	2.30	76/1934 (3.9%)	2.46	125/2605 (4.8%)
1	E	2.25	81/1934 (4.2%)	2.54	146/2605 (5.6%)
1	F	2.29	83/1934 (4.3%)	2.42	123/2605 (4.7%)
1	G	2.25	72/1934 (3.7%)	2.42	129/2605 (5.0%)
1	a	2.30	70/1892 (3.7%)	2.44	120/2549 (4.7%)
1	b	2.22	65/1892 (3.4%)	2.49	134/2549 (5.3%)
1	c	2.23	70/1892 (3.7%)	2.37	108/2549 (4.2%)
1	d	2.27	72/1892 (3.8%)	2.48	136/2549 (5.3%)
1	e	2.31	69/1892 (3.6%)	2.41	123/2549 (4.8%)
1	f	2.27	68/1892 (3.6%)	2.46	131/2549 (5.1%)
1	g	2.26	69/1892 (3.6%)	2.43	122/2549 (4.8%)
2	1	2.30	65/1573 (4.1%)	2.47	101/2121 (4.8%)
2	2	2.25	66/1573 (4.2%)	2.36	83/2121 (3.9%)
2	3	2.25	60/1573 (3.8%)	2.42	111/2121 (5.2%)
2	4	2.27	67/1573 (4.3%)	2.40	113/2121 (5.3%)
2	5	3.20	76/1573 (4.8%)	2.57	126/2121 (5.9%)
2	6	2.32	61/1573 (3.9%)	2.42	95/2121 (4.5%)
2	7	2.22	57/1573 (3.6%)	2.41	103/2121 (4.9%)
2	h	2.24	59/1573 (3.8%)	2.36	91/2121 (4.3%)
2	i	2.28	58/1573 (3.7%)	2.48	114/2121 (5.4%)
2	j	2.35	75/1573 (4.8%)	2.47	113/2121 (5.3%)
2	k	2.27	60/1573 (3.8%)	2.51	121/2121 (5.7%)
2	l	3.21	77/1573 (4.9%)	2.55	121/2121 (5.7%)
2	m	2.29	52/1573 (3.3%)	2.48	92/2121 (4.3%)
2	n	2.28	63/1573 (4.0%)	2.43	98/2121 (4.6%)
3	H	2.33	129/3146 (4.1%)	2.44	210/4240 (5.0%)
3	I	2.27	130/3146 (4.1%)	2.57	255/4240 (6.0%)
3	J	2.25	113/3146 (3.6%)	2.42	203/4240 (4.8%)
3	K	2.27	122/3146 (3.9%)	2.51	237/4240 (5.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	L	2.30	143/3146 (4.5%)	2.51	228/4240 (5.4%)
3	M	2.23	106/3146 (3.4%)	2.49	222/4240 (5.2%)
All	All	2.33	2667/67680 (3.9%)	2.46	4603/91212 (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	10
1	B	0	11
1	C	0	10
1	D	0	7
1	E	0	7
1	F	0	9
1	G	0	11
1	a	0	8
1	b	0	10
1	c	0	9
1	d	0	8
1	e	0	8
1	f	0	10
1	g	0	6
2	1	0	8
2	2	0	7
2	3	0	5
2	4	0	6
2	5	0	7
2	6	0	4
2	7	0	7
2	h	0	6
2	i	0	9
2	j	0	4
2	k	0	11
2	l	0	10
2	m	0	4
2	n	0	8
3	H	0	18
3	I	0	12
3	J	0	16
3	K	0	18

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	17
3	M	0	20
All	All	0	321

All (2667) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	CZ-NH1	57.24	2.12	1.32
2	5	170	ARG	CZ-NH1	56.05	2.11	1.32
2	l	211	PHE	CG-CD2	34.94	2.12	1.38
2	l	211	PHE	CG-CD1	34.00	2.10	1.38
2	5	211	PHE	CG-CD1	32.43	2.06	1.38
2	5	211	PHE	CG-CD2	31.50	2.05	1.38
2	l	211	PHE	CE1-CZ	23.31	2.08	1.38
2	5	211	PHE	CE1-CZ	23.20	2.08	1.38
2	5	211	PHE	CD2-CE2	21.84	2.04	1.38
2	l	211	PHE	CD2-CE2	21.31	2.02	1.38
2	5	211	PHE	CD1-CE1	21.25	2.02	1.38
2	5	211	PHE	CE2-CZ	20.85	2.01	1.38
2	l	211	PHE	CD1-CE1	20.20	1.99	1.38
2	l	211	PHE	CE2-CZ	19.54	1.97	1.38
1	f	105	GLU	CA-C	-12.94	1.42	1.52
3	J	293	LEU	CA-C	-12.82	1.37	1.52
3	J	398	VAL	C-O	-11.58	1.00	1.23
3	I	398	VAL	C-O	-11.56	1.00	1.23
3	L	398	VAL	C-O	-11.56	1.00	1.23
3	M	398	VAL	C-O	-11.56	1.00	1.23
3	H	398	VAL	C-OXT	-11.55	1.00	1.23
3	I	398	VAL	C-OXT	-11.55	1.00	1.23
3	M	398	VAL	C-OXT	-11.54	1.00	1.23
3	L	398	VAL	C-OXT	-11.54	1.00	1.23
3	K	398	VAL	C-OXT	-11.53	1.00	1.23
3	H	398	VAL	C-O	-11.53	1.00	1.23
3	K	398	VAL	C-O	-11.53	1.00	1.23
3	J	398	VAL	C-OXT	-11.53	1.00	1.23
2	5	159	ILE	CA-C	-11.32	1.38	1.52
2	l	41	ALA	CA-C	-11.29	1.43	1.52
2	5	178	ARG	NE-CZ	11.08	1.45	1.33
3	H	340	ALA	N-CA	-11.04	1.32	1.46
2	6	104	PHE	N-CA	-10.94	1.36	1.46
1	c	78	THR	CA-C	-10.53	1.40	1.52
1	C	148	TYR	CA-C	-10.47	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	341	ARG	NE-CZ	10.38	1.44	1.33
3	H	105	ARG	NE-CZ	10.32	1.44	1.33
1	A	47	ILE	CA-C	-10.27	1.40	1.52
1	a	94	ILE	C-N	10.26	1.47	1.33
2	5	100	SER	CA-C	-10.11	1.39	1.52
1	D	212	GLY	CA-C	-10.11	1.43	1.51
2	5	21	ASP	N-CA	-10.07	1.37	1.46
3	I	299	ARG	NE-CZ	10.05	1.44	1.33
3	K	126	MET	C-N	9.86	1.43	1.33
2	6	156	THR	CA-C	-9.85	1.42	1.52
3	M	247	ALA	CA-C	-9.84	1.40	1.52
1	c	21	LEU	CA-C	-9.77	1.40	1.52
1	F	168	ARG	CD-NE	9.68	1.59	1.46
1	D	71	ASP	CA-C	-9.66	1.41	1.52
2	3	113	GLY	CA-C	-9.62	1.41	1.51
1	C	222	LYS	CA-C	-9.60	1.40	1.52
1	b	20	ARG	NE-CZ	9.57	1.43	1.33
2	j	158	GLU	CA-C	-9.53	1.43	1.53
1	a	241	ARG	N-CA	-9.34	1.35	1.46
2	n	81	ARG	NE-CZ	9.30	1.43	1.33
1	G	21	LEU	CA-C	-9.30	1.41	1.52
1	A	197	GLY	CA-C	-9.29	1.41	1.52
2	3	148	TYR	CA-C	-9.29	1.40	1.52
1	e	148	TYR	CA-C	-9.28	1.41	1.52
1	c	42	CYS	CA-CB	9.28	1.67	1.53
1	d	163	ALA	CA-C	-9.26	1.41	1.52
3	J	262	GLN	CA-C	-9.22	1.40	1.52
2	5	212	ARG	CD-NE	9.18	1.59	1.46
1	A	175	PHE	CA-C	-9.17	1.40	1.52
2	5	12	THR	C-N	9.14	1.44	1.33
1	C	169	ASN	CA-C	-9.13	1.41	1.52
2	5	177	LYS	CA-C	-9.09	1.41	1.52
1	b	161	ALA	CA-C	-9.07	1.40	1.52
1	G	91	ARG	NE-CZ	9.06	1.43	1.33
2	l	51	ARG	NE-CZ	9.03	1.43	1.33
1	f	130	ARG	CD-NE	9.02	1.58	1.46
2	i	83	ARG	CD-NE	9.01	1.58	1.46
3	I	49	ARG	NE-CZ	9.00	1.43	1.33
1	A	177	LYS	CA-C	-9.00	1.41	1.53
1	c	69	LYS	N-CA	-8.99	1.35	1.46
3	H	301	GLY	CA-C	-8.97	1.39	1.51
3	I	132	VAL	CA-CB	-8.96	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	20	ARG	CA-C	-8.95	1.41	1.52
1	F	44	GLU	C-N	8.92	1.42	1.32
1	b	186	ASP	CA-CB	8.89	1.67	1.53
1	G	73	HIS	CA-C	-8.89	1.40	1.52
2	5	126	ASP	C-N	-8.88	1.26	1.33
1	G	144	VAL	CA-C	8.84	1.58	1.52
2	n	59	SER	C-N	8.84	1.45	1.33
2	7	132	ILE	CA-C	-8.83	1.42	1.52
1	d	53	ARG	CD-NE	8.83	1.58	1.46
3	K	112	THR	N-CA	-8.82	1.36	1.46
1	B	73	HIS	ND1-CE1	8.78	1.41	1.32
2	7	49	ALA	CA-C	-8.74	1.42	1.52
1	C	82	VAL	CA-C	-8.74	1.41	1.52
3	H	46	ARG	NE-CZ	8.73	1.42	1.33
2	1	178	ARG	NE-CZ	8.69	1.42	1.33
2	1	153	ASP	CA-C	-8.67	1.41	1.52
1	f	61	ALA	CA-C	-8.67	1.43	1.53
2	k	28	GLU	CA-C	-8.67	1.42	1.52
3	I	148	VAL	CA-C	8.67	1.64	1.52
2	1	88	ARG	CD-NE	8.65	1.58	1.46
1	B	67	ILE	CA-C	-8.63	1.41	1.52
1	F	11	ALA	CA-C	-8.63	1.41	1.52
1	f	191	LEU	C-N	8.62	1.44	1.34
2	n	56	THR	N-CA	-8.60	1.35	1.46
3	L	371	THR	CA-C	-8.58	1.42	1.52
2	4	107	LEU	CA-C	-8.57	1.44	1.53
1	g	225	SER	CA-CB	8.54	1.67	1.53
3	H	124	ASP	CA-CB	8.54	1.66	1.54
3	K	289	ARG	CD-NE	8.54	1.58	1.46
1	f	139	ALA	CA-C	-8.52	1.42	1.52
1	f	111	GLU	CA-C	-8.51	1.41	1.52
1	C	230	LYS	CA-C	-8.50	1.42	1.52
2	h	104	PHE	C-N	8.49	1.44	1.33
1	F	20	ARG	NE-CZ	8.43	1.42	1.33
3	L	78	VAL	CA-C	-8.42	1.42	1.52
2	m	58	GLY	CA-C	-8.42	1.41	1.52
1	b	45	GLY	CA-C	-8.41	1.43	1.52
3	K	266	MET	CA-C	-8.38	1.41	1.52
2	m	83	ARG	N-CA	-8.37	1.35	1.46
3	L	376	THR	C-N	8.36	1.45	1.33
1	g	22	PHE	CA-C	-8.36	1.41	1.52
2	i	96	ASN	CA-C	-8.35	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	108	VAL	CA-C	-8.35	1.42	1.52
1	e	162	THR	CA-C	-8.34	1.42	1.52
1	d	33	ARG	C-N	8.34	1.43	1.32
1	a	210	GLU	CA-C	-8.34	1.42	1.52
3	H	244	ASP	CA-C	8.34	1.63	1.52
1	d	161	ALA	C-N	8.32	1.44	1.33
2	5	30	ARG	CA-C	-8.32	1.43	1.52
3	L	278	ARG	NE-CZ	8.32	1.42	1.33
2	l	155	PHE	C-N	8.31	1.42	1.33
2	4	123	TYR	CA-C	-8.31	1.42	1.52
2	m	196	PHE	CA-C	-8.28	1.42	1.53
1	C	144	VAL	C-O	8.27	1.30	1.24
2	h	88	ARG	NE-CZ	8.27	1.42	1.33
2	1	172	ILE	N-CA	8.24	1.57	1.46
3	M	324	HIS	ND1-CE1	8.23	1.40	1.32
2	5	33	MET	CA-CB	8.22	1.66	1.54
2	l	178	ARG	CA-C	-8.21	1.40	1.52
1	F	208	ASN	N-CA	-8.21	1.39	1.46
2	m	71	LYS	CA-C	-8.20	1.42	1.52
2	5	140	THR	CA-C	-8.19	1.42	1.52
1	E	10	ARG	NE-CZ	8.17	1.42	1.33
2	n	42	ALA	CA-C	8.16	1.62	1.52
2	7	122	ILE	CA-C	-8.16	1.43	1.52
2	i	179	ASP	CA-C	-8.15	1.42	1.52
2	j	38	ALA	C-N	8.14	1.43	1.33
1	C	33	ARG	CD-NE	8.13	1.57	1.46
3	H	265	MET	CA-CB	8.13	1.66	1.53
2	4	180	SER	N-CA	-8.12	1.36	1.46
2	n	104	PHE	CA-CB	8.11	1.64	1.53
1	f	86	ARG	N-CA	-8.10	1.36	1.46
2	i	27	THR	C-N	8.10	1.45	1.33
1	B	91	ARG	NE-CZ	8.09	1.42	1.33
2	k	73	GLU	N-CA	-8.07	1.36	1.46
1	B	106	PRO	CA-C	8.06	1.62	1.52
1	c	208	ASN	CA-C	8.06	1.62	1.53
1	F	10	ARG	CD-NE	8.06	1.57	1.46
3	H	263	ARG	CD-NE	8.05	1.57	1.46
1	c	192	GLY	N-CA	8.04	1.55	1.45
1	G	96	ALA	CA-C	-8.04	1.42	1.52
1	a	236	ALA	CA-CB	8.03	1.65	1.53
2	3	68	ARG	NE-CZ	8.03	1.41	1.33
1	b	143	GLU	C-N	8.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	65	GLU	N-CA	-7.99	1.35	1.46
3	J	66	GLY	N-CA	-7.97	1.36	1.45
3	J	364	ARG	CD-NE	7.97	1.57	1.46
2	j	50	ASP	C-N	7.94	1.46	1.33
2	6	102	ARG	CD-NE	7.93	1.57	1.46
2	m	42	ALA	CA-C	-7.93	1.43	1.52
1	C	147	LEU	CA-C	-7.92	1.44	1.52
3	J	230	ALA	C-N	7.92	1.44	1.33
2	4	212	ARG	CD-NE	7.92	1.57	1.46
3	M	207	VAL	CA-CB	-7.92	1.43	1.55
1	E	164	ILE	CA-C	-7.91	1.44	1.52
2	5	24	VAL	CA-C	-7.91	1.43	1.52
1	B	148	TYR	CA-C	-7.89	1.42	1.52
2	1	137	ILE	C-N	7.89	1.41	1.33
1	c	86	ARG	CA-C	-7.88	1.42	1.52
2	7	113	GLY	N-CA	-7.88	1.37	1.45
2	k	204	VAL	N-CA	-7.87	1.37	1.46
1	E	235	ARG	NE-CZ	7.87	1.41	1.33
3	M	29	ARG	NE-CZ	7.87	1.41	1.33
3	I	309	VAL	CA-C	7.87	1.61	1.52
1	a	236	ALA	N-CA	-7.86	1.37	1.46
1	f	28	ARG	NE-CZ	7.85	1.41	1.33
3	K	289	ARG	NE-CZ	7.84	1.41	1.33
2	m	68	ARG	CA-C	-7.84	1.42	1.52
1	C	149	GLU	CA-CB	7.83	1.66	1.53
1	f	239	ARG	C-N	7.83	1.43	1.33
1	d	245	LYS	C-N	7.82	1.44	1.33
3	L	200	ARG	CD-NE	7.82	1.57	1.46
1	e	45	GLY	CA-C	-7.81	1.42	1.52
1	G	68	TYR	CA-CB	7.80	1.64	1.53
2	h	18	VAL	N-CA	-7.79	1.36	1.46
2	m	171	ALA	CA-C	-7.77	1.43	1.52
2	5	115	ILE	N-CA	-7.76	1.37	1.46
3	K	310	PRO	CA-C	-7.76	1.43	1.52
1	d	64	ILE	CA-C	-7.76	1.43	1.52
3	L	263	ARG	NE-CZ	7.75	1.41	1.33
2	i	102	ARG	CA-C	-7.75	1.41	1.52
3	M	179	LEU	CA-CB	7.74	1.62	1.53
2	m	81	ARG	CZ-NH2	7.73	1.43	1.33
3	M	43	ARG	NE-CZ	7.73	1.41	1.33
2	7	128	ILE	CA-CB	-7.72	1.45	1.54
1	F	54	VAL	CA-C	-7.71	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	224	VAL	N-CA	-7.71	1.38	1.46
1	G	115	LYS	CA-C	-7.71	1.42	1.52
1	a	241	ARG	CD-NE	7.70	1.57	1.46
1	f	28	ARG	N-CA	-7.69	1.37	1.46
3	I	381	LYS	C-N	7.68	1.43	1.33
1	D	117	CYS	N-CA	-7.68	1.36	1.46
1	C	193	LEU	C-N	7.67	1.43	1.33
3	I	46	ARG	CZ-NH1	7.67	1.43	1.32
1	B	44	GLU	C-N	7.67	1.41	1.32
1	G	146	LYS	CA-C	-7.66	1.43	1.52
3	H	308	GLU	C-N	7.66	1.40	1.33
3	M	259	ARG	CD-NE	7.66	1.56	1.46
1	B	211	VAL	CA-C	-7.66	1.43	1.52
2	1	64	GLN	CA-C	-7.66	1.43	1.52
2	i	42	ALA	C-N	7.65	1.43	1.33
1	d	80	GLY	N-CA	7.64	1.53	1.45
1	b	180	ARG	N-CA	-7.63	1.35	1.45
1	g	91	ARG	CD-NE	7.61	1.56	1.46
2	j	198	GLN	CA-C	-7.61	1.43	1.52
3	K	221	ARG	NE-CZ	7.61	1.41	1.33
2	j	102	ARG	NE-CZ	7.61	1.41	1.33
2	l	88	ARG	NE-CZ	7.61	1.41	1.33
3	H	154	ARG	CA-C	-7.61	1.42	1.52
1	A	164	ILE	C-N	7.60	1.42	1.32
2	6	42	ALA	CA-C	-7.60	1.43	1.52
3	M	391	ASP	C-N	7.60	1.43	1.33
3	L	152	GLU	CA-CB	7.60	1.65	1.53
1	C	138	ILE	CA-C	-7.59	1.43	1.52
3	L	16	LEU	C-N	7.59	1.44	1.34
3	J	224	ARG	NE-CZ	7.59	1.41	1.33
3	K	305	ARG	CD-NE	7.58	1.56	1.46
2	k	120	LYS	CA-C	-7.58	1.43	1.52
1	C	235	ARG	CA-C	-7.58	1.43	1.52
2	i	133	GLU	N-CA	-7.58	1.37	1.46
3	H	174	PRO	N-CD	-7.57	1.37	1.47
3	H	224	ARG	CD-NE	7.57	1.56	1.46
2	l	18	VAL	CA-C	-7.57	1.44	1.52
2	2	198	GLN	CA-C	-7.56	1.43	1.52
1	C	37	ALA	CA-C	-7.55	1.43	1.52
1	e	29	GLU	CA-C	-7.54	1.42	1.52
3	L	144	GLY	CA-C	-7.54	1.41	1.51
2	k	196	PHE	CA-C	-7.54	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	GLN	N-CA	-7.54	1.37	1.46
2	n	68	ARG	CD-NE	7.54	1.56	1.46
3	L	24	ARG	CD-NE	7.54	1.56	1.46
2	h	195	GLU	CA-C	-7.53	1.43	1.52
2	i	102	ARG	CD-NE	7.52	1.56	1.46
3	M	46	ARG	CD-NE	7.52	1.56	1.46
2	5	32	THR	C-N	7.51	1.45	1.33
2	4	146	THR	CA-CB	7.51	1.65	1.53
3	H	223	VAL	CA-CB	-7.50	1.45	1.54
3	L	66	GLY	CA-C	-7.50	1.43	1.51
1	c	168	ARG	NE-CZ	7.50	1.41	1.33
1	G	186	ASP	CA-C	-7.49	1.43	1.52
1	D	239	ARG	CD-NE	7.49	1.56	1.46
2	2	25	MET	CA-C	-7.48	1.43	1.52
1	a	52	LYS	N-CA	7.48	1.55	1.46
3	K	85	PRO	CA-C	-7.48	1.44	1.53
3	K	310	PRO	N-CD	-7.48	1.37	1.47
2	n	37	ILE	CA-C	-7.48	1.44	1.52
1	a	79	SER	N-CA	-7.47	1.37	1.46
1	f	52	LYS	CA-C	-7.46	1.42	1.52
2	h	51	ARG	N-CA	-7.46	1.36	1.46
3	H	278	ARG	CD-NE	7.46	1.56	1.46
2	k	55	THR	CA-C	-7.46	1.43	1.52
3	H	157	VAL	C-N	7.46	1.43	1.33
1	d	211	VAL	C-N	7.45	1.41	1.33
1	e	83	ALA	N-CA	-7.45	1.37	1.46
2	i	189	VAL	CA-C	-7.45	1.43	1.52
3	H	50	ARG	NE-CZ	7.45	1.41	1.33
2	j	157	PRO	C-N	7.45	1.43	1.33
3	H	156	ALA	C-N	7.45	1.43	1.33
3	K	178	VAL	N-CA	-7.45	1.37	1.46
3	M	303	PHE	CA-C	-7.45	1.42	1.52
1	f	226	PRO	N-CA	7.45	1.57	1.47
2	h	70	ILE	CA-CB	-7.44	1.45	1.54
3	I	250	ARG	CD-NE	7.44	1.56	1.46
1	F	168	ARG	NE-CZ	7.44	1.41	1.33
1	E	239	ARG	N-CA	-7.43	1.37	1.46
2	m	74	ALA	C-N	7.43	1.43	1.33
1	D	168	ARG	CZ-NH1	7.43	1.43	1.32
1	a	93	ARG	CA-CB	7.43	1.64	1.53
2	6	87	VAL	N-CA	7.42	1.55	1.46
2	1	52	MET	N-CA	7.42	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	118	VAL	CA-CB	-7.41	1.45	1.54
1	g	20	ARG	CA-C	-7.41	1.43	1.53
2	3	78	GLU	CA-C	-7.41	1.43	1.52
2	k	178	ARG	CZ-NH2	7.41	1.43	1.33
2	m	88	ARG	NE-CZ	7.41	1.41	1.33
2	4	62	ASP	CA-CB	7.40	1.64	1.53
2	l	71	LYS	CA-C	-7.40	1.43	1.52
3	I	44	TYR	CA-C	-7.40	1.42	1.52
2	n	18	VAL	N-CA	-7.39	1.37	1.46
1	A	30	ALA	CA-C	-7.38	1.42	1.52
1	D	95	GLU	C-N	7.38	1.43	1.33
3	L	49	ARG	N-CA	-7.38	1.37	1.46
1	a	143	GLU	C-N	7.38	1.40	1.33
1	c	229	LEU	N-CA	-7.38	1.37	1.46
3	H	180	LEU	N-CA	7.37	1.55	1.46
1	A	139	ALA	CA-C	-7.37	1.43	1.52
2	5	103	TYR	C-N	7.36	1.41	1.33
3	L	53	SER	C-N	7.35	1.43	1.33
1	e	236	ALA	C-N	7.35	1.43	1.34
1	f	212	GLY	CA-C	7.35	1.59	1.51
2	5	107	LEU	CA-C	-7.35	1.44	1.52
2	k	14	THR	CA-C	-7.34	1.43	1.52
2	h	65	PHE	CA-CB	7.33	1.65	1.53
2	2	116	ASP	CA-C	-7.31	1.43	1.52
2	4	30	ARG	NE-CZ	7.31	1.41	1.33
3	K	376	THR	N-CA	-7.31	1.37	1.46
3	L	46	ARG	NE-CZ	7.31	1.41	1.33
3	K	91	THR	C-N	7.31	1.39	1.33
3	J	49	ARG	CA-CB	7.31	1.64	1.53
1	E	193	LEU	CA-CB	7.30	1.64	1.53
1	d	130	ARG	CD-NE	7.30	1.56	1.46
2	1	203	GLU	N-CA	-7.30	1.37	1.46
1	G	94	ILE	CA-C	-7.29	1.43	1.52
1	C	68	TYR	N-CA	-7.29	1.36	1.45
1	d	199	SER	C-N	7.29	1.41	1.34
3	L	115	ILE	CA-C	-7.29	1.44	1.52
3	K	339	LEU	N-CA	-7.29	1.37	1.46
1	a	65	GLU	CA-C	-7.29	1.43	1.52
1	b	38	ILE	CA-C	-7.29	1.44	1.52
3	I	60	SER	C-N	7.29	1.42	1.33
1	D	130	ARG	CD-NE	7.27	1.56	1.46
1	B	43	LYS	CA-C	-7.26	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	GLY	CA-C	-7.26	1.44	1.52
2	1	212	ARG	NE-CZ	7.25	1.41	1.33
3	L	240	ILE	CA-C	-7.25	1.43	1.52
2	k	182	SER	CA-C	-7.25	1.43	1.52
2	n	83	ARG	CD-NE	7.25	1.56	1.46
3	J	346	ALA	C-N	7.24	1.43	1.33
3	L	194	ALA	N-CA	-7.24	1.37	1.46
1	A	38	ILE	N-CA	-7.24	1.37	1.46
2	1	152	GLU	CA-C	7.24	1.62	1.52
3	M	28	ARG	CZ-NH1	7.24	1.42	1.32
2	4	155	PHE	CA-CB	7.23	1.62	1.53
2	h	80	ARG	CZ-NH2	7.23	1.42	1.33
1	F	10	ARG	CZ-NH1	7.22	1.42	1.32
1	e	53	ARG	CA-CB	7.22	1.65	1.53
1	a	75	CYS	CA-C	-7.21	1.43	1.52
2	i	193	GLU	CA-C	-7.21	1.43	1.52
2	l	173	TYR	CA-C	7.21	1.62	1.52
2	m	154	ARG	CD-NE	7.21	1.56	1.46
3	K	177	GLY	CA-C	-7.20	1.43	1.51
1	G	73	HIS	ND1-CE1	7.19	1.39	1.32
2	2	113	GLY	N-CA	-7.19	1.37	1.44
1	c	24	VAL	CA-CB	-7.19	1.44	1.54
1	g	97	GLN	C-N	7.18	1.43	1.33
1	B	13	THR	C-N	7.18	1.41	1.33
2	n	144	SER	N-CA	-7.18	1.37	1.46
2	j	48	ILE	CA-C	-7.18	1.43	1.52
1	F	218	ASP	CA-C	-7.18	1.42	1.52
3	I	171	GLY	C-N	7.17	1.43	1.33
3	K	147	ASP	C-N	7.17	1.41	1.33
1	a	43	LYS	CA-CB	7.16	1.63	1.53
1	A	168	ARG	NE-CZ	7.16	1.41	1.33
1	a	73	HIS	C-N	7.16	1.43	1.33
3	J	57	ARG	CD-NE	7.16	1.56	1.46
1	e	106	PRO	CA-C	-7.15	1.44	1.52
3	M	326	ARG	CD-NE	7.15	1.56	1.46
1	b	86	ARG	NE-CZ	7.15	1.41	1.33
2	j	100	SER	CA-CB	7.15	1.64	1.53
2	3	17	LEU	CA-C	-7.14	1.43	1.52
2	6	81	ARG	NE-CZ	7.14	1.41	1.33
2	2	101	TYR	CA-CB	7.14	1.62	1.52
3	J	29	ARG	CD-NE	7.14	1.56	1.46
2	1	68	ARG	CD-NE	7.13	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	65	PHE	CA-C	-7.13	1.43	1.52
3	I	326	ARG	NE-CZ	7.13	1.40	1.33
1	g	20	ARG	CZ-NH1	7.13	1.42	1.32
3	I	56	GLU	N-CA	-7.13	1.37	1.46
2	2	209	ALA	C-N	7.12	1.44	1.33
1	a	205	VAL	CA-C	-7.12	1.45	1.52
3	K	310	PRO	N-CA	-7.11	1.38	1.47
2	i	190	LYS	CA-C	-7.11	1.44	1.52
2	k	81	ARG	NE-CZ	7.11	1.40	1.33
2	5	19	CYS	CA-CB	7.11	1.64	1.53
2	6	24	VAL	CA-CB	-7.11	1.45	1.54
2	6	60	VAL	N-CA	-7.11	1.38	1.46
2	j	16	GLY	C-N	7.10	1.43	1.33
3	I	246	ILE	CA-C	-7.10	1.43	1.52
1	A	141	VAL	CA-C	-7.10	1.43	1.52
2	7	68	ARG	NE-CZ	7.09	1.40	1.33
1	a	125	GLN	CA-C	-7.09	1.43	1.52
2	3	154	ARG	NE-CZ	7.09	1.40	1.33
1	C	145	PRO	CA-CB	7.08	1.62	1.53
1	F	79	SER	C-N	7.08	1.41	1.33
1	g	153	SER	CA-C	-7.08	1.43	1.52
3	K	119	LEU	CA-C	-7.08	1.43	1.52
3	M	106	VAL	CA-C	-7.07	1.44	1.52
1	c	119	PHE	CA-CB	7.07	1.64	1.53
1	D	48	LEU	CA-C	-7.07	1.44	1.52
1	D	61	ALA	CA-C	-7.07	1.42	1.52
2	n	121	SER	C-N	7.07	1.42	1.33
1	d	210	GLU	N-CA	-7.07	1.37	1.46
2	l	93	LEU	CA-C	-7.06	1.43	1.52
3	J	331	ALA	CA-C	-7.06	1.44	1.53
2	k	30	ARG	NE-CZ	7.05	1.40	1.33
1	f	109	VAL	C-O	-7.05	1.16	1.24
1	G	108	THR	N-CA	-7.05	1.37	1.45
2	m	115	ILE	N-CA	-7.05	1.37	1.46
2	6	178	ARG	CD-NE	7.05	1.56	1.46
1	E	174	PHE	CA-CB	7.05	1.64	1.53
3	H	43	ARG	NE-CZ	7.04	1.40	1.33
2	k	24	VAL	CA-CB	-7.03	1.45	1.54
2	l	147	ALA	N-CA	7.03	1.55	1.46
1	g	149	GLU	CA-C	-7.03	1.44	1.52
2	j	60	VAL	N-CA	-7.03	1.38	1.46
3	L	190	LEU	C-N	7.02	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	81	ARG	NE-CZ	7.02	1.40	1.33
1	E	230	LYS	CA-CB	7.01	1.62	1.53
2	j	70	ILE	N-CA	-7.00	1.38	1.46
3	L	105	ARG	CD-NE	7.00	1.56	1.46
3	M	271	GLU	C-N	7.00	1.43	1.33
2	2	170	ARG	NE-CZ	7.00	1.40	1.33
1	B	239	ARG	NE-CZ	6.99	1.40	1.33
3	L	317	ARG	CA-C	-6.99	1.43	1.52
2	6	37	ILE	N-CA	-6.99	1.38	1.46
1	G	129	VAL	C-N	6.99	1.43	1.33
1	a	223	GLU	CA-CB	6.99	1.62	1.53
2	2	206	GLN	C-N	6.98	1.42	1.33
2	n	203	GLU	CA-CB	6.98	1.64	1.53
3	I	201	ALA	C-N	6.98	1.42	1.33
3	M	244	ASP	CA-C	-6.98	1.43	1.52
2	5	172	ILE	CA-CB	6.98	1.63	1.54
3	I	195	VAL	C-N	6.98	1.43	1.33
3	L	299	ARG	NE-CZ	6.98	1.40	1.33
3	K	283	VAL	CA-C	-6.97	1.44	1.52
1	B	209	ILE	C-N	6.97	1.43	1.33
2	6	107	LEU	CA-C	-6.97	1.44	1.52
3	M	389	ILE	CA-C	-6.97	1.46	1.52
2	5	211	PHE	CA-C	-6.96	1.43	1.52
3	H	29	ARG	NE-CZ	6.96	1.40	1.33
3	K	152	GLU	C-N	6.96	1.42	1.33
3	J	127	VAL	CA-C	-6.96	1.44	1.52
1	g	63	THR	C-N	6.96	1.41	1.33
3	L	264	THR	CA-C	-6.95	1.43	1.52
1	C	139	ALA	CA-C	-6.94	1.44	1.52
1	B	59	LEU	CA-C	-6.94	1.44	1.52
3	K	19	ASP	CA-CB	6.94	1.64	1.53
1	F	18	ASP	C-N	6.93	1.44	1.33
3	M	50	ARG	CZ-NH2	6.93	1.42	1.33
2	i	61	GLY	CA-C	-6.93	1.44	1.51
1	D	14	VAL	CA-CB	-6.93	1.46	1.54
3	L	317	ARG	C-N	6.92	1.42	1.33
3	L	362	ALA	CA-C	-6.92	1.43	1.52
3	J	371	THR	CA-C	-6.92	1.45	1.53
1	d	138	ILE	CA-CB	6.92	1.61	1.53
2	i	54	MET	C-N	6.92	1.42	1.33
1	E	239	ARG	NE-CZ	6.91	1.40	1.33
2	m	154	ARG	C-N	6.91	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	ALA	CA-CB	6.91	1.64	1.53
3	K	71	ILE	N-CA	-6.91	1.38	1.46
1	F	193	LEU	C-N	6.91	1.42	1.33
1	F	28	ARG	NE-CZ	6.91	1.40	1.33
2	2	107	LEU	C-O	6.91	1.31	1.24
3	L	46	ARG	CD-NE	6.91	1.55	1.46
1	F	138	ILE	N-CA	-6.90	1.37	1.46
2	7	18	VAL	CA-C	-6.90	1.43	1.52
1	G	20	ARG	NE-CZ	6.89	1.40	1.33
2	l	81	ARG	CZ-NH1	6.89	1.42	1.32
1	B	20	ARG	NE-CZ	6.88	1.40	1.33
1	f	88	LEU	CA-CB	6.88	1.64	1.53
1	C	53	ARG	CZ-NH2	6.88	1.42	1.33
2	k	115	ILE	N-CA	-6.88	1.38	1.46
2	m	120	LYS	CA-C	-6.88	1.44	1.52
2	7	29	LYS	CA-CB	6.88	1.64	1.53
3	K	262	GLN	CA-C	-6.88	1.43	1.52
3	J	341	ARG	NE-CZ	6.88	1.40	1.33
1	c	235	ARG	NE-CZ	6.87	1.40	1.33
1	c	149	GLU	CA-C	-6.87	1.44	1.52
2	j	39	SER	CA-C	-6.87	1.44	1.52
1	c	32	LYS	C-N	6.86	1.42	1.33
1	c	96	ALA	CA-C	-6.86	1.44	1.52
1	G	188	ALA	C-N	6.86	1.42	1.33
2	l	148	TYR	CA-C	6.86	1.61	1.52
1	F	196	MET	CA-CB	6.85	1.64	1.53
2	7	44	LYS	N-CA	-6.85	1.36	1.45
1	a	41	LYS	N-CA	-6.84	1.37	1.46
3	M	299	ARG	CA-C	6.84	1.60	1.53
3	M	360	MET	N-CA	-6.84	1.38	1.46
1	D	63	THR	CA-C	-6.84	1.44	1.52
3	K	260	GLU	C-N	6.84	1.42	1.33
1	D	116	ILE	CA-C	6.84	1.62	1.52
3	M	203	PHE	CA-C	-6.83	1.44	1.52
1	B	42	CYS	C-N	6.82	1.43	1.33
2	j	75	ASN	CA-CB	6.82	1.64	1.53
3	M	82	SER	CA-CB	6.82	1.64	1.53
3	M	249	ARG	CA-CB	6.82	1.65	1.53
1	D	239	ARG	NE-CZ	6.82	1.40	1.33
3	L	303	PHE	CA-C	-6.81	1.46	1.53
2	h	68	ARG	CD-NE	6.81	1.55	1.46
1	d	33	ARG	NE-CZ	6.80	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	100	LEU	CA-C	-6.80	1.44	1.52
1	C	179	TYR	C-N	6.80	1.42	1.33
2	j	103	TYR	CA-CB	6.79	1.64	1.53
1	D	153	SER	N-CA	-6.79	1.38	1.46
2	7	34	GLY	CA-C	-6.79	1.42	1.51
2	m	147	ALA	C-N	6.79	1.43	1.34
1	b	16	SER	C-N	6.79	1.41	1.34
3	H	97	GLU	C-N	6.79	1.42	1.33
1	F	241	ARG	NE-CZ	6.78	1.40	1.33
2	5	113	GLY	C-N	6.78	1.40	1.33
3	L	390	PRO	CA-C	-6.78	1.44	1.52
1	A	149	GLU	CA-C	6.78	1.60	1.52
2	2	39	SER	CA-C	-6.78	1.44	1.52
3	H	161	LEU	CA-CB	6.77	1.64	1.53
3	H	254	ASP	CA-C	-6.77	1.43	1.52
3	J	308	GLU	CA-CB	6.77	1.61	1.53
3	L	242	GLU	C-N	6.77	1.42	1.33
3	K	51	LEU	CA-C	-6.76	1.43	1.52
1	G	81	LEU	CA-CB	6.75	1.62	1.53
2	i	46	TYR	N-CA	-6.75	1.37	1.46
1	b	238	GLU	CA-CB	6.75	1.63	1.53
2	4	80	ARG	NE-CZ	6.75	1.40	1.33
2	h	131	ALA	CA-CB	6.74	1.63	1.53
1	d	194	VAL	N-CA	-6.74	1.38	1.46
2	6	39	SER	CA-C	6.74	1.60	1.52
1	c	86	ARG	CD-NE	6.74	1.55	1.46
1	d	151	ASP	CA-C	6.74	1.58	1.52
2	h	20	LYS	CA-C	-6.74	1.43	1.52
3	K	41	ARG	CA-CB	6.73	1.63	1.53
1	e	242	GLU	N-CA	-6.73	1.38	1.46
3	J	378	ALA	C-N	6.73	1.42	1.33
1	E	212	GLY	N-CA	-6.73	1.38	1.44
2	j	88	ARG	CD-NE	6.73	1.55	1.46
1	a	214	VAL	CA-CB	-6.73	1.45	1.54
2	i	90	ILE	CA-CB	-6.72	1.45	1.54
1	A	133	GLY	C-N	6.72	1.40	1.33
2	6	57	ALA	CA-C	-6.72	1.44	1.52
2	1	123	TYR	CA-C	-6.71	1.44	1.52
2	1	138	VAL	CA-CB	-6.71	1.48	1.55
1	e	66	LYS	N-CA	-6.71	1.37	1.46
2	2	212	ARG	NE-CZ	6.71	1.40	1.33
3	I	30	LEU	CA-CB	6.71	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	354	ILE	C-N	6.71	1.42	1.33
3	L	269	LEU	C-N	6.71	1.43	1.33
3	H	210	GLU	CA-CB	6.71	1.64	1.53
1	f	33	ARG	NE-CZ	6.71	1.40	1.33
3	H	281	VAL	C-N	6.70	1.42	1.33
1	D	131	PRO	C-N	6.70	1.42	1.33
3	J	233	LYS	CA-C	-6.70	1.44	1.52
2	l	212	ARG	NE-CZ	6.69	1.40	1.33
1	B	170	ALA	C-N	6.69	1.42	1.33
2	n	178	ARG	CD-NE	6.69	1.55	1.46
1	d	128	GLY	CA-C	-6.69	1.40	1.51
2	2	178	ARG	CD-NE	6.69	1.55	1.46
3	J	154	ARG	N-CA	-6.68	1.38	1.46
1	E	36	THR	C-N	6.68	1.42	1.33
1	C	57	LYS	CA-C	-6.68	1.42	1.52
2	l	50	ASP	N-CA	-6.68	1.37	1.46
2	7	85	PRO	CA-CB	6.68	1.63	1.53
2	h	56	THR	CA-C	-6.67	1.44	1.52
3	K	65	VAL	CA-C	-6.67	1.44	1.52
1	A	197	GLY	C-O	-6.67	1.16	1.23
1	F	140	GLY	CA-C	-6.67	1.43	1.51
2	l	164	ALA	CA-C	-6.67	1.44	1.52
3	I	259	ARG	CD-NE	6.67	1.55	1.46
3	J	70	ASP	C-N	6.67	1.42	1.33
2	7	173	TYR	C-N	6.66	1.42	1.33
3	H	367	ARG	CZ-NH1	6.66	1.42	1.32
3	I	329	LYS	N-CA	-6.66	1.38	1.46
3	J	87	PHE	CA-C	-6.66	1.44	1.52
1	e	151	ASP	CA-CB	6.65	1.62	1.54
3	L	329	LYS	N-CA	-6.65	1.37	1.46
3	L	49	ARG	CD-NE	6.65	1.55	1.46
1	D	83	ALA	CA-C	-6.64	1.44	1.52
1	D	105	GLU	CA-C	6.64	1.59	1.52
1	A	230	LYS	CA-C	-6.64	1.44	1.52
1	B	90	ASP	CA-C	-6.63	1.44	1.52
1	B	141	VAL	N-CA	-6.63	1.36	1.46
3	K	49	ARG	NE-CZ	6.63	1.40	1.33
2	2	60	VAL	CA-C	-6.63	1.44	1.52
3	J	97	GLU	C-N	6.63	1.43	1.34
2	3	178	ARG	CD-NE	6.62	1.55	1.46
2	3	196	PHE	N-CA	-6.62	1.38	1.46
1	A	136	LEU	N-CA	-6.62	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	201	PRO	C-N	6.62	1.42	1.33
2	2	181	ALA	C-N	6.62	1.43	1.33
2	m	187	ASP	CA-C	-6.62	1.44	1.52
3	K	318	ILE	N-CA	-6.61	1.38	1.46
2	2	183	GLY	CA-C	6.61	1.61	1.51
3	M	39	SER	CA-CB	6.61	1.63	1.53
3	M	211	PHE	C-N	6.61	1.42	1.33
3	J	200	ARG	CZ-NH2	6.61	1.42	1.33
2	h	199	TYR	N-CA	-6.61	1.37	1.46
3	H	105	ARG	N-CA	-6.61	1.37	1.46
2	h	154	ARG	N-CA	6.60	1.54	1.46
3	K	195	VAL	CA-C	-6.60	1.44	1.52
3	M	276	ASP	C-N	6.60	1.41	1.33
1	a	89	ILE	C-N	6.59	1.42	1.33
1	C	168	ARG	NE-CZ	6.59	1.40	1.33
1	A	53	ARG	C-N	6.59	1.39	1.33
1	c	42	CYS	CA-C	-6.59	1.44	1.52
3	I	118	VAL	C-O	-6.59	1.17	1.24
3	H	164	PRO	N-CA	-6.59	1.38	1.47
2	5	85	PRO	CA-C	-6.59	1.46	1.53
2	n	111	LEU	N-CA	-6.59	1.38	1.46
2	6	171	ALA	CA-C	-6.58	1.44	1.52
3	I	332	GLU	CA-CB	6.58	1.62	1.53
1	D	162	THR	CA-CB	6.58	1.63	1.53
1	F	130	ARG	CZ-NH1	6.58	1.42	1.32
3	M	268	LEU	CA-C	-6.58	1.44	1.52
2	2	126	ASP	C-N	6.58	1.41	1.34
2	6	83	ARG	NE-CZ	6.58	1.40	1.33
3	H	60	SER	CA-CB	6.58	1.62	1.53
1	b	201	GLU	CA-C	-6.57	1.45	1.53
3	M	302	ARG	NE-CZ	6.57	1.40	1.33
1	f	205	VAL	CA-CB	-6.57	1.48	1.54
2	i	180	SER	CA-C	-6.57	1.43	1.52
2	i	12	THR	N-CA	6.56	1.58	1.46
1	A	207	GLU	CA-C	-6.56	1.44	1.52
2	3	189	VAL	N-CA	-6.56	1.38	1.46
2	k	56	THR	C-N	6.56	1.42	1.33
2	m	56	THR	CA-C	-6.55	1.44	1.52
1	f	235	ARG	NE-CZ	6.55	1.40	1.33
2	3	183	GLY	CA-C	-6.54	1.42	1.51
1	c	96	ALA	CA-CB	6.54	1.63	1.53
1	G	112	LEU	CA-C	-6.54	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	ARG	CA-CB	6.54	1.64	1.53
3	I	226	VAL	N-CA	-6.54	1.38	1.46
3	K	50	ARG	CD-NE	6.54	1.55	1.46
1	d	244	LEU	CA-CB	6.54	1.62	1.53
2	m	135	LYS	CA-C	-6.54	1.44	1.52
2	7	83	ARG	N-CA	-6.54	1.37	1.46
2	k	91	ALA	N-CA	-6.53	1.38	1.46
2	1	106	TYR	CA-C	6.53	1.60	1.52
1	B	172	THR	C-N	6.53	1.42	1.33
1	f	236	ALA	C-N	6.53	1.42	1.33
1	A	235	ARG	NE-CZ	6.53	1.40	1.33
1	C	20	ARG	CA-C	-6.53	1.44	1.52
2	n	82	GLU	CA-C	-6.53	1.45	1.53
3	H	192	ALA	N-CA	-6.53	1.38	1.46
2	2	155	PHE	C-N	6.52	1.41	1.32
3	H	329	LYS	CA-C	6.52	1.60	1.52
1	e	205	VAL	CA-C	6.52	1.57	1.52
2	6	139	ALA	C-N	6.52	1.42	1.33
2	3	197	TYR	CA-C	-6.52	1.44	1.52
1	D	20	ARG	CD-NE	6.51	1.55	1.46
3	I	339	LEU	CA-CB	6.51	1.63	1.53
3	H	388	PRO	CA-CB	6.51	1.62	1.53
2	m	28	GLU	CA-C	-6.51	1.45	1.52
3	H	53	SER	N-CA	-6.51	1.38	1.46
3	L	250	ARG	CD-NE	6.51	1.55	1.46
3	M	134	GLU	CA-CB	6.51	1.64	1.53
3	M	174	PRO	CA-C	-6.51	1.46	1.52
1	E	157	LEU	CA-C	-6.50	1.44	1.52
3	J	231	LYS	CA-CB	6.50	1.63	1.53
3	J	176	LYS	C-N	6.50	1.43	1.33
2	2	76	LEU	N-CA	-6.50	1.38	1.46
2	6	18	VAL	CA-CB	6.50	1.62	1.54
1	c	114	LYS	CA-C	-6.50	1.44	1.52
1	G	133	GLY	CA-C	-6.50	1.42	1.51
1	e	139	ALA	CA-C	-6.50	1.45	1.52
1	e	235	ARG	C-N	6.49	1.42	1.33
2	n	163	GLU	N-CA	-6.49	1.38	1.46
2	l	154	ARG	CZ-NH2	6.49	1.41	1.33
3	J	277	PRO	CA-CB	-6.49	1.45	1.53
2	5	88	ARG	NE-CZ	6.49	1.40	1.33
1	C	133	GLY	CA-C	6.48	1.60	1.51
1	g	233	VAL	CA-C	-6.48	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	93	ARG	CD-NE	6.48	1.55	1.46
3	K	59	ARG	NE-CZ	6.48	1.40	1.33
2	n	20	LYS	CA-CB	6.48	1.65	1.53
3	H	239	PHE	N-CA	-6.48	1.38	1.46
1	c	28	ARG	CZ-NH1	6.48	1.41	1.32
3	K	177	GLY	C-N	6.48	1.41	1.33
1	A	137	LEU	CA-C	-6.48	1.45	1.52
1	D	241	ARG	CA-C	-6.48	1.44	1.52
3	M	204	ILE	N-CA	-6.47	1.38	1.46
1	E	239	ARG	C-N	6.47	1.42	1.33
2	m	168	ALA	CA-C	-6.47	1.44	1.52
1	f	46	VAL	CA-C	-6.47	1.44	1.52
1	g	241	ARG	NE-CZ	6.47	1.40	1.33
1	A	81	LEU	C-N	6.46	1.42	1.33
1	b	28	ARG	NE-CZ	6.46	1.40	1.33
3	I	390	PRO	C-N	6.46	1.42	1.33
3	H	239	PHE	CA-CB	6.46	1.62	1.53
3	K	307	ILE	CA-C	-6.46	1.44	1.52
1	d	70	ILE	C-N	6.46	1.42	1.33
3	L	179	LEU	CA-CB	6.45	1.62	1.53
1	d	205	VAL	C-O	-6.45	1.19	1.24
2	4	160	GLY	CA-C	-6.45	1.45	1.52
3	J	77	VAL	CA-C	-6.45	1.44	1.52
1	B	146	LYS	CA-C	-6.45	1.44	1.52
1	E	239	ARG	CZ-NH2	6.45	1.41	1.33
2	1	80	ARG	NE-CZ	6.44	1.40	1.33
2	4	126	ASP	N-CA	-6.44	1.37	1.45
3	H	49	ARG	CD-NE	6.44	1.55	1.46
3	I	148	VAL	CA-CB	-6.44	1.46	1.54
2	1	89	ALA	C-N	6.44	1.41	1.33
3	J	55	VAL	C-N	6.44	1.42	1.33
2	2	81	ARG	NE-CZ	6.43	1.40	1.33
3	L	306	ILE	CA-C	6.43	1.60	1.52
3	I	278	ARG	N-CA	-6.43	1.38	1.46
2	6	121	SER	CA-C	-6.43	1.44	1.52
2	6	106	TYR	C-O	6.43	1.28	1.23
1	G	239	ARG	N-CA	-6.43	1.38	1.46
2	3	68	ARG	CD-NE	6.43	1.55	1.46
2	j	179	ASP	CA-C	-6.43	1.44	1.52
2	j	62	ASP	CA-CB	6.42	1.63	1.53
3	J	319	GLN	CA-C	-6.42	1.44	1.52
1	g	137	LEU	C-N	6.42	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	29	ARG	CZ-NH2	6.42	1.41	1.33
1	e	148	TYR	N-CA	-6.42	1.38	1.45
3	H	258	ASP	CA-C	-6.42	1.45	1.53
1	E	105	GLU	N-CA	-6.42	1.35	1.45
3	H	283	VAL	CA-CB	-6.42	1.46	1.54
2	3	134	GLU	CA-CB	6.41	1.61	1.53
2	5	167	LEU	CA-C	-6.41	1.44	1.52
1	B	125	GLN	CA-CB	6.41	1.63	1.53
1	E	168	ARG	CA-C	-6.41	1.44	1.52
1	F	120	LYS	CA-C	-6.41	1.44	1.52
2	6	167	LEU	CA-C	-6.41	1.44	1.52
2	3	212	ARG	CD-NE	6.40	1.55	1.46
1	C	93	ARG	CD-NE	6.40	1.55	1.46
1	G	122	GLN	CA-C	-6.40	1.44	1.52
1	A	168	ARG	CZ-NH1	6.40	1.41	1.32
1	B	244	LEU	C-N	6.40	1.42	1.33
1	C	211	VAL	CA-C	-6.40	1.44	1.52
2	j	202	GLU	N-CA	-6.39	1.38	1.46
2	k	68	ARG	CZ-NH1	6.39	1.41	1.32
3	K	28	ARG	N-CA	6.39	1.53	1.46
1	d	168	ARG	CZ-NH2	6.39	1.41	1.33
2	1	154	ARG	NE-CZ	6.39	1.40	1.33
3	M	326	ARG	CA-CB	6.39	1.63	1.53
2	l	170	ARG	NE-CZ	6.39	1.40	1.33
1	D	111	GLU	C-N	6.39	1.42	1.33
3	H	380	GLU	CA-C	-6.39	1.44	1.52
3	K	120	PRO	N-CA	-6.38	1.39	1.47
3	M	172	ILE	CA-C	-6.38	1.44	1.52
2	3	201	PRO	N-CD	-6.38	1.38	1.47
1	d	93	ARG	NE-CZ	6.38	1.40	1.33
2	3	148	TYR	N-CA	-6.38	1.38	1.46
2	l	41	ALA	C-N	6.38	1.42	1.33
1	D	28	ARG	C-N	6.38	1.43	1.33
1	C	8	TYR	CA-C	6.37	1.62	1.52
2	7	89	ALA	N-CA	-6.37	1.38	1.46
3	I	261	VAL	CA-CB	-6.37	1.46	1.54
1	d	65	GLU	C-N	6.37	1.42	1.33
3	H	250	ARG	CA-C	-6.37	1.44	1.53
3	I	383	LEU	C-N	6.37	1.42	1.33
2	1	189	VAL	CA-CB	-6.37	1.46	1.54
2	n	183	GLY	CA-C	-6.37	1.41	1.52
3	H	92	SER	CA-CB	6.37	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	61	GLY	C-N	6.36	1.42	1.33
2	7	81	ARG	CD-NE	6.36	1.55	1.46
3	K	155	GLU	C-N	6.36	1.43	1.33
1	G	219	ARG	C-N	6.36	1.41	1.33
1	B	22	PHE	N-CA	-6.36	1.37	1.46
2	l	35	ASN	C-O	-6.36	1.17	1.23
3	M	40	GLU	CA-CB	6.36	1.63	1.53
1	B	219	ARG	CZ-NH1	6.36	1.41	1.32
1	G	68	TYR	C-N	6.36	1.41	1.33
2	i	161	VAL	CA-C	6.36	1.62	1.52
3	I	50	ARG	CD-NE	6.36	1.55	1.46
3	I	294	ASP	CA-C	-6.36	1.45	1.53
3	I	341	ARG	CD-NE	6.36	1.55	1.46
3	M	326	ARG	CZ-NH2	6.36	1.41	1.33
1	A	50	ALA	C-N	6.36	1.42	1.33
1	A	37	ALA	C-N	6.35	1.42	1.33
2	7	47	GLN	CA-CB	6.35	1.61	1.53
1	A	28	ARG	NE-CZ	6.35	1.40	1.33
2	l	163	GLU	CA-CB	6.35	1.63	1.53
3	J	28	ARG	CZ-NH1	6.35	1.41	1.32
1	A	143	GLU	CA-C	-6.35	1.44	1.52
1	g	79	SER	N-CA	-6.35	1.38	1.46
1	g	157	LEU	CA-C	-6.35	1.44	1.52
2	6	198	GLN	N-CA	-6.35	1.38	1.46
3	I	229	LEU	N-CA	-6.35	1.38	1.46
3	K	224	ARG	CD-NE	6.35	1.55	1.46
3	K	36	PHE	C-N	6.35	1.42	1.33
1	F	239	ARG	NE-CZ	6.34	1.40	1.33
2	l	97	LEU	CA-C	6.34	1.60	1.52
2	l	127	PRO	CA-C	6.34	1.61	1.52
1	a	37	ALA	N-CA	-6.34	1.38	1.46
1	G	93	ARG	CZ-NH2	6.34	1.41	1.33
1	F	78	THR	CA-C	6.34	1.60	1.52
1	c	130	ARG	CZ-NH1	6.34	1.41	1.32
3	M	61	PRO	CA-C	-6.34	1.46	1.52
2	j	58	GLY	C-O	6.33	1.27	1.24
3	I	45	GLU	CA-C	-6.33	1.44	1.52
1	a	170	ALA	N-CA	-6.33	1.38	1.46
3	J	241	ASP	C-N	6.33	1.42	1.33
3	J	250	ARG	CD-NE	6.33	1.55	1.46
2	h	102	ARG	NE-CZ	6.33	1.40	1.33
1	f	59	LEU	CA-CB	6.33	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	ILE	CA-C	-6.33	1.44	1.52
2	j	70	ILE	CA-CB	6.33	1.62	1.54
2	4	17	LEU	C-N	6.32	1.41	1.33
1	D	39	GLY	CA-C	-6.32	1.46	1.52
2	6	201	PRO	C-N	6.32	1.41	1.33
1	A	214	VAL	CA-CB	-6.32	1.46	1.54
2	5	108	VAL	N-CA	-6.32	1.38	1.46
3	L	221	ARG	CA-C	-6.32	1.44	1.52
1	B	177	LYS	N-CA	-6.31	1.38	1.46
1	c	180	ARG	CD-NE	6.31	1.55	1.46
2	h	186	ILE	CA-C	-6.31	1.44	1.52
1	F	226	PRO	CA-C	6.31	1.62	1.52
3	M	77	VAL	C-N	6.31	1.40	1.33
2	5	170	ARG	CA-C	-6.30	1.44	1.52
3	I	238	ILE	N-CA	-6.30	1.38	1.46
3	K	276	ASP	N-CA	-6.30	1.40	1.46
2	1	121	SER	C-N	6.30	1.41	1.33
2	1	122	ILE	CA-C	-6.30	1.44	1.52
2	l	125	ILE	CA-C	-6.30	1.44	1.52
2	j	166	GLU	CA-C	-6.30	1.44	1.52
1	C	234	GLU	CA-CB	6.30	1.63	1.53
2	n	105	PRO	CA-C	-6.30	1.44	1.52
3	H	69	SER	N-CA	-6.30	1.37	1.46
2	h	138	VAL	C-N	6.29	1.41	1.33
1	E	79	SER	CA-C	-6.29	1.44	1.52
2	2	210	LYS	CA-C	-6.29	1.44	1.52
1	a	87	VAL	N-CA	-6.29	1.38	1.46
1	C	6	MET	N-CA	-6.29	1.38	1.46
1	C	168	ARG	CD-NE	6.29	1.55	1.46
2	2	180	SER	CA-C	-6.29	1.44	1.52
3	H	48	VAL	CA-CB	-6.29	1.46	1.54
1	G	11	ALA	CA-C	-6.29	1.44	1.52
2	h	51	ARG	CD-NE	6.29	1.55	1.46
3	M	69	SER	CA-C	-6.29	1.45	1.52
1	D	144	VAL	N-CA	-6.28	1.40	1.46
2	i	56	THR	C-N	6.28	1.42	1.33
2	i	107	LEU	CA-C	-6.28	1.45	1.52
2	3	30	ARG	CZ-NH1	6.28	1.41	1.32
2	5	193	GLU	CA-C	-6.28	1.44	1.52
2	n	166	GLU	C-N	6.28	1.42	1.33
1	E	156	LEU	CA-C	-6.28	1.45	1.52
3	K	258	ASP	C-N	6.27	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	VAL	N-CA	-6.27	1.41	1.46
3	L	298	LEU	CA-CB	6.27	1.63	1.53
1	e	170	ALA	N-CA	-6.27	1.39	1.46
2	5	83	ARG	NE-CZ	6.27	1.40	1.33
3	I	381	LYS	N-CA	-6.27	1.38	1.46
3	J	26	LEU	C-N	6.27	1.43	1.33
3	J	125	PRO	C-N	6.27	1.42	1.33
3	K	71	ILE	CA-C	-6.26	1.45	1.52
2	3	37	ILE	CA-C	-6.26	1.44	1.52
1	F	144	VAL	N-CA	-6.26	1.41	1.46
2	h	112	ILE	CA-C	-6.26	1.45	1.52
3	I	87	PHE	CA-C	6.25	1.60	1.52
2	2	14	THR	N-CA	-6.25	1.37	1.45
2	j	22	GLY	N-CA	-6.25	1.39	1.45
1	b	235	ARG	NE-CZ	6.25	1.40	1.33
1	F	191	LEU	CA-C	-6.25	1.44	1.52
1	f	202	SER	CA-C	-6.25	1.44	1.52
3	I	357	GLU	C-N	6.25	1.42	1.33
1	a	235	ARG	C-N	6.25	1.41	1.33
2	l	23	VAL	CA-C	-6.25	1.44	1.52
3	L	207	VAL	C-O	-6.25	1.17	1.23
2	5	172	ILE	C-N	6.25	1.43	1.33
3	I	383	LEU	CA-C	-6.25	1.43	1.52
3	K	26	LEU	C-N	6.24	1.42	1.33
2	5	154	ARG	NE-CZ	6.24	1.40	1.33
3	L	38	GLU	N-CA	-6.24	1.38	1.46
1	e	212	GLY	CA-C	-6.24	1.47	1.52
2	1	96	ASN	N-CA	-6.24	1.38	1.46
1	E	196	MET	N-CA	-6.24	1.38	1.46
2	h	172	ILE	CA-CB	-6.24	1.46	1.54
3	K	201	ALA	CA-C	-6.24	1.44	1.52
1	d	28	ARG	CZ-NH1	6.23	1.41	1.32
1	c	87	VAL	CA-C	-6.23	1.45	1.52
3	K	239	PHE	N-CA	-6.23	1.38	1.46
1	b	239	ARG	CZ-NH1	6.23	1.41	1.32
2	5	136	ASP	CA-C	-6.23	1.44	1.52
3	H	260	GLU	CA-C	-6.23	1.44	1.52
2	i	148	TYR	CA-CB	6.23	1.63	1.53
3	M	89	VAL	CA-C	-6.23	1.45	1.52
1	D	67	ILE	C-N	6.23	1.42	1.33
3	H	134	GLU	CA-CB	6.22	1.64	1.53
3	H	241	ASP	CA-CB	6.22	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	322	LYS	C-N	6.22	1.41	1.33
3	K	326	ARG	CA-CB	6.22	1.63	1.53
1	c	35	ALA	CA-CB	6.22	1.63	1.53
2	7	107	LEU	CA-CB	6.22	1.62	1.53
1	e	145	PRO	CA-C	-6.22	1.44	1.52
1	A	7	GLY	C-N	6.22	1.42	1.33
1	C	65	GLU	CA-C	-6.21	1.45	1.52
1	g	87	VAL	CA-C	-6.21	1.43	1.52
2	1	107	LEU	CA-C	-6.21	1.44	1.52
1	a	100	ARG	CD-NE	6.21	1.54	1.46
1	A	135	SER	CA-C	-6.20	1.45	1.52
1	a	33	ARG	N-CA	-6.20	1.38	1.46
1	e	80	GLY	C-N	6.20	1.41	1.33
1	F	174	PHE	CA-C	-6.20	1.44	1.52
3	K	265	MET	CA-C	-6.20	1.45	1.52
2	3	187	ASP	CA-C	-6.20	1.45	1.52
3	H	278	ARG	CZ-NH2	6.20	1.41	1.33
3	J	158	GLU	C-N	6.20	1.41	1.33
1	G	61	ALA	N-CA	-6.20	1.38	1.46
2	2	73	GLU	CA-CB	6.20	1.63	1.53
3	I	88	VAL	N-CA	-6.20	1.38	1.46
2	n	103	TYR	CA-CB	6.20	1.64	1.53
3	H	243	LEU	CA-C	-6.20	1.44	1.52
3	J	198	GLN	N-CA	-6.20	1.38	1.46
3	L	350	ASP	CA-C	-6.19	1.44	1.52
3	J	63	LEU	N-CA	-6.19	1.39	1.46
3	K	187	GLY	CA-C	-6.19	1.43	1.51
1	g	27	ALA	CA-C	-6.19	1.44	1.52
2	h	41	ALA	C-O	-6.19	1.17	1.24
3	K	358	ALA	CA-C	-6.19	1.44	1.52
1	E	176	GLU	C-O	-6.19	1.16	1.24
2	6	92	THR	N-CA	-6.19	1.38	1.46
3	J	49	ARG	CZ-NH2	6.19	1.41	1.33
2	4	131	ALA	N-CA	-6.18	1.38	1.46
2	4	140	THR	CA-C	-6.18	1.44	1.52
3	H	309	VAL	CA-C	-6.18	1.46	1.52
3	L	370	VAL	CA-C	-6.18	1.44	1.52
3	M	34	LYS	CA-C	6.18	1.61	1.52
2	3	102	ARG	CD-NE	6.18	1.54	1.46
2	j	170	ARG	CD-NE	6.18	1.54	1.46
1	g	86	ARG	CZ-NH2	6.17	1.41	1.33
3	L	303	PHE	CA-CB	6.17	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	224	ARG	CD-NE	6.17	1.54	1.46
1	d	99	ASN	N-CA	-6.17	1.38	1.46
2	1	29	LYS	CA-C	-6.17	1.44	1.52
3	I	52	ARG	CA-CB	6.17	1.63	1.53
3	K	199	THR	CA-C	-6.17	1.44	1.52
3	K	282	LYS	CA-C	-6.17	1.44	1.52
3	K	335	ASP	CA-CB	6.17	1.62	1.53
3	M	154	ARG	NE-CZ	6.17	1.39	1.33
1	a	73	HIS	ND1-CE1	6.17	1.38	1.32
1	B	53	ARG	CZ-NH1	6.17	1.41	1.32
1	F	120	LYS	C-N	6.17	1.42	1.34
2	h	112	ILE	C-N	6.17	1.40	1.33
2	3	81	ARG	CZ-NH1	6.17	1.41	1.32
2	l	189	VAL	CA-CB	-6.17	1.45	1.54
1	a	117	CYS	CA-C	-6.17	1.44	1.52
2	2	102	ARG	NE-CZ	6.16	1.39	1.33
2	5	166	GLU	N-CA	-6.16	1.38	1.46
3	L	162	LEU	CA-CB	6.16	1.63	1.53
2	4	36	PHE	N-CA	-6.16	1.38	1.46
3	H	113	LEU	N-CA	-6.16	1.38	1.46
1	F	229	LEU	C-N	6.16	1.42	1.33
1	g	73	HIS	N-CA	-6.16	1.38	1.46
2	l	31	ALA	N-CA	-6.16	1.38	1.45
3	I	341	ARG	NE-CZ	6.16	1.39	1.33
2	5	24	VAL	N-CA	-6.16	1.39	1.46
3	J	84	GLY	C-N	6.16	1.41	1.33
3	M	196	ALA	C-O	-6.16	1.16	1.24
3	L	361	PHE	C-N	6.15	1.42	1.33
2	1	96	ASN	CA-CB	6.15	1.62	1.53
1	c	131	PRO	CA-CB	6.15	1.62	1.53
3	M	241	ASP	CA-CB	6.15	1.61	1.53
2	5	180	SER	N-CA	-6.15	1.38	1.47
2	l	85	PRO	C-N	6.15	1.41	1.33
2	7	154	ARG	CD-NE	6.15	1.54	1.46
3	H	17	GLU	CA-CB	6.15	1.62	1.53
1	b	79	SER	C-N	6.15	1.42	1.33
2	4	178	ARG	NE-CZ	6.14	1.39	1.33
1	c	174	PHE	CA-CB	6.14	1.63	1.53
1	e	241	ARG	CZ-NH1	6.14	1.41	1.32
2	2	59	SER	CA-C	-6.14	1.44	1.52
2	j	136	ASP	C-N	6.14	1.41	1.33
2	n	47	GLN	CA-C	-6.14	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	285	GLY	CA-C	-6.14	1.43	1.51
2	7	137	ILE	CA-C	-6.13	1.45	1.52
2	n	188	VAL	C-N	6.13	1.41	1.33
3	J	259	ARG	CD-NE	6.13	1.54	1.46
1	d	231	PRO	N-CA	-6.13	1.39	1.47
3	H	372	MET	C-N	6.13	1.42	1.33
2	4	108	VAL	N-CA	-6.13	1.38	1.46
2	n	190	LYS	C-N	6.13	1.41	1.33
2	j	176	MET	C-N	6.12	1.41	1.33
1	B	109	VAL	CA-CB	-6.12	1.46	1.54
2	2	185	GLY	C-N	6.12	1.42	1.33
2	k	209	ALA	CA-C	-6.12	1.44	1.52
2	h	141	GLY	N-CA	-6.12	1.36	1.44
2	2	124	SER	CA-CB	6.12	1.62	1.53
2	h	185	GLY	C-N	6.12	1.41	1.33
1	e	73	HIS	CG-CD2	6.12	1.42	1.35
1	G	23	GLN	CA-C	-6.12	1.44	1.52
2	m	199	TYR	N-CA	-6.12	1.39	1.46
2	7	162	ASP	C-N	6.12	1.42	1.33
3	L	41	ARG	CD-NE	6.12	1.54	1.46
1	F	177	LYS	N-CA	-6.11	1.38	1.46
2	k	98	LEU	CB-CG	6.11	1.65	1.53
2	m	111	LEU	CA-C	6.11	1.59	1.52
3	K	276	ASP	CA-C	6.11	1.60	1.52
2	i	168	ALA	N-CA	-6.11	1.39	1.46
3	L	80	LYS	C-N	6.11	1.41	1.33
1	c	176	GLU	CA-CB	6.10	1.63	1.53
1	d	76	ALA	CA-C	-6.10	1.45	1.52
1	G	152	PRO	N-CA	-6.10	1.39	1.47
1	c	113	ALA	N-CA	-6.10	1.39	1.46
2	4	188	VAL	CA-C	-6.10	1.45	1.52
3	H	46	ARG	CD-NE	6.10	1.54	1.46
2	6	99	ASN	C-N	6.10	1.41	1.33
2	1	60	VAL	CA-CB	6.09	1.61	1.54
2	7	81	ARG	NE-CZ	6.09	1.39	1.33
3	L	123	LYS	CA-C	6.09	1.60	1.53
1	e	134	VAL	CA-C	-6.09	1.44	1.52
3	M	37	ILE	C-N	6.09	1.42	1.33
1	a	201	GLU	C-N	6.09	1.41	1.33
1	f	219	ARG	NE-CZ	6.09	1.39	1.33
3	K	215	TYR	CA-C	-6.09	1.44	1.52
3	J	366	GLU	CA-C	-6.09	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	105	PRO	CA-C	-6.09	1.43	1.52
3	H	12	LYS	CA-CB	6.09	1.62	1.53
2	n	48	ILE	N-CA	-6.08	1.37	1.46
1	g	85	ALA	CA-CB	6.08	1.62	1.53
1	b	53	ARG	NE-CZ	6.08	1.39	1.33
2	i	86	THR	N-CA	-6.08	1.38	1.45
2	6	33	MET	C-N	6.08	1.41	1.33
2	7	161	VAL	N-CA	-6.08	1.38	1.46
3	I	239	PHE	CA-CB	6.08	1.61	1.53
3	K	92	SER	CA-C	-6.08	1.47	1.53
3	K	332	GLU	CA-C	-6.08	1.45	1.52
3	J	189	THR	C-N	6.08	1.42	1.33
1	c	189	MET	C-N	6.08	1.41	1.33
1	E	117	CYS	C-N	6.08	1.42	1.34
3	J	111	GLN	CA-C	-6.08	1.44	1.52
3	J	162	LEU	C-N	6.08	1.41	1.33
1	G	87	VAL	CA-C	-6.07	1.43	1.52
3	I	333	ASP	N-CA	-6.07	1.40	1.46
3	L	214	LYS	N-CA	-6.07	1.38	1.46
1	E	153	SER	CA-CB	6.07	1.64	1.53
3	H	320	ILE	C-N	6.07	1.41	1.33
3	L	378	ALA	N-CA	-6.07	1.39	1.46
3	L	48	VAL	CA-C	-6.07	1.45	1.52
1	E	163	ALA	C-N	6.06	1.41	1.33
2	n	51	ARG	CZ-NH1	6.06	1.41	1.32
3	H	366	GLU	CA-C	-6.06	1.44	1.52
1	e	134	VAL	N-CA	-6.06	1.39	1.46
1	F	171	VAL	N-CA	-6.06	1.38	1.46
2	h	42	ALA	C-N	6.06	1.41	1.33
2	h	167	LEU	CA-CB	6.06	1.62	1.53
2	1	81	ARG	CA-C	-6.06	1.44	1.52
3	I	57	ARG	CZ-NH2	6.06	1.41	1.33
1	f	245	LYS	C-N	6.06	1.41	1.33
2	j	80	ARG	CZ-NH1	6.06	1.41	1.32
3	I	231	LYS	C-N	6.06	1.42	1.33
1	a	38	ILE	C-N	6.05	1.41	1.32
1	e	183	LEU	CA-C	-6.05	1.45	1.52
3	J	243	LEU	CA-CB	6.05	1.60	1.52
1	E	200	ILE	C-O	-6.05	1.17	1.24
1	F	93	ARG	CZ-NH1	6.05	1.41	1.32
1	a	214	VAL	N-CA	-6.05	1.38	1.46
2	5	26	ALA	N-CA	-6.05	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	93	LEU	CA-C	6.05	1.60	1.52
2	7	197	TYR	C-O	-6.05	1.16	1.23
3	J	260	GLU	CA-CB	6.05	1.62	1.53
2	j	115	ILE	CA-CB	-6.05	1.47	1.54
1	B	150	THR	N-CA	-6.05	1.38	1.46
1	B	183	LEU	CA-CB	6.05	1.63	1.53
3	I	305	ARG	CD-NE	6.05	1.54	1.46
1	C	64	ILE	CA-C	-6.04	1.45	1.52
2	j	34	GLY	CA-C	-6.04	1.44	1.52
1	E	62	ASP	CA-CB	6.04	1.61	1.53
2	2	54	MET	N-CA	-6.04	1.38	1.46
2	3	49	ALA	CA-CB	6.04	1.62	1.53
2	3	212	ARG	CZ-NH1	6.04	1.41	1.32
2	4	68	ARG	NE-CZ	6.04	1.39	1.33
1	f	174	PHE	CA-CB	6.04	1.62	1.53
3	M	333	ASP	C-N	6.04	1.41	1.33
1	c	145	PRO	C-N	6.04	1.41	1.33
1	c	226	PRO	C-N	6.04	1.42	1.33
2	n	56	THR	CA-C	-6.04	1.45	1.52
3	J	396	MET	CA-C	-6.04	1.45	1.52
1	C	134	VAL	N-CA	-6.03	1.39	1.46
2	l	35	ASN	CA-CB	6.03	1.62	1.53
1	B	125	GLN	N-CA	-6.03	1.39	1.46
3	K	238	ILE	N-CA	-6.03	1.39	1.46
3	L	49	ARG	CZ-NH1	6.03	1.41	1.32
3	M	325	THR	N-CA	-6.03	1.39	1.46
1	E	16	SER	CA-C	-6.03	1.45	1.53
1	E	219	ARG	CZ-NH2	6.03	1.41	1.33
2	l	36	PHE	CA-C	-6.03	1.45	1.52
3	J	222	LEU	N-CA	-6.03	1.38	1.46
1	g	28	ARG	NE-CZ	6.02	1.39	1.33
1	d	197	GLY	CA-C	-6.02	1.44	1.51
2	7	80	ARG	CZ-NH2	6.02	1.41	1.33
1	d	46	VAL	N-CA	-6.02	1.39	1.46
2	j	182	SER	CA-C	-6.02	1.45	1.52
1	A	33	ARG	CD-NE	6.02	1.54	1.46
1	d	177	LYS	CA-CB	6.01	1.63	1.53
2	j	105	PRO	C-N	6.01	1.42	1.33
2	k	75	ASN	N-CA	6.01	1.53	1.46
2	l	112	ILE	CA-C	-6.01	1.44	1.52
1	d	160	LYS	CA-CB	6.01	1.63	1.53
3	I	81	SER	CA-C	-6.01	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	130	ARG	NE-CZ	6.01	1.39	1.33
1	E	31	VAL	CA-C	-6.01	1.45	1.52
1	e	86	ARG	NE-CZ	6.01	1.39	1.33
2	6	79	ILE	C-N	6.01	1.42	1.33
3	J	40	GLU	CA-C	-6.01	1.44	1.52
1	B	134	VAL	CA-C	-6.00	1.45	1.52
2	6	166	GLU	N-CA	-6.00	1.39	1.46
1	G	180	ARG	CZ-NH2	6.00	1.41	1.33
1	b	112	LEU	C-N	6.00	1.41	1.33
3	L	305	ARG	CZ-NH1	6.00	1.41	1.32
1	F	76	ALA	N-CA	-6.00	1.38	1.46
1	F	101	LEU	CA-CB	6.00	1.62	1.53
2	6	202	GLU	C-N	6.00	1.41	1.33
2	7	37	ILE	CA-C	-6.00	1.46	1.52
1	a	99	ASN	CA-C	6.00	1.60	1.52
3	L	259	ARG	NE-CZ	6.00	1.39	1.33
1	B	188	ALA	CA-C	-5.99	1.45	1.52
2	i	71	LYS	CA-CB	5.99	1.62	1.53
3	K	289	ARG	CA-C	-5.99	1.45	1.52
1	F	121	GLN	CA-C	-5.99	1.44	1.52
3	H	215	TYR	CA-C	-5.99	1.45	1.52
2	l	26	ALA	CA-C	-5.99	1.45	1.52
2	7	159	ILE	N-CA	-5.99	1.39	1.46
3	M	364	ARG	NE-CZ	5.99	1.39	1.33
1	A	155	ALA	N-CA	-5.99	1.38	1.45
1	G	217	ASP	C-N	5.99	1.41	1.33
2	h	172	ILE	C-N	5.99	1.41	1.33
1	D	218	ASP	CA-C	-5.99	1.44	1.52
2	2	197	TYR	C-O	-5.98	1.16	1.24
2	k	122	ILE	N-CA	-5.98	1.39	1.46
2	5	40	LYS	C-N	5.98	1.41	1.33
1	a	180	ARG	N-CA	5.98	1.53	1.45
3	J	241	ASP	N-CA	-5.98	1.38	1.45
1	G	207	GLU	CA-CB	5.98	1.64	1.53
1	g	107	ILE	CA-CB	-5.98	1.48	1.54
2	h	24	VAL	N-CA	-5.98	1.39	1.46
1	D	22	PHE	N-CA	-5.98	1.38	1.46
3	L	289	ARG	NE-CZ	5.98	1.39	1.33
3	L	397	PHE	CA-C	-5.98	1.44	1.52
1	e	219	ARG	CZ-NH2	5.98	1.41	1.33
2	4	124	SER	N-CA	-5.97	1.38	1.46
3	I	370	VAL	CA-C	-5.97	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	LYS	CA-CB	5.97	1.65	1.53
1	G	40	ILE	CA-C	-5.97	1.45	1.52
3	M	230	ALA	C-O	-5.97	1.17	1.24
1	b	180	ARG	NE-CZ	5.96	1.39	1.33
2	3	28	GLU	CA-C	-5.96	1.45	1.52
2	5	109	GLN	N-CA	-5.96	1.38	1.46
2	l	205	GLU	C-N	5.96	1.42	1.33
2	6	101	TYR	CA-C	-5.96	1.45	1.52
3	I	76	ARG	NE-CZ	5.96	1.39	1.33
3	I	99	GLU	C-O	-5.96	1.17	1.24
1	c	186	ASP	CA-CB	5.96	1.62	1.53
3	M	278	ARG	CD-NE	5.96	1.54	1.46
3	H	16	LEU	CA-C	-5.96	1.45	1.52
1	b	34	GLY	C-N	5.96	1.41	1.33
1	d	204	LEU	CA-C	-5.96	1.44	1.53
2	j	102	ARG	CD-NE	5.96	1.54	1.46
2	l	154	ARG	CD-NE	5.95	1.54	1.46
1	D	55	GLY	C-N	5.95	1.42	1.33
1	c	203	GLU	CA-C	-5.95	1.45	1.52
1	G	200	ILE	C-N	5.95	1.42	1.33
2	5	152	GLU	C-N	5.95	1.41	1.33
1	B	193	LEU	C-N	5.95	1.41	1.33
2	1	55	THR	C-N	5.95	1.42	1.33
1	B	173	GLU	N-CA	-5.95	1.39	1.46
1	c	79	SER	C-N	5.95	1.43	1.32
1	d	201	GLU	CA-CB	5.95	1.62	1.53
3	K	157	VAL	CA-C	-5.95	1.45	1.52
1	e	86	ARG	CD-NE	5.95	1.54	1.46
2	4	104	PHE	CA-C	-5.95	1.45	1.53
3	J	187	GLY	N-CA	-5.95	1.36	1.45
3	J	298	LEU	CA-CB	5.95	1.63	1.53
2	i	105	PRO	CA-C	-5.94	1.45	1.52
2	4	53	ALA	CA-C	-5.94	1.45	1.52
2	l	180	SER	C-N	5.94	1.42	1.33
2	7	173	TYR	N-CA	-5.94	1.39	1.46
3	K	392	LEU	CA-C	5.94	1.60	1.52
1	D	38	ILE	CA-C	-5.94	1.45	1.52
2	h	83	ARG	CZ-NH1	5.94	1.41	1.32
1	b	164	ILE	C-N	5.94	1.40	1.33
1	F	170	ALA	CA-CB	5.94	1.63	1.53
1	A	73	HIS	ND1-CE1	5.93	1.38	1.32
1	D	233	VAL	CA-C	-5.93	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	36	PHE	C-N	5.93	1.40	1.33
3	I	206	VAL	C-N	5.93	1.40	1.33
1	F	236	ALA	C-N	5.93	1.41	1.34
3	K	249	ARG	NE-CZ	5.93	1.39	1.33
3	L	352	LYS	C-N	5.93	1.41	1.33
1	b	90	ASP	C-N	5.93	1.42	1.33
2	n	175	ALA	C-N	5.93	1.42	1.34
1	E	33	ARG	CA-C	-5.93	1.45	1.52
2	5	26	ALA	CA-C	-5.93	1.45	1.52
3	I	321	PHE	N-CA	-5.93	1.39	1.46
1	e	163	ALA	CA-C	-5.92	1.45	1.52
2	3	71	LYS	C-O	-5.92	1.17	1.24
3	H	202	THR	CA-C	-5.92	1.44	1.52
2	3	106	TYR	CA-CB	5.92	1.63	1.53
1	D	240	ILE	N-CA	5.92	1.53	1.46
2	6	158	GLU	CA-C	-5.92	1.45	1.53
3	H	314	PHE	CA-C	-5.92	1.45	1.52
1	D	192	GLY	CA-C	-5.91	1.44	1.51
2	n	134	GLU	CA-C	5.91	1.59	1.52
2	l	30	ARG	N-CA	-5.91	1.38	1.46
2	h	33	MET	C-N	5.91	1.42	1.33
3	L	183	PRO	CA-CB	-5.91	1.46	1.54
1	A	157	LEU	N-CA	-5.91	1.38	1.46
1	E	119	PHE	CA-C	5.91	1.60	1.52
2	m	80	ARG	CA-C	-5.91	1.45	1.52
3	L	16	LEU	N-CA	-5.91	1.39	1.46
3	L	19	ASP	C-N	5.91	1.42	1.34
1	G	241	ARG	CD-NE	5.91	1.54	1.46
1	d	86	ARG	CZ-NH1	5.91	1.41	1.32
1	F	84	ASP	CA-C	-5.91	1.45	1.52
2	i	145	LEU	C-O	-5.91	1.17	1.24
3	J	60	SER	CA-C	-5.91	1.46	1.53
1	e	86	ARG	C-N	5.90	1.41	1.33
2	4	185	GLY	N-CA	-5.90	1.36	1.45
3	I	327	LYS	C-N	5.90	1.39	1.33
3	K	185	GLY	N-CA	-5.90	1.36	1.45
3	J	200	ARG	CA-CB	5.90	1.62	1.53
1	C	78	THR	CA-C	5.90	1.59	1.52
1	E	21	LEU	CA-C	-5.90	1.45	1.52
1	f	148	TYR	N-CA	-5.90	1.38	1.45
2	7	24	VAL	N-CA	-5.90	1.39	1.46
1	C	180	ARG	NE-CZ	5.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	335	ASP	CA-CB	5.90	1.62	1.53
1	b	193	LEU	CA-C	-5.90	1.45	1.52
1	g	39	GLY	C-N	5.90	1.41	1.33
2	l	120	LYS	CA-C	5.90	1.59	1.52
3	K	243	LEU	CA-C	5.89	1.59	1.52
3	K	271	GLU	C-N	5.89	1.41	1.33
3	M	378	ALA	CA-C	-5.89	1.44	1.52
1	B	41	LYS	C-N	5.89	1.41	1.33
2	4	106	TYR	N-CA	-5.89	1.38	1.46
1	E	152	PRO	C-N	5.89	1.42	1.33
3	I	248	ALA	CA-C	-5.89	1.45	1.52
3	L	94	TYR	C-N	5.89	1.41	1.33
3	J	43	ARG	NE-CZ	5.89	1.39	1.33
1	A	60	GLU	C-O	-5.89	1.16	1.23
1	F	86	ARG	CA-C	-5.89	1.45	1.52
2	4	151	LEU	CA-C	-5.89	1.45	1.52
3	J	132	VAL	C-O	-5.89	1.17	1.24
1	C	143	GLU	C-N	5.88	1.38	1.33
2	m	80	ARG	CD-NE	5.88	1.54	1.46
2	m	186	ILE	CA-CB	5.88	1.60	1.54
3	K	284	ILE	CA-C	5.88	1.59	1.52
1	b	10	ARG	CZ-NH1	5.88	1.41	1.32
2	6	59	SER	CA-C	-5.88	1.45	1.52
1	c	22	PHE	N-CA	-5.88	1.39	1.46
2	n	89	ALA	CA-C	-5.88	1.45	1.52
3	L	302	ARG	NE-CZ	5.88	1.39	1.33
3	M	27	TYR	CA-CB	5.88	1.62	1.53
3	L	337	LYS	C-N	5.87	1.42	1.34
1	g	230	LYS	N-CA	-5.87	1.40	1.46
1	e	20	ARG	CZ-NH2	5.87	1.41	1.33
1	D	242	GLU	CA-CB	5.87	1.62	1.53
1	e	62	ASP	CA-C	-5.87	1.45	1.52
2	3	68	ARG	N-CA	-5.87	1.39	1.46
1	F	236	ALA	CA-C	-5.86	1.45	1.52
2	6	180	SER	C-N	5.86	1.41	1.33
1	E	209	ILE	CA-CB	-5.86	1.44	1.55
3	K	28	ARG	NE-CZ	5.86	1.39	1.33
3	M	170	VAL	CA-C	-5.86	1.45	1.52
2	4	91	ALA	CA-C	-5.86	1.45	1.52
3	M	263	ARG	NE-CZ	5.86	1.39	1.33
2	h	46	TYR	N-CA	-5.86	1.38	1.46
2	l	20	LYS	CA-CB	5.86	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	126	ASP	CA-CB	5.86	1.61	1.53
2	l	171	ALA	CA-C	-5.86	1.45	1.52
2	m	181	ALA	CA-C	-5.86	1.45	1.52
2	m	40	LYS	CA-C	-5.86	1.45	1.52
1	D	90	ASP	N-CA	-5.85	1.39	1.46
2	j	204	VAL	CA-C	-5.85	1.45	1.52
2	5	71	LYS	C-N	5.85	1.41	1.33
1	d	190	VAL	C-N	5.85	1.41	1.33
3	L	333	ASP	C-N	5.85	1.41	1.33
2	2	78	GLU	N-CA	-5.85	1.39	1.46
2	j	30	ARG	N-CA	-5.85	1.39	1.46
3	K	203	PHE	N-CA	-5.85	1.38	1.46
3	M	67	VAL	CA-C	5.85	1.59	1.52
1	D	175	PHE	CA-C	-5.84	1.44	1.52
1	f	197	GLY	N-CA	-5.84	1.38	1.45
2	i	83	ARG	CZ-NH1	5.84	1.41	1.32
1	F	152	PRO	C-N	5.84	1.42	1.33
1	C	213	TYR	CA-C	-5.84	1.45	1.52
1	F	25	GLU	CA-C	-5.84	1.44	1.52
3	I	133	GLU	C-N	5.84	1.42	1.33
1	f	12	ILE	CA-CB	-5.84	1.46	1.54
2	n	207	ILE	C-N	5.84	1.42	1.33
1	D	172	THR	CA-CB	5.84	1.62	1.53
1	a	184	SER	CA-C	-5.84	1.45	1.53
1	C	241	ARG	CA-CB	5.84	1.62	1.53
2	m	83	ARG	CD-NE	5.84	1.54	1.46
3	I	192	ALA	CA-C	-5.84	1.45	1.52
3	I	309	VAL	CA-CB	-5.84	1.46	1.54
1	a	104	ASP	C-N	5.83	1.39	1.33
2	h	37	ILE	N-CA	-5.83	1.39	1.46
1	c	241	ARG	NE-CZ	5.83	1.39	1.33
1	D	203	GLU	CA-CB	5.83	1.62	1.53
2	j	186	ILE	C-N	5.83	1.41	1.33
3	M	149	GLN	N-CA	-5.83	1.39	1.46
1	g	100	ARG	NE-CZ	5.83	1.39	1.33
3	M	136	PRO	C-N	5.83	1.41	1.33
1	c	196	MET	C-N	5.83	1.41	1.33
2	6	51	ARG	CZ-NH1	5.83	1.41	1.32
2	1	130	GLY	N-CA	-5.83	1.36	1.45
2	l	47	GLN	CA-C	-5.83	1.45	1.52
3	H	205	ARG	CZ-NH1	5.83	1.41	1.32
1	A	135	SER	N-CA	-5.82	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLU	CA-C	-5.82	1.45	1.52
3	I	118	VAL	CA-C	-5.82	1.46	1.52
2	6	138	VAL	CA-C	-5.82	1.46	1.52
3	H	172	ILE	N-CA	-5.82	1.39	1.46
1	A	170	ALA	CA-C	-5.82	1.45	1.52
1	D	108	THR	CA-C	5.82	1.60	1.52
3	L	140	TYR	N-CA	-5.82	1.38	1.46
1	a	33	ARG	CD-NE	5.82	1.54	1.46
3	K	325	THR	CA-CB	-5.82	1.43	1.53
3	M	200	ARG	CD-NE	5.81	1.54	1.46
1	G	143	GLU	N-CA	-5.81	1.38	1.46
2	h	44	LYS	C-N	5.81	1.40	1.33
2	k	126	ASP	C-N	5.81	1.41	1.34
1	d	181	ASP	C-N	5.81	1.41	1.33
3	K	281	VAL	CA-C	-5.81	1.45	1.52
1	A	49	ILE	CA-C	-5.81	1.45	1.52
3	L	272	LEU	CA-C	-5.81	1.45	1.52
2	k	53	ALA	N-CA	-5.81	1.38	1.45
1	e	165	GLY	C-N	5.80	1.41	1.33
1	f	17	PRO	C-N	5.80	1.42	1.33
2	h	169	VAL	CA-C	-5.80	1.45	1.52
3	M	73	GLU	CA-C	-5.80	1.43	1.52
1	A	220	THR	CA-C	-5.80	1.45	1.52
1	G	119	PHE	C-N	5.80	1.41	1.33
3	L	334	VAL	C-N	5.80	1.41	1.33
2	k	156	THR	N-CA	-5.80	1.40	1.46
3	J	140	TYR	C-N	5.80	1.42	1.33
1	C	159	TYR	CA-C	-5.80	1.45	1.52
3	L	108	LEU	CA-C	-5.80	1.46	1.52
3	L	317	ARG	CZ-NH1	5.80	1.40	1.32
1	f	79	SER	CA-C	-5.79	1.45	1.52
3	L	158	GLU	CA-C	5.79	1.60	1.52
1	f	181	ASP	CA-C	-5.79	1.45	1.52
3	J	181	TYR	C-N	5.79	1.42	1.33
1	G	19	GLY	CA-C	-5.79	1.44	1.51
3	J	370	VAL	C-N	5.79	1.39	1.33
1	e	180	ARG	CZ-NH1	5.78	1.40	1.32
3	I	16	LEU	C-N	5.78	1.41	1.33
1	E	23	GLN	C-N	5.78	1.40	1.33
2	l	191	ILE	CA-CB	-5.78	1.46	1.53
3	L	319	GLN	N-CA	-5.78	1.39	1.46
2	1	205	GLU	CA-C	-5.78	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	165	GLY	C-O	-5.78	1.20	1.24
2	7	184	ASP	CA-C	-5.78	1.45	1.52
3	J	126	MET	CA-CB	5.77	1.63	1.53
3	J	282	LYS	N-CA	-5.77	1.39	1.45
1	B	92	ALA	CA-C	-5.77	1.45	1.52
2	j	33	MET	N-CA	-5.77	1.39	1.46
1	D	88	LEU	CA-C	-5.77	1.45	1.52
1	F	64	ILE	C-N	5.77	1.41	1.33
1	g	172	THR	C-N	5.77	1.41	1.33
2	3	74	ALA	C-N	5.77	1.41	1.33
3	J	36	PHE	N-CA	5.77	1.53	1.46
1	C	162	THR	C-O	-5.77	1.17	1.23
3	K	171	GLY	CA-C	-5.77	1.43	1.51
1	A	89	ILE	C-N	5.77	1.41	1.33
1	F	100	ARG	CZ-NH1	5.76	1.40	1.32
2	k	77	TYR	N-CA	-5.76	1.39	1.46
2	k	90	ILE	CA-CB	5.76	1.62	1.54
3	J	299	ARG	CD-NE	5.76	1.54	1.46
1	f	91	ARG	CD-NE	5.76	1.54	1.46
2	h	191	ILE	N-CA	-5.76	1.39	1.46
3	J	165	GLU	C-N	5.76	1.42	1.34
1	b	51	ASP	CA-CB	5.76	1.61	1.53
1	e	55	GLY	C-N	5.76	1.41	1.33
2	1	73	GLU	N-CA	-5.76	1.39	1.46
3	L	14	LYS	N-CA	-5.76	1.39	1.46
1	G	73	HIS	N-CA	-5.76	1.38	1.46
1	g	42	CYS	CA-C	-5.76	1.45	1.53
1	g	70	ILE	CA-C	-5.76	1.46	1.53
2	h	139	ALA	N-CA	-5.76	1.39	1.46
2	i	138	VAL	CA-C	-5.76	1.45	1.52
2	i	170	ARG	CZ-NH2	5.76	1.41	1.33
3	H	302	ARG	NE-CZ	5.75	1.39	1.33
1	B	163	ALA	N-CA	-5.75	1.38	1.45
1	e	49	ILE	N-CA	-5.75	1.39	1.46
1	g	32	LYS	N-CA	5.75	1.53	1.46
2	5	70	ILE	CA-CB	-5.75	1.46	1.54
2	m	203	GLU	C-N	5.75	1.41	1.33
3	H	299	ARG	C-N	5.75	1.40	1.33
1	b	239	ARG	NE-CZ	5.75	1.39	1.33
3	I	249	ARG	CZ-NH1	5.75	1.40	1.32
3	J	310	PRO	C-N	5.75	1.42	1.33
3	L	47	GLU	CA-C	-5.75	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	95	SER	N-CA	-5.75	1.39	1.46
2	l	153	ASP	N-CA	-5.75	1.39	1.46
3	J	278	ARG	NE-CZ	5.75	1.39	1.33
2	4	56	THR	CA-C	-5.75	1.45	1.52
2	k	156	THR	C-N	5.75	1.38	1.33
3	J	128	TYR	C-N	5.75	1.39	1.33
1	b	107	ILE	CB-CG1	5.75	1.65	1.53
2	5	95	SER	C-N	5.75	1.41	1.33
3	K	309	VAL	N-CA	-5.75	1.39	1.46
1	e	22	PHE	C-N	5.74	1.41	1.34
1	f	17	PRO	CA-CB	5.74	1.63	1.53
2	2	128	ILE	CB-CG1	5.74	1.65	1.53
2	i	57	ALA	CA-C	-5.74	1.45	1.52
1	C	173	GLU	C-N	5.74	1.41	1.33
1	c	47	ILE	CB-CG1	5.74	1.65	1.53
2	2	73	GLU	C-N	5.74	1.41	1.33
2	i	162	ASP	N-CA	-5.74	1.39	1.46
2	h	134	GLU	CA-C	-5.74	1.45	1.52
2	6	156	THR	C-N	-5.74	1.27	1.34
1	g	20	ARG	CZ-NH2	5.74	1.41	1.33
3	J	170	VAL	CA-C	-5.74	1.46	1.52
2	h	33	MET	C-O	5.74	1.30	1.23
2	h	178	ARG	NE-CZ	5.74	1.39	1.33
1	g	244	LEU	CA-CB	5.73	1.62	1.53
1	d	217	ASP	CA-CB	5.73	1.61	1.53
1	E	19	GLY	CA-C	-5.73	1.43	1.51
1	g	177	LYS	C-N	5.73	1.41	1.33
3	J	144	GLY	C-N	5.73	1.41	1.33
2	n	132	ILE	C-N	5.73	1.40	1.33
1	b	26	TYR	C-N	5.73	1.41	1.33
1	C	86	ARG	CD-NE	5.73	1.54	1.46
1	d	100	ARG	CD-NE	5.73	1.54	1.46
1	f	214	VAL	CA-C	-5.73	1.45	1.52
2	2	198	GLN	C-N	5.73	1.41	1.33
2	3	131	ALA	CA-C	-5.73	1.45	1.52
2	6	39	SER	N-CA	-5.73	1.39	1.46
2	m	123	TYR	N-CA	-5.73	1.39	1.46
3	H	46	ARG	CA-CB	5.73	1.62	1.53
3	M	226	VAL	N-CA	-5.73	1.39	1.46
1	c	13	THR	CA-CB	5.73	1.61	1.52
2	7	100	SER	CA-C	-5.73	1.45	1.52
1	A	219	ARG	CA-CB	5.72	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	51	ARG	CD-NE	5.72	1.54	1.46
1	C	14	VAL	CA-C	-5.72	1.45	1.52
1	D	196	MET	N-CA	-5.72	1.39	1.46
1	g	98	ILE	C-N	5.72	1.41	1.33
2	4	203	GLU	C-N	5.72	1.40	1.33
3	L	210	GLU	CA-CB	5.72	1.63	1.53
1	d	174	PHE	N-CA	-5.72	1.39	1.46
3	H	43	ARG	CD-NE	5.72	1.54	1.46
3	H	104	ALA	C-O	-5.72	1.17	1.24
1	a	171	VAL	CA-C	-5.72	1.45	1.52
1	b	204	LEU	CA-CB	5.72	1.62	1.53
3	H	65	VAL	N-CA	-5.72	1.39	1.46
3	I	74	ASP	C-N	5.72	1.40	1.33
2	7	105	PRO	CA-C	-5.72	1.44	1.52
2	n	47	GLN	N-CA	-5.72	1.39	1.46
3	H	278	ARG	NE-CZ	5.72	1.39	1.33
1	C	111	GLU	CA-C	-5.71	1.45	1.52
1	A	139	ALA	C-N	5.71	1.39	1.33
1	A	198	LEU	N-CA	-5.71	1.39	1.46
1	C	66	LYS	C-N	5.71	1.41	1.33
1	c	85	ALA	CA-C	-5.71	1.45	1.52
3	H	305	ARG	NE-CZ	5.71	1.39	1.33
3	L	219	GLY	CA-C	-5.71	1.45	1.51
3	L	364	ARG	CZ-NH1	5.71	1.40	1.32
2	2	22	GLY	N-CA	-5.71	1.39	1.45
1	e	82	VAL	CA-C	-5.71	1.44	1.52
1	b	125	GLN	CA-CB	5.71	1.62	1.53
1	G	203	GLU	C-N	5.70	1.41	1.33
2	l	39	SER	N-CA	-5.70	1.38	1.46
3	I	276	ASP	C-N	5.70	1.41	1.33
1	a	12	ILE	N-CA	-5.70	1.38	1.46
2	k	120	LYS	N-CA	-5.70	1.38	1.46
2	h	154	ARG	C-N	5.70	1.41	1.33
1	E	182	ASP	CA-C	-5.70	1.45	1.52
2	h	79	ILE	N-CA	-5.70	1.39	1.46
2	j	68	ARG	C-N	5.70	1.41	1.33
3	I	221	ARG	CA-CB	5.70	1.62	1.53
3	I	387	THR	CA-C	-5.70	1.45	1.52
2	j	23	VAL	CA-C	-5.69	1.45	1.52
2	k	30	ARG	CA-C	-5.69	1.45	1.52
2	k	132	ILE	CA-C	-5.69	1.45	1.52
2	3	81	ARG	NE-CZ	5.69	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	11	ALA	CA-C	-5.69	1.45	1.52
3	K	316	GLY	C-N	5.69	1.41	1.33
3	H	273	ASP	CA-CB	-5.69	1.45	1.53
1	A	180	ARG	CZ-NH2	5.69	1.40	1.33
1	b	134	VAL	CA-CB	-5.69	1.47	1.55
1	D	245	LYS	CA-C	-5.69	1.45	1.52
3	M	224	ARG	CZ-NH2	5.69	1.40	1.33
1	b	180	ARG	CD-NE	5.69	1.54	1.46
3	M	293	LEU	CA-C	-5.69	1.45	1.52
1	C	126	TYR	CA-CB	5.68	1.62	1.53
3	L	105	ARG	N-CA	5.68	1.53	1.46
1	B	73	HIS	C-N	5.68	1.40	1.33
1	d	210	GLU	CA-C	5.68	1.59	1.52
1	D	235	ARG	CD-NE	5.68	1.54	1.46
2	i	153	ASP	CA-C	-5.68	1.45	1.52
2	n	63	ALA	N-CA	-5.68	1.39	1.46
1	d	239	ARG	CD-NE	5.67	1.54	1.46
1	g	124	THR	N-CA	-5.67	1.39	1.46
1	C	191	LEU	CA-C	-5.67	1.45	1.52
1	C	235	ARG	NE-CZ	5.67	1.39	1.33
3	I	14	LYS	C-O	-5.67	1.17	1.24
3	K	278	ARG	CD-NE	5.67	1.54	1.46
1	d	31	VAL	CA-C	-5.66	1.45	1.52
3	H	263	ARG	CZ-NH1	5.66	1.40	1.32
1	F	60	GLU	CA-CB	5.66	1.62	1.53
1	F	164	ILE	CA-CB	-5.66	1.45	1.55
2	2	118	GLU	CA-C	-5.66	1.45	1.52
3	L	59	ARG	CZ-NH2	5.66	1.40	1.33
3	M	171	GLY	CA-C	-5.66	1.43	1.51
1	c	129	VAL	CA-CB	-5.66	1.45	1.55
3	H	104	ALA	C-N	5.66	1.41	1.33
2	n	19	CYS	C-N	5.66	1.41	1.33
3	I	59	ARG	CD-NE	5.66	1.54	1.46
1	B	86	ARG	CZ-NH2	5.66	1.40	1.33
1	D	142	ASP	CA-C	-5.66	1.45	1.52
1	G	155	ALA	CA-C	-5.66	1.46	1.52
3	K	395	VAL	C-N	5.66	1.41	1.34
1	B	112	LEU	N-CA	-5.65	1.39	1.46
2	h	25	MET	CA-C	-5.65	1.45	1.52
2	l	83	ARG	CA-C	-5.65	1.45	1.52
1	a	28	ARG	CA-C	-5.65	1.45	1.52
1	G	136	LEU	CA-C	-5.65	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	169	ASN	C-N	5.65	1.41	1.33
2	j	51	ARG	NE-CZ	5.65	1.39	1.33
2	1	63	ALA	C-N	5.65	1.41	1.33
2	i	52	MET	CA-C	-5.65	1.45	1.52
3	K	304	ASP	CA-C	5.65	1.60	1.52
3	M	385	LYS	C-N	5.65	1.41	1.33
3	J	238	ILE	C-N	5.65	1.41	1.33
1	B	28	ARG	CZ-NH2	5.65	1.40	1.33
1	C	100	ARG	CZ-NH1	5.65	1.40	1.32
1	e	27	ALA	N-CA	-5.65	1.38	1.46
3	J	132	VAL	CA-CB	5.65	1.61	1.54
1	G	40	ILE	N-CA	-5.64	1.39	1.46
1	G	47	ILE	CA-C	-5.64	1.45	1.52
2	7	69	ILE	C-N	5.64	1.41	1.33
1	B	84	ASP	CA-C	5.64	1.60	1.52
1	B	168	ARG	CA-C	-5.64	1.45	1.52
1	b	221	PHE	CA-C	5.64	1.59	1.52
2	7	195	GLU	N-CA	-5.64	1.39	1.46
1	b	24	VAL	CA-CB	-5.64	1.47	1.54
1	e	53	ARG	CD-NE	5.64	1.54	1.46
2	m	167	LEU	C-N	5.64	1.41	1.33
3	K	156	ALA	CA-C	-5.64	1.45	1.52
1	a	85	ALA	CA-C	5.63	1.60	1.52
3	I	83	THR	CA-C	5.63	1.60	1.52
1	b	32	LYS	CA-CB	-5.63	1.44	1.53
1	C	210	GLU	C-N	5.63	1.40	1.33
2	7	79	ILE	CA-C	-5.63	1.45	1.52
1	a	73	HIS	CD2-NE2	5.63	1.44	1.37
1	F	67	ILE	CA-CB	5.63	1.60	1.54
1	F	219	ARG	NE-CZ	5.63	1.39	1.33
2	k	115	ILE	CA-C	-5.63	1.46	1.52
2	l	21	ASP	N-CA	-5.63	1.39	1.46
1	D	83	ALA	CA-CB	-5.63	1.44	1.53
1	F	223	GLU	CA-C	-5.63	1.45	1.52
2	1	17	LEU	C-N	5.63	1.40	1.33
3	I	170	VAL	CA-CB	-5.63	1.47	1.54
3	L	166	LEU	CA-C	-5.63	1.45	1.52
1	e	37	ALA	CA-C	-5.62	1.45	1.52
1	f	241	ARG	CD-NE	5.62	1.54	1.46
1	G	63	THR	CA-C	-5.62	1.46	1.52
2	k	121	SER	CA-C	-5.62	1.45	1.52
2	1	202	GLU	CA-CB	5.62	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	139	SER	CA-C	-5.62	1.47	1.53
3	M	278	ARG	CZ-NH2	5.62	1.40	1.33
3	J	278	ARG	CZ-NH1	5.62	1.40	1.32
2	m	140	THR	N-CA	-5.62	1.39	1.46
1	C	103	TYR	C-N	5.62	1.41	1.33
1	F	104	ASP	CA-C	-5.62	1.45	1.53
1	g	184	SER	C-N	5.62	1.41	1.33
2	h	170	ARG	NE-CZ	5.62	1.39	1.33
2	l	64	GLN	N-CA	-5.62	1.39	1.46
3	I	110	GLN	N-CA	5.62	1.53	1.46
3	J	173	GLU	N-CA	-5.62	1.38	1.46
1	d	207	GLU	N-CA	-5.62	1.40	1.46
2	l	80	ARG	CA-C	-5.62	1.45	1.52
2	i	98	LEU	CA-C	-5.61	1.45	1.52
2	k	201	PRO	CA-CB	-5.61	1.45	1.53
1	D	153	SER	C-N	5.61	1.41	1.33
1	G	137	LEU	CA-C	-5.61	1.46	1.52
1	g	130	ARG	CD-NE	5.61	1.54	1.46
2	k	64	GLN	C-N	5.61	1.41	1.33
3	L	28	ARG	CZ-NH2	5.61	1.40	1.33
1	d	162	THR	C-N	5.61	1.40	1.33
1	f	223	GLU	C-O	-5.61	1.17	1.23
2	3	30	ARG	CA-C	-5.61	1.45	1.52
3	H	327	LYS	CA-C	-5.61	1.45	1.52
3	K	189	THR	C-N	5.61	1.41	1.33
1	D	142	ASP	CA-CB	5.61	1.62	1.53
1	F	90	ASP	N-CA	-5.61	1.39	1.46
2	j	102	ARG	CZ-NH1	5.61	1.40	1.32
3	J	215	TYR	C-N	5.61	1.41	1.33
1	B	239	ARG	CD-NE	5.60	1.54	1.46
1	a	239	ARG	CZ-NH2	5.60	1.40	1.33
1	A	232	TYR	C-N	5.60	1.40	1.33
1	B	53	ARG	CD-NE	5.60	1.54	1.46
3	L	209	SER	CA-C	5.60	1.60	1.52
1	f	177	LYS	C-N	5.60	1.40	1.33
3	K	113	LEU	C-N	5.60	1.40	1.33
2	1	145	LEU	C-N	5.60	1.41	1.33
2	n	210	LYS	N-CA	-5.60	1.38	1.46
1	D	150	THR	CA-C	-5.59	1.46	1.52
2	2	155	PHE	CA-CB	5.59	1.61	1.53
1	D	214	VAL	N-CA	-5.59	1.38	1.46
2	7	184	ASP	C-N	5.59	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	248	ALA	C-N	5.59	1.40	1.33
1	e	53	ARG	CZ-NH2	5.59	1.40	1.33
2	1	176	MET	CA-C	-5.59	1.45	1.52
2	4	153	ASP	CA-CB	5.59	1.62	1.53
3	H	196	ALA	CA-C	-5.59	1.45	1.52
1	b	95	GLU	CA-C	-5.59	1.45	1.52
1	E	234	GLU	CA-CB	5.59	1.62	1.53
1	e	169	ASN	N-CA	-5.59	1.39	1.46
2	j	62	ASP	CA-C	-5.59	1.45	1.52
3	L	358	ALA	CA-CB	5.59	1.62	1.53
1	g	156	LEU	CA-CB	5.59	1.61	1.53
1	e	160	LYS	N-CA	-5.59	1.37	1.45
1	F	198	LEU	CA-C	-5.59	1.45	1.52
2	7	102	ARG	CD-NE	5.59	1.54	1.46
2	n	117	SER	C-O	5.59	1.30	1.24
3	I	146	LEU	N-CA	-5.59	1.40	1.46
1	e	178	GLU	CA-C	5.58	1.59	1.52
3	K	63	LEU	N-CA	-5.58	1.39	1.46
3	M	198	GLN	CA-C	-5.58	1.45	1.52
2	j	80	ARG	NE-CZ	5.58	1.39	1.33
3	J	24	ARG	CD-NE	5.58	1.54	1.46
3	I	78	VAL	CA-C	-5.58	1.45	1.52
3	K	213	GLN	C-N	5.58	1.40	1.33
1	C	195	ALA	N-CA	-5.58	1.39	1.46
3	M	199	THR	C-N	5.58	1.41	1.33
1	c	129	VAL	CA-C	-5.58	1.46	1.52
1	c	131	PRO	N-CD	-5.58	1.40	1.47
1	D	20	ARG	CA-C	-5.58	1.46	1.52
2	j	88	ARG	NE-CZ	5.58	1.39	1.33
2	5	158	GLU	N-CA	-5.58	1.39	1.46
1	F	66	LYS	C-N	5.57	1.40	1.33
3	I	305	ARG	CZ-NH2	5.57	1.40	1.33
3	L	105	ARG	CZ-NH1	5.57	1.40	1.32
1	E	30	ALA	CA-CB	5.57	1.61	1.53
1	A	33	ARG	CA-C	-5.57	1.45	1.52
1	c	179	TYR	N-CA	5.57	1.52	1.46
1	E	184	SER	C-N	5.57	1.41	1.33
1	G	27	ALA	N-CA	-5.57	1.38	1.46
2	m	193	GLU	CA-CB	5.57	1.62	1.53
2	1	102	ARG	NE-CZ	5.57	1.39	1.33
1	a	21	LEU	CA-C	-5.56	1.45	1.53
1	C	50	ALA	C-N	5.56	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	58	LEU	CA-CB	5.56	1.62	1.53
1	C	105	GLU	CA-C	-5.56	1.47	1.53
2	n	75	ASN	CA-CB	5.56	1.62	1.53
2	3	67	ALA	N-CA	-5.56	1.39	1.46
2	m	128	ILE	CA-C	-5.56	1.46	1.53
3	I	209	SER	CA-CB	5.56	1.63	1.53
2	6	108	VAL	CA-C	5.56	1.59	1.52
1	F	170	ALA	CA-C	-5.55	1.45	1.52
3	K	157	VAL	N-CA	-5.55	1.39	1.46
1	E	130	ARG	C-N	5.55	1.40	1.33
1	E	239	ARG	CA-C	-5.55	1.45	1.52
2	h	68	ARG	NE-CZ	5.55	1.39	1.33
1	G	8	TYR	CA-C	-5.55	1.44	1.52
1	g	234	GLU	CA-CB	5.55	1.62	1.53
2	i	191	ILE	CB-CG1	5.55	1.64	1.53
2	m	139	ALA	CA-C	-5.55	1.45	1.52
1	c	86	ARG	CA-CB	5.55	1.61	1.53
1	F	113	ALA	C-N	5.55	1.41	1.33
1	g	229	LEU	CA-CB	5.55	1.61	1.53
2	3	198	GLN	CA-C	-5.55	1.46	1.52
3	H	328	MET	CA-C	-5.55	1.47	1.53
1	F	69	LYS	CA-CB	5.54	1.62	1.53
1	c	101	LEU	CA-CB	5.54	1.62	1.53
1	E	167	GLY	C-N	5.54	1.40	1.33
1	f	180	ARG	NE-CZ	5.54	1.39	1.33
2	j	124	SER	CA-CB	-5.54	1.43	1.53
2	4	51	ARG	CD-NE	5.54	1.54	1.46
3	I	391	ASP	CA-CB	5.54	1.62	1.53
2	i	31	ALA	CA-C	5.54	1.59	1.52
1	d	166	MET	N-CA	-5.54	1.39	1.46
2	1	69	ILE	C-N	5.54	1.40	1.33
1	e	208	ASN	N-CA	-5.54	1.40	1.46
2	k	174	SER	CA-CB	5.54	1.62	1.53
1	A	123	TYR	CG-CD2	5.54	1.50	1.39
1	b	182	ASP	CA-CB	5.54	1.61	1.53
2	n	54	MET	CA-C	-5.54	1.45	1.52
3	J	52	ARG	CD-NE	5.54	1.54	1.46
2	k	45	ILE	C-N	5.54	1.42	1.33
1	C	234	GLU	CA-C	-5.53	1.46	1.52
1	c	185	PHE	C-N	5.53	1.41	1.33
3	M	201	ALA	N-CA	5.53	1.52	1.45
1	b	27	ALA	CA-C	5.53	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	115	LYS	C-N	-5.53	1.27	1.33
3	K	320	ILE	CA-C	-5.53	1.45	1.52
1	C	50	ALA	CA-C	-5.53	1.45	1.52
2	j	122	ILE	CA-C	-5.53	1.45	1.52
2	i	105	PRO	CA-CB	-5.53	1.46	1.53
2	3	88	ARG	CZ-NH2	5.52	1.40	1.33
2	j	77	TYR	N-CA	-5.52	1.39	1.46
2	6	98	LEU	CA-CB	5.52	1.62	1.53
3	I	141	GLU	CA-C	-5.52	1.45	1.52
1	A	184	SER	CA-C	5.52	1.60	1.53
1	F	159	TYR	N-CA	-5.52	1.38	1.45
2	2	149	GLY	N-CA	-5.52	1.37	1.45
3	L	371	THR	CA-CB	5.52	1.62	1.53
2	h	68	ARG	CA-CB	5.52	1.62	1.53
3	M	247	ALA	C-N	5.52	1.40	1.33
1	A	91	ARG	CA-CB	5.51	1.62	1.53
2	2	88	ARG	NE-CZ	5.51	1.39	1.33
2	m	108	VAL	C-N	5.51	1.40	1.33
2	7	204	VAL	CA-C	5.51	1.59	1.52
3	I	267	GLN	C-N	5.51	1.41	1.33
2	4	113	GLY	N-CA	-5.51	1.39	1.45
3	K	221	ARG	CD-NE	5.51	1.53	1.46
2	2	145	LEU	C-N	5.51	1.41	1.33
2	j	50	ASP	CA-C	-5.51	1.45	1.52
3	H	155	GLU	CA-C	-5.51	1.45	1.52
3	H	262	GLN	N-CA	-5.51	1.38	1.46
1	d	40	ILE	N-CA	-5.51	1.39	1.46
2	5	114	GLY	CA-C	-5.51	1.45	1.52
1	g	122	GLN	C-N	5.51	1.41	1.33
2	m	32	THR	N-CA	-5.51	1.39	1.45
1	D	201	GLU	CA-C	-5.50	1.46	1.53
2	k	124	SER	C-N	-5.50	1.26	1.33
1	E	138	ILE	CA-C	-5.50	1.46	1.52
1	g	140	GLY	N-CA	-5.50	1.39	1.45
1	g	208	ASN	CA-CB	5.50	1.63	1.53
3	L	221	ARG	NE-CZ	5.50	1.39	1.33
3	J	274	GLY	CA-C	5.50	1.58	1.52
3	L	48	VAL	C-N	5.50	1.40	1.33
3	J	302	ARG	CA-CB	5.50	1.63	1.53
1	a	41	LYS	CA-C	-5.50	1.46	1.52
1	g	53	ARG	CD-NE	5.50	1.53	1.46
3	H	115	ILE	C-N	-5.50	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	107	ALA	CA-C	-5.50	1.46	1.52
2	n	118	GLU	CA-C	-5.50	1.45	1.52
3	I	46	ARG	CA-CB	5.50	1.62	1.53
2	6	147	ALA	CA-CB	5.50	1.61	1.53
1	B	101	LEU	C-O	-5.49	1.17	1.24
2	k	15	VAL	N-CA	5.49	1.52	1.46
1	C	95	GLU	C-N	5.49	1.41	1.33
1	E	133	GLY	CA-C	-5.49	1.44	1.51
1	e	16	SER	CA-C	-5.49	1.45	1.53
1	F	205	VAL	CA-C	-5.49	1.47	1.52
1	f	153	SER	N-CA	-5.49	1.39	1.46
1	C	80	GLY	C-N	5.49	1.40	1.33
1	G	6	MET	CA-CB	5.49	1.62	1.53
3	J	76	ARG	NE-CZ	5.49	1.39	1.33
2	k	26	ALA	N-CA	-5.49	1.39	1.46
1	A	239	ARG	CD-NE	5.49	1.53	1.46
1	F	213	TYR	N-CA	-5.49	1.39	1.46
1	G	54	VAL	C-N	5.49	1.41	1.32
2	3	37	ILE	CA-CB	5.49	1.61	1.54
2	5	155	PHE	CA-C	-5.49	1.45	1.52
3	L	97	GLU	N-CA	-5.49	1.39	1.46
2	3	165	VAL	CA-CB	-5.48	1.47	1.54
3	L	244	ASP	CA-CB	5.48	1.60	1.53
1	C	213	TYR	CA-CB	5.48	1.63	1.53
2	2	79	ILE	CA-C	-5.48	1.45	1.52
2	2	123	TYR	CA-C	-5.48	1.46	1.52
2	j	154	ARG	N-CA	-5.48	1.39	1.46
2	4	76	LEU	C-N	5.48	1.41	1.33
2	6	170	ARG	CZ-NH1	5.48	1.40	1.32
3	J	222	LEU	CA-CB	5.48	1.62	1.53
1	c	43	LYS	C-N	5.48	1.42	1.33
1	e	100	ARG	CD-NE	5.48	1.53	1.46
1	f	190	VAL	N-CA	-5.48	1.39	1.46
2	j	14	THR	CA-C	-5.48	1.46	1.52
2	5	179	ASP	N-CA	-5.48	1.39	1.45
3	M	68	VAL	CA-C	-5.48	1.46	1.52
3	J	142	ASP	CB-CG	5.48	1.65	1.52
2	3	170	ARG	CD-NE	5.48	1.53	1.46
1	c	239	ARG	CA-C	-5.48	1.45	1.52
2	1	80	ARG	N-CA	-5.48	1.39	1.46
2	3	35	ASN	CA-C	-5.48	1.46	1.52
3	L	190	LEU	CA-CB	5.48	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	249	ARG	CD-NE	5.48	1.53	1.46
2	4	196	PHE	N-CA	-5.48	1.39	1.46
2	l	83	ARG	NE-CZ	5.48	1.39	1.33
1	C	41	LYS	N-CA	-5.47	1.39	1.46
1	F	128	GLY	C-N	5.47	1.39	1.33
2	i	129	GLY	CA-C	-5.47	1.46	1.51
2	j	84	LYS	CA-C	-5.47	1.46	1.52
1	E	131	PRO	C-N	5.47	1.41	1.33
2	j	131	ALA	N-CA	-5.47	1.39	1.46
2	k	167	LEU	CA-C	-5.47	1.45	1.52
3	M	395	VAL	CA-CB	-5.47	1.48	1.54
1	A	218	ASP	C-N	5.47	1.41	1.33
1	D	120	LYS	CA-C	-5.47	1.45	1.52
1	e	97	GLN	N-CA	5.47	1.52	1.46
2	2	37	ILE	C-N	5.47	1.40	1.33
2	3	206	GLN	N-CA	-5.47	1.38	1.46
2	l	13	THR	C-N	5.47	1.41	1.33
1	A	71	ASP	CA-C	-5.47	1.45	1.52
1	b	181	ASP	CA-C	-5.47	1.45	1.52
1	e	103	TYR	CA-C	-5.47	1.44	1.52
3	L	203	PHE	CA-CB	5.47	1.60	1.53
1	C	86	ARG	NE-CZ	5.47	1.39	1.33
1	D	20	ARG	CZ-NH2	5.46	1.40	1.33
1	E	126	TYR	N-CA	-5.46	1.38	1.46
3	I	105	ARG	CD-NE	5.46	1.53	1.46
3	I	127	VAL	CA-CB	-5.46	1.47	1.54
3	I	252	ASN	C-N	5.46	1.41	1.33
1	F	107	ILE	CA-CB	5.46	1.59	1.54
1	F	209	ILE	CA-C	-5.46	1.46	1.52
2	1	69	ILE	N-CA	-5.46	1.40	1.46
2	4	51	ARG	NE-CZ	5.46	1.39	1.33
1	b	19	GLY	C-N	5.46	1.41	1.33
2	n	196	PHE	CA-C	-5.46	1.47	1.53
1	G	131	PRO	CA-C	-5.46	1.45	1.52
2	3	166	GLU	CA-C	-5.46	1.45	1.52
3	I	295	PRO	C-N	-5.46	1.26	1.33
2	h	91	ALA	N-CA	-5.46	1.39	1.46
2	j	89	ALA	N-CA	-5.45	1.39	1.46
3	H	83	THR	CA-CB	-5.45	1.44	1.53
3	I	335	ASP	CA-C	-5.45	1.47	1.53
1	f	64	ILE	C-N	5.45	1.41	1.33
3	I	386	THR	CA-C	-5.45	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	13	THR	CA-C	-5.45	1.45	1.52
1	E	114	LYS	CA-CB	5.45	1.61	1.53
1	e	59	LEU	CB-CG	5.45	1.64	1.53
1	D	42	CYS	CA-CB	-5.45	1.46	1.53
1	f	142	ASP	CA-CB	5.45	1.62	1.53
2	1	178	ARG	C-N	5.45	1.40	1.33
2	j	211	PHE	CA-CB	5.45	1.62	1.53
3	L	41	ARG	C-N	5.45	1.40	1.33
3	H	309	VAL	C-O	-5.44	1.18	1.23
3	L	181	TYR	CA-C	-5.44	1.45	1.52
1	a	20	ARG	NE-CZ	5.44	1.39	1.33
1	f	228	GLU	N-CA	-5.44	1.39	1.45
2	4	78	GLU	CA-CB	5.44	1.61	1.53
1	A	119	PHE	C-O	5.44	1.30	1.24
2	h	147	ALA	CA-CB	5.44	1.61	1.53
2	3	30	ARG	CZ-NH2	5.44	1.40	1.33
2	7	182	SER	CA-C	-5.44	1.46	1.52
3	I	247	ALA	CA-CB	5.44	1.62	1.53
3	L	152	GLU	C-O	-5.44	1.17	1.24
1	G	239	ARG	CZ-NH2	5.44	1.40	1.33
2	2	68	ARG	NE-CZ	5.44	1.39	1.33
2	k	79	ILE	C-N	5.44	1.41	1.33
1	f	241	ARG	NE-CZ	5.43	1.39	1.33
2	n	20	LYS	CA-C	-5.43	1.45	1.52
1	D	166	MET	CA-CB	5.43	1.61	1.53
2	k	42	ALA	N-CA	-5.43	1.39	1.45
2	7	193	GLU	C-N	5.43	1.41	1.33
3	L	159	LEU	N-CA	-5.43	1.41	1.46
3	M	237	ILE	C-N	5.43	1.41	1.33
1	f	130	ARG	NE-CZ	5.43	1.39	1.33
2	l	150	VAL	C-N	5.43	1.41	1.33
1	d	214	VAL	N-CA	-5.43	1.39	1.46
1	g	92	ALA	N-CA	-5.43	1.39	1.46
2	k	62	ASP	N-CA	-5.43	1.39	1.46
3	M	367	ARG	CZ-NH2	5.43	1.40	1.33
1	f	112	LEU	N-CA	-5.43	1.40	1.46
2	1	195	GLU	N-CA	-5.43	1.39	1.45
3	L	41	ARG	CZ-NH1	5.43	1.40	1.32
1	E	242	GLU	N-CA	-5.42	1.39	1.46
3	I	53	SER	C-N	5.42	1.41	1.33
2	k	73	GLU	CA-C	-5.42	1.45	1.52
1	G	47	ILE	CB-CG1	5.42	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	180	ARG	CD-NE	5.42	1.53	1.46
1	g	219	ARG	CA-C	-5.42	1.46	1.53
2	6	162	ASP	CA-CB	5.42	1.61	1.53
3	K	85	PRO	N-CA	-5.42	1.40	1.47
3	M	64	LEU	CA-CB	5.42	1.61	1.53
1	B	33	ARG	CA-C	-5.42	1.45	1.52
2	l	46	TYR	CA-C	-5.42	1.46	1.52
2	l	107	LEU	CA-C	-5.42	1.47	1.53
3	I	361	PHE	C-O	-5.42	1.17	1.24
1	D	58	LEU	C-N	5.42	1.41	1.33
1	G	55	GLY	C-N	5.42	1.41	1.33
1	G	129	VAL	CA-CB	-5.42	1.49	1.55
2	l	132	ILE	C-N	5.42	1.41	1.33
3	L	295	PRO	C-N	5.42	1.40	1.33
3	J	355	CYS	CA-C	-5.42	1.45	1.52
1	B	12	ILE	CA-CB	5.42	1.62	1.54
1	B	235	ARG	NE-CZ	5.41	1.39	1.33
1	F	10	ARG	NE-CZ	5.41	1.39	1.33
2	l	152	GLU	CA-C	-5.41	1.45	1.52
1	G	28	ARG	NE-CZ	5.41	1.39	1.33
1	G	41	LYS	CA-C	-5.41	1.46	1.52
1	G	238	GLU	C-N	5.41	1.41	1.33
3	H	316	GLY	CA-C	-5.41	1.45	1.52
1	d	119	PHE	C-N	5.41	1.41	1.33
3	K	295	PRO	CA-C	-5.41	1.44	1.52
3	K	41	ARG	CD-NE	5.41	1.53	1.46
3	H	27	TYR	N-CA	-5.41	1.39	1.46
3	M	52	ARG	NE-CZ	5.41	1.39	1.33
3	M	80	LYS	CA-C	-5.41	1.46	1.52
3	K	160	PRO	CA-C	-5.40	1.43	1.52
3	L	241	ASP	C-N	5.40	1.40	1.33
1	A	164	ILE	CA-C	5.40	1.59	1.52
2	2	208	LEU	N-CA	5.40	1.53	1.46
2	m	168	ALA	N-CA	-5.40	1.39	1.46
1	C	223	GLU	C-N	5.40	1.39	1.33
1	E	142	ASP	N-CA	-5.40	1.39	1.46
1	E	211	VAL	CA-C	5.40	1.59	1.52
3	H	182	GLY	CA-C	-5.40	1.44	1.51
3	L	36	PHE	C-N	5.40	1.40	1.33
3	M	41	ARG	CZ-NH2	5.40	1.40	1.33
2	2	83	ARG	CZ-NH1	5.40	1.40	1.32
2	i	154	ARG	CA-CB	-5.40	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	51	ARG	CD-NE	5.40	1.53	1.46
1	b	196	MET	C-O	-5.40	1.17	1.24
1	D	86	ARG	CZ-NH2	5.40	1.40	1.33
2	i	51	ARG	CD-NE	5.40	1.53	1.46
2	m	107	LEU	CA-CB	5.40	1.60	1.53
3	J	232	GLU	CA-C	5.40	1.60	1.52
1	G	208	ASN	CA-CB	5.40	1.63	1.53
1	F	40	ILE	C-O	-5.39	1.18	1.24
2	k	196	PHE	CA-CB	5.39	1.60	1.53
3	H	73	GLU	C-N	5.39	1.41	1.33
1	A	187	ASP	C-N	5.39	1.41	1.33
1	E	168	ARG	CD-NE	5.39	1.53	1.46
1	f	202	SER	N-CA	-5.39	1.39	1.46
1	g	141	VAL	CA-C	-5.39	1.45	1.52
2	5	34	GLY	CA-C	5.39	1.59	1.51
3	H	115	ILE	C-O	-5.39	1.18	1.24
3	H	192	ALA	CA-C	5.39	1.59	1.52
1	d	219	ARG	CD-NE	5.39	1.53	1.46
1	g	202	SER	CA-CB	5.39	1.61	1.53
2	4	29	LYS	CA-CB	5.39	1.60	1.53
1	a	228	GLU	C-N	5.39	1.41	1.34
2	h	67	ALA	CA-C	-5.39	1.45	1.52
3	K	259	ARG	CA-CB	-5.39	1.44	1.53
1	B	166	MET	C-N	5.39	1.42	1.33
2	h	33	MET	CA-C	-5.39	1.45	1.52
1	A	167	GLY	C-N	5.39	1.40	1.33
1	f	15	PHE	N-CA	-5.39	1.39	1.46
1	f	44	GLU	C-N	5.39	1.41	1.32
2	h	47	GLN	CA-C	-5.39	1.46	1.52
2	h	196	PHE	C-N	5.39	1.41	1.33
1	B	230	LYS	CA-C	5.38	1.58	1.52
1	B	241	ARG	CZ-NH2	5.38	1.40	1.33
2	j	70	ILE	C-O	-5.38	1.17	1.24
2	l	32	THR	CA-C	-5.38	1.46	1.52
1	D	144	VAL	C-N	5.38	1.39	1.33
3	H	47	GLU	C-N	5.38	1.40	1.33
3	J	24	ARG	NE-CZ	5.38	1.39	1.33
1	A	43	LYS	N-CA	-5.38	1.39	1.46
2	2	83	ARG	NE-CZ	5.38	1.39	1.33
3	K	299	ARG	C-N	5.38	1.39	1.34
1	d	49	ILE	CB-CG1	5.38	1.64	1.53
2	1	204	VAL	C-O	5.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	364	ARG	CA-C	-5.38	1.45	1.52
3	M	238	ILE	N-CA	-5.38	1.39	1.46
1	E	156	LEU	CA-CB	5.38	1.63	1.53
2	4	43	LYS	CA-CB	5.38	1.61	1.53
2	5	191	ILE	CA-CB	5.38	1.61	1.54
1	c	122	GLN	C-N	5.38	1.41	1.33
1	E	122	GLN	CA-C	-5.38	1.45	1.52
2	i	168	ALA	CA-C	-5.37	1.45	1.52
3	H	258	ASP	CA-CB	-5.37	1.47	1.53
3	J	205	ARG	C-N	5.37	1.40	1.33
1	b	152	PRO	N-CA	5.37	1.53	1.47
1	D	74	ILE	CB-CG1	5.37	1.64	1.53
3	I	255	THR	CA-C	-5.37	1.45	1.52
3	K	214	LYS	C-N	5.37	1.41	1.33
1	d	88	LEU	N-CA	-5.37	1.40	1.46
2	n	107	LEU	CA-C	-5.37	1.45	1.52
3	L	396	MET	CA-CB	5.37	1.62	1.53
2	2	165	VAL	CA-C	-5.37	1.45	1.52
2	i	81	ARG	NE-CZ	5.37	1.39	1.33
2	5	49	ALA	CA-C	-5.37	1.46	1.53
3	J	183	PRO	CA-C	-5.37	1.47	1.52
1	G	70	ILE	CA-C	-5.37	1.46	1.52
2	6	95	SER	CA-C	-5.37	1.46	1.52
3	H	139	SER	CA-CB	5.37	1.64	1.54
3	J	25	GLU	C-N	5.37	1.41	1.33
3	J	305	ARG	NE-CZ	5.37	1.39	1.33
2	1	151	LEU	CA-C	-5.36	1.46	1.52
2	h	159	ILE	CA-CB	-5.36	1.47	1.54
2	k	110	LEU	C-O	5.36	1.30	1.23
2	5	171	ALA	CA-C	-5.36	1.45	1.52
2	6	106	TYR	N-CA	-5.36	1.42	1.47
2	l	147	ALA	CA-CB	5.36	1.61	1.53
1	a	209	ILE	CA-C	-5.36	1.46	1.52
2	m	117	SER	CA-C	-5.36	1.45	1.52
3	I	34	LYS	C-N	5.36	1.41	1.33
1	C	178	GLU	C-N	5.36	1.40	1.33
2	i	70	ILE	N-CA	-5.36	1.40	1.46
2	j	83	ARG	N-CA	-5.36	1.39	1.45
2	4	212	ARG	NE-CZ	5.36	1.39	1.33
1	B	50	ALA	CA-C	-5.36	1.46	1.52
1	C	195	ALA	C-N	5.36	1.41	1.33
3	I	64	LEU	CA-C	-5.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	154	ARG	N-CA	-5.36	1.39	1.46
1	b	144	VAL	C-O	-5.35	1.20	1.24
1	b	206	PRO	CA-C	-5.35	1.43	1.52
2	j	54	MET	CA-C	-5.35	1.46	1.52
1	b	213	TYR	CA-C	-5.35	1.46	1.52
2	k	72	ILE	C-N	5.35	1.41	1.33
1	D	173	GLU	CA-C	-5.35	1.45	1.52
3	H	299	ARG	NE-CZ	5.35	1.39	1.33
3	K	289	ARG	CZ-NH2	5.35	1.40	1.33
1	F	60	GLU	CA-C	-5.35	1.45	1.52
2	6	105	PRO	CA-CB	-5.35	1.46	1.53
3	I	289	ARG	NE-CZ	5.35	1.39	1.33
2	5	145	LEU	CA-C	-5.35	1.46	1.52
3	K	368	ALA	CA-C	-5.35	1.45	1.52
1	a	130	ARG	C-N	5.34	1.40	1.33
3	I	52	ARG	CZ-NH2	5.34	1.40	1.33
3	L	317	ARG	N-CA	-5.34	1.39	1.46
1	g	74	ILE	CA-C	-5.34	1.46	1.52
2	6	154	ARG	CZ-NH2	5.34	1.40	1.33
3	H	209	SER	N-CA	-5.34	1.39	1.46
1	E	238	GLU	N-CA	-5.34	1.40	1.46
1	f	148	TYR	CA-C	-5.34	1.46	1.52
2	2	28	GLU	CA-C	-5.34	1.46	1.52
2	7	69	ILE	CA-CB	-5.34	1.48	1.54
1	a	133	GLY	CA-C	-5.34	1.44	1.51
1	D	153	SER	CA-CB	5.34	1.61	1.53
1	d	135	SER	CA-C	5.34	1.59	1.52
2	4	79	ILE	CA-C	-5.34	1.46	1.52
3	K	162	LEU	CA-C	-5.34	1.45	1.52
3	L	287	THR	N-CA	-5.34	1.39	1.45
1	B	77	ALA	CA-C	-5.33	1.45	1.53
1	d	135	SER	C-N	5.33	1.41	1.33
2	m	108	VAL	CA-C	-5.33	1.46	1.52
3	L	76	ARG	C-N	5.33	1.40	1.33
1	a	149	GLU	CA-C	-5.33	1.46	1.52
1	E	201	GLU	C-N	5.33	1.40	1.33
1	G	205	VAL	N-CA	-5.33	1.40	1.46
2	5	200	SER	CA-CB	5.33	1.61	1.53
1	c	53	ARG	NE-CZ	5.33	1.39	1.33
2	4	195	GLU	CA-C	-5.33	1.46	1.52
3	H	53	SER	CA-C	-5.33	1.46	1.52
1	e	12	ILE	CA-C	-5.33	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	131	PRO	C-N	5.33	1.40	1.33
2	k	19	CYS	CA-C	-5.33	1.46	1.52
2	6	16	GLY	C-O	-5.33	1.16	1.23
3	L	29	ARG	CA-CB	5.33	1.61	1.53
3	M	77	VAL	CA-CB	-5.33	1.47	1.54
1	a	168	ARG	CA-CB	5.33	1.61	1.53
2	i	99	ASN	CA-C	5.33	1.59	1.52
3	L	266	MET	CA-CB	5.32	1.61	1.53
1	e	184	SER	C-O	5.32	1.30	1.23
1	e	122	GLN	CD-NE2	5.32	1.44	1.33
1	F	77	ALA	CA-C	-5.32	1.46	1.52
1	g	76	ALA	N-CA	-5.32	1.39	1.45
2	1	72	ILE	C-N	5.32	1.41	1.33
2	l	123	TYR	CA-C	-5.32	1.46	1.52
2	m	102	ARG	CZ-NH1	5.32	1.40	1.32
1	D	29	GLU	C-N	5.32	1.41	1.33
1	g	164	ILE	CA-C	-5.32	1.46	1.52
3	I	367	ARG	CZ-NH2	5.32	1.40	1.33
1	d	51	ASP	N-CA	-5.32	1.39	1.46
2	2	85	PRO	N-CA	-5.32	1.40	1.46
2	3	148	TYR	C-O	-5.32	1.17	1.24
2	l	68	ARG	CD-NE	5.32	1.53	1.46
3	L	134	GLU	CA-C	-5.32	1.45	1.52
1	c	98	ILE	CB-CG1	5.31	1.64	1.53
1	g	58	LEU	CA-C	-5.31	1.45	1.52
1	g	219	ARG	NE-CZ	5.31	1.38	1.33
3	M	121	THR	C-N	5.31	1.40	1.33
1	a	91	ARG	CZ-NH2	5.31	1.40	1.33
1	b	205	VAL	C-O	-5.31	1.20	1.24
1	F	42	CYS	CA-C	-5.31	1.46	1.52
1	g	157	LEU	C-N	5.31	1.41	1.33
2	i	19	CYS	CA-CB	-5.31	1.45	1.53
2	5	74	ALA	CA-CB	5.31	1.61	1.53
3	M	249	ARG	NE-CZ	5.31	1.38	1.33
1	C	241	ARG	NE-CZ	5.30	1.38	1.33
1	e	32	LYS	N-CA	-5.30	1.40	1.46
1	G	195	ALA	CA-C	5.30	1.59	1.52
2	7	54	MET	N-CA	-5.30	1.39	1.46
3	M	109	ASN	N-CA	-5.30	1.39	1.46
3	M	358	ALA	CA-CB	5.30	1.61	1.53
3	J	131	GLU	C-N	5.30	1.40	1.33
1	b	142	ASP	CA-C	-5.30	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	63	THR	C-N	5.30	1.40	1.33
3	K	28	ARG	CZ-NH2	5.30	1.40	1.33
1	d	146	LYS	CA-C	-5.30	1.46	1.52
1	f	180	ARG	CZ-NH2	5.30	1.40	1.33
3	I	171	GLY	N-CA	-5.30	1.37	1.45
3	L	225	GLU	CA-C	-5.30	1.45	1.52
1	a	47	ILE	C-N	5.30	1.40	1.33
1	B	41	LYS	CA-CB	5.30	1.62	1.53
1	D	93	ARG	CZ-NH2	5.30	1.40	1.33
3	I	28	ARG	CZ-NH2	5.30	1.40	1.33
2	6	134	GLU	C-N	5.30	1.40	1.33
3	H	334	VAL	CA-CB	-5.30	1.47	1.54
3	M	43	ARG	CD-NE	5.30	1.53	1.46
1	A	107	ILE	CA-C	-5.29	1.46	1.52
1	D	216	VAL	C-O	-5.29	1.18	1.24
2	2	88	ARG	CZ-NH2	5.29	1.40	1.33
3	M	178	VAL	C-N	5.29	1.41	1.33
1	c	65	GLU	N-CA	-5.29	1.39	1.46
2	i	85	PRO	N-CA	-5.29	1.40	1.46
2	3	17	LEU	N-CA	5.29	1.52	1.46
3	H	70	ASP	N-CA	-5.29	1.39	1.45
3	H	82	SER	CA-CB	5.29	1.62	1.53
3	L	279	GLY	C-N	5.29	1.39	1.33
3	M	133	GLU	N-CA	-5.29	1.40	1.46
3	J	259	ARG	NE-CZ	5.29	1.38	1.33
1	b	168	ARG	NE-CZ	5.29	1.38	1.33
1	D	86	ARG	CD-NE	5.29	1.53	1.46
2	n	108	VAL	N-CA	-5.29	1.40	1.46
3	J	200	ARG	CD-NE	5.29	1.53	1.46
1	a	58	LEU	N-CA	-5.29	1.39	1.46
2	j	14	THR	C-N	5.29	1.40	1.33
3	H	341	ARG	CD-NE	5.29	1.53	1.46
2	i	171	ALA	CA-C	-5.28	1.46	1.52
1	a	100	ARG	CZ-NH1	5.28	1.40	1.32
1	D	184	SER	N-CA	-5.28	1.38	1.45
1	G	68	TYR	N-CA	-5.28	1.39	1.46
2	2	177	LYS	CA-C	-5.28	1.45	1.52
2	n	150	VAL	C-N	5.28	1.40	1.33
1	e	239	ARG	C-N	5.28	1.40	1.33
1	f	147	LEU	N-CA	-5.28	1.39	1.46
3	L	114	ALA	C-O	-5.28	1.17	1.23
1	D	56	SER	C-N	5.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	78	THR	N-CA	-5.27	1.39	1.45
1	d	239	ARG	CA-C	-5.27	1.45	1.52
1	g	93	ARG	CD-NE	5.27	1.53	1.46
2	3	117	SER	N-CA	-5.27	1.39	1.46
2	n	116	ASP	CA-C	-5.27	1.46	1.52
3	H	155	GLU	C-N	5.27	1.41	1.33
3	J	319	GLN	C-N	5.27	1.40	1.33
1	c	113	ALA	C-N	5.27	1.40	1.33
1	G	111	GLU	N-CA	-5.27	1.39	1.46
1	D	123	TYR	CA-CB	5.27	1.61	1.53
1	f	190	VAL	C-N	5.27	1.41	1.33
2	6	158	GLU	C-O	-5.27	1.17	1.23
3	K	297	ILE	N-CA	-5.27	1.39	1.46
1	E	231	PRO	CA-C	5.27	1.60	1.52
1	F	243	LEU	CA-C	-5.27	1.45	1.52
2	6	134	GLU	CA-C	-5.27	1.46	1.52
3	H	259	ARG	NE-CZ	5.27	1.38	1.33
1	C	48	LEU	N-CA	-5.27	1.40	1.46
2	k	45	ILE	CA-C	-5.27	1.46	1.52
2	l	57	ALA	N-CA	-5.27	1.39	1.46
3	M	251	THR	CA-C	5.27	1.58	1.52
1	B	211	VAL	N-CA	-5.26	1.40	1.46
1	e	53	ARG	NE-CZ	5.26	1.38	1.33
2	1	21	ASP	CA-C	-5.26	1.45	1.52
2	j	209	ALA	N-CA	-5.26	1.39	1.46
1	g	36	THR	C-N	5.26	1.40	1.33
1	g	148	TYR	C-N	5.26	1.40	1.33
3	J	93	GLN	C-N	5.26	1.40	1.33
1	a	164	ILE	C-O	-5.26	1.18	1.23
1	b	13	THR	C-O	-5.26	1.17	1.23
1	d	183	LEU	C-N	5.26	1.40	1.33
1	E	226	PRO	N-CA	-5.26	1.40	1.47
1	F	91	ARG	CA-CB	-5.26	1.45	1.53
1	G	229	LEU	N-CA	-5.26	1.39	1.46
2	l	189	VAL	C-N	5.26	1.40	1.33
3	M	302	ARG	CZ-NH2	5.26	1.40	1.33
1	A	211	VAL	N-CA	-5.26	1.40	1.46
2	1	147	ALA	CA-C	5.26	1.59	1.52
3	H	138	VAL	C-N	-5.26	1.26	1.33
2	6	161	VAL	CA-C	-5.26	1.45	1.52
3	K	263	ARG	CD-NE	5.26	1.53	1.46
2	k	166	GLU	C-N	5.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	26	LEU	CA-C	-5.25	1.46	1.52
1	c	59	LEU	C-N	5.25	1.41	1.33
1	F	185	PHE	CA-CB	5.25	1.61	1.53
3	H	353	ALA	N-CA	-5.25	1.39	1.46
3	L	123	LYS	C-N	5.25	1.39	1.33
3	L	305	ARG	CD-NE	5.25	1.53	1.46
3	L	27	TYR	C-N	5.25	1.40	1.33
3	M	336	PHE	N-CA	-5.25	1.39	1.46
1	a	60	GLU	N-CA	-5.25	1.39	1.45
2	i	30	ARG	CZ-NH2	5.25	1.40	1.33
3	J	32	ASP	CA-C	-5.25	1.46	1.52
1	B	15	PHE	CG-CD1	5.25	1.49	1.38
1	C	46	VAL	N-CA	5.25	1.52	1.46
1	c	67	ILE	CA-C	-5.25	1.46	1.52
2	6	83	ARG	N-CA	-5.25	1.39	1.46
3	H	336	PHE	C-N	5.25	1.41	1.33
3	K	278	ARG	C-N	5.25	1.39	1.33
3	L	29	ARG	NE-CZ	5.25	1.38	1.33
2	j	142	SER	CA-C	-5.25	1.45	1.52
3	I	210	GLU	N-CA	5.25	1.52	1.46
2	2	175	ALA	C-N	5.25	1.40	1.33
2	4	101	TYR	N-CA	-5.25	1.39	1.46
3	J	159	LEU	N-CA	-5.25	1.41	1.46
1	a	156	LEU	C-N	5.24	1.40	1.33
1	a	181	ASP	C-N	5.24	1.40	1.33
2	j	18	VAL	N-CA	-5.24	1.39	1.46
1	E	17	PRO	C-N	5.24	1.41	1.33
1	a	81	LEU	N-CA	-5.24	1.39	1.45
2	n	180	SER	CA-CB	5.24	1.59	1.52
1	b	180	ARG	CZ-NH1	5.24	1.40	1.32
1	E	117	CYS	N-CA	-5.24	1.39	1.46
2	1	139	ALA	C-N	5.24	1.40	1.33
2	n	209	ALA	CA-C	-5.24	1.45	1.52
3	L	329	LYS	C-N	5.24	1.41	1.33
1	E	177	LYS	C-N	5.24	1.40	1.33
1	E	19	GLY	N-CA	-5.24	1.37	1.45
3	L	27	TYR	C-O	-5.24	1.18	1.24
3	L	127	VAL	C-N	5.24	1.41	1.33
1	d	87	VAL	CA-CB	-5.23	1.47	1.54
2	4	18	VAL	CA-CB	-5.23	1.47	1.54
3	K	69	SER	CA-C	-5.23	1.45	1.52
1	B	28	ARG	CZ-NH1	5.23	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	166	GLU	N-CA	-5.23	1.39	1.46
2	3	67	ALA	C-O	-5.23	1.17	1.24
2	k	106	TYR	CA-CB	5.23	1.63	1.53
3	L	305	ARG	CZ-NH2	5.23	1.40	1.33
1	E	219	ARG	NE-CZ	5.23	1.38	1.33
1	E	239	ARG	CZ-NH1	5.23	1.40	1.32
2	3	117	SER	CA-C	5.23	1.59	1.52
2	4	78	GLU	C-N	5.23	1.40	1.33
3	L	378	ALA	C-N	5.23	1.40	1.33
2	l	132	ILE	N-CA	5.23	1.52	1.46
3	L	322	LYS	CA-C	-5.23	1.45	1.52
2	1	52	MET	CA-C	-5.22	1.46	1.52
3	I	259	ARG	CZ-NH1	5.22	1.40	1.32
1	d	142	ASP	CA-C	-5.22	1.45	1.52
1	f	79	SER	C-N	5.22	1.37	1.33
2	j	194	ASP	N-CA	-5.22	1.39	1.46
1	c	82	VAL	C-N	5.22	1.40	1.33
2	6	111	LEU	C-N	5.22	1.40	1.33
1	b	151	ASP	N-CA	5.22	1.50	1.45
1	F	143	GLU	CA-C	-5.22	1.45	1.52
1	E	34	GLY	C-N	5.22	1.40	1.33
2	i	61	GLY	C-N	5.22	1.40	1.33
1	g	98	ILE	N-CA	-5.22	1.40	1.46
1	g	130	ARG	NE-CZ	5.22	1.38	1.33
2	2	129	GLY	N-CA	5.22	1.51	1.45
2	4	43	LYS	CA-C	-5.22	1.46	1.52
2	5	170	ARG	CD-NE	5.22	1.53	1.46
2	6	108	VAL	CA-CB	-5.22	1.49	1.55
2	m	206	GLN	N-CA	-5.22	1.39	1.46
3	K	203	PHE	CA-C	-5.22	1.45	1.52
3	L	229	LEU	CA-C	-5.22	1.46	1.52
3	J	55	VAL	CA-CB	5.22	1.60	1.54
2	3	174	SER	C-N	5.21	1.41	1.34
2	k	195	GLU	N-CA	-5.21	1.39	1.46
2	5	35	ASN	CA-C	5.21	1.58	1.52
2	n	18	VAL	CA-C	-5.21	1.46	1.52
3	M	151	GLU	CA-CB	-5.21	1.45	1.53
3	M	242	GLU	C-N	5.21	1.41	1.34
3	J	259	ARG	CZ-NH1	5.21	1.40	1.32
3	L	128	TYR	CA-CB	5.21	1.61	1.53
1	A	75	CYS	N-CA	-5.21	1.39	1.45
2	1	54	MET	N-CA	-5.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	44	GLU	N-CA	-5.21	1.40	1.46
1	G	125	GLN	CA-C	-5.21	1.46	1.52
1	b	40	ILE	CA-C	-5.21	1.46	1.52
2	4	72	ILE	CA-C	5.21	1.59	1.52
2	k	165	VAL	CA-CB	-5.21	1.48	1.54
2	5	208	LEU	CB-CG	5.21	1.63	1.53
3	M	207	VAL	CA-C	-5.21	1.46	1.52
1	B	174	PHE	CA-CB	5.21	1.61	1.53
1	C	175	PHE	C-N	5.21	1.41	1.34
1	f	180	ARG	CA-C	-5.21	1.46	1.52
2	1	207	ILE	CA-C	-5.21	1.45	1.52
2	5	178	ARG	CZ-NH2	5.21	1.40	1.33
2	6	155	PHE	CA-CB	5.21	1.61	1.53
3	L	59	ARG	CZ-NH1	5.21	1.40	1.32
1	A	214	VAL	C-O	-5.20	1.18	1.24
1	B	150	THR	C-N	5.20	1.41	1.32
1	b	66	LYS	C-N	5.20	1.40	1.33
2	i	73	GLU	N-CA	-5.20	1.39	1.46
2	4	21	ASP	C-N	5.20	1.41	1.33
2	6	45	ILE	C-N	5.20	1.40	1.33
2	m	31	ALA	CA-CB	-5.20	1.45	1.53
2	7	76	LEU	C-O	-5.20	1.18	1.24
3	L	228	GLN	CA-C	-5.20	1.46	1.52
3	J	131	GLU	CA-CB	5.20	1.63	1.53
2	2	146	THR	CA-C	-5.20	1.46	1.52
2	k	93	LEU	N-CA	-5.20	1.40	1.46
3	M	230	ALA	N-CA	5.20	1.52	1.46
1	c	98	ILE	CA-CB	5.20	1.61	1.54
1	c	243	LEU	CB-CG	5.20	1.63	1.53
1	f	80	GLY	N-CA	-5.20	1.39	1.45
2	1	68	ARG	CZ-NH1	5.20	1.40	1.32
1	D	43	LYS	CA-C	-5.20	1.45	1.52
2	5	129	GLY	CA-C	-5.20	1.45	1.52
3	L	269	LEU	N-CA	-5.20	1.39	1.46
2	2	26	ALA	C-N	5.20	1.40	1.33
2	l	116	ASP	N-CA	-5.20	1.39	1.46
3	I	123	LYS	C-N	5.20	1.40	1.33
3	M	214	LYS	CA-C	-5.20	1.45	1.52
1	a	168	ARG	C-N	5.20	1.40	1.33
1	b	104	ASP	C-N	5.20	1.39	1.33
1	b	134	VAL	N-CA	-5.20	1.40	1.46
1	C	223	GLU	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	170	ARG	CZ-NH1	5.20	1.40	1.32
2	i	178	ARG	NE-CZ	5.20	1.38	1.33
3	H	124	ASP	N-CA	5.20	1.51	1.46
1	d	123	TYR	CA-C	-5.19	1.45	1.52
2	4	73	GLU	CA-C	-5.19	1.45	1.52
3	K	37	ILE	C-N	5.19	1.40	1.33
1	A	171	VAL	C-N	5.19	1.40	1.33
1	A	183	LEU	CA-C	-5.19	1.46	1.52
1	A	239	ARG	CZ-NH1	5.19	1.40	1.32
1	B	31	VAL	CA-CB	5.19	1.61	1.54
1	B	53	ARG	N-CA	5.19	1.52	1.46
1	E	74	ILE	CA-CB	-5.19	1.47	1.54
2	3	47	GLN	CA-C	-5.19	1.46	1.52
3	H	289	ARG	C-N	5.19	1.39	1.33
3	K	274	GLY	N-CA	5.19	1.52	1.45
1	C	227	GLU	C-N	5.19	1.41	1.33
3	H	326	ARG	CD-NE	5.19	1.53	1.46
2	j	195	GLU	CA-C	-5.19	1.45	1.52
2	j	212	ARG	NE-CZ	5.19	1.38	1.33
2	5	104	PHE	CA-C	-5.19	1.47	1.52
3	I	154	ARG	CZ-NH1	5.19	1.40	1.32
3	K	109	ASN	C-N	5.19	1.40	1.33
3	K	260	GLU	CA-C	-5.19	1.46	1.52
1	a	83	ALA	CA-CB	5.19	1.61	1.53
1	F	70	ILE	N-CA	-5.19	1.39	1.46
2	m	75	ASN	N-CA	-5.19	1.40	1.46
2	l	18	VAL	N-CA	-5.19	1.40	1.46
3	I	278	ARG	NE-CZ	5.19	1.38	1.33
1	A	31	VAL	C-N	5.18	1.40	1.33
2	1	13	THR	CA-C	5.18	1.59	1.52
2	3	211	PHE	CA-CB	5.18	1.61	1.53
3	J	154	ARG	NE-CZ	5.18	1.38	1.33
3	J	305	ARG	CZ-NH1	5.18	1.40	1.32
1	b	130	ARG	CA-C	-5.18	1.46	1.52
1	b	184	SER	C-O	-5.18	1.16	1.23
1	c	177	LYS	CA-CB	5.18	1.62	1.53
2	i	49	ALA	N-CA	-5.18	1.39	1.46
2	3	194	ASP	CA-C	-5.18	1.45	1.52
2	k	54	MET	N-CA	-5.18	1.39	1.46
3	J	118	VAL	CA-C	-5.18	1.46	1.52
1	A	236	ALA	CA-C	-5.18	1.46	1.52
1	d	148	TYR	C-N	5.18	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	174	PHE	CA-C	-5.18	1.46	1.52
2	h	68	ARG	CA-C	-5.18	1.45	1.52
3	I	315	GLU	CA-C	-5.18	1.46	1.52
2	5	25	MET	CA-C	-5.18	1.46	1.52
1	F	232	TYR	N-CA	5.18	1.52	1.46
1	g	100	ARG	CD-NE	5.18	1.53	1.46
1	d	74	ILE	N-CA	-5.17	1.40	1.46
2	7	88	ARG	NE-CZ	5.17	1.38	1.33
2	i	108	VAL	CA-CB	-5.17	1.50	1.55
3	K	341	ARG	CZ-NH1	5.17	1.40	1.32
3	L	161	LEU	C-O	-5.17	1.18	1.24
1	E	185	PHE	N-CA	-5.17	1.40	1.46
1	g	112	LEU	CA-C	-5.17	1.46	1.52
1	g	208	ASN	CG-ND2	5.17	1.44	1.33
2	3	154	ARG	CZ-NH1	5.17	1.40	1.32
2	j	83	ARG	NE-CZ	5.17	1.38	1.33
2	4	187	ASP	CA-C	-5.17	1.46	1.52
3	I	172	ILE	CA-C	-5.17	1.46	1.52
3	K	327	LYS	C-N	5.17	1.40	1.33
2	h	164	ALA	N-CA	-5.17	1.39	1.46
2	7	83	ARG	CZ-NH2	5.17	1.40	1.33
2	n	119	GLY	CA-C	-5.17	1.44	1.51
1	A	165	GLY	C-N	5.17	1.41	1.33
1	B	75	CYS	C-N	5.17	1.40	1.33
1	D	14	VAL	CA-C	-5.17	1.46	1.52
2	1	124	SER	CA-C	-5.17	1.46	1.52
2	j	58	GLY	CA-C	-5.17	1.46	1.52
1	b	168	ARG	CD-NE	5.17	1.53	1.46
1	D	26	TYR	CA-CB	-5.16	1.45	1.53
1	f	62	ASP	CA-CB	5.16	1.62	1.53
1	f	76	ALA	CA-C	-5.16	1.46	1.52
2	j	65	PHE	CA-CB	5.16	1.61	1.53
2	4	57	ALA	CA-C	5.16	1.58	1.52
2	m	58	GLY	C-N	5.16	1.40	1.33
3	L	263	ARG	C-N	5.16	1.41	1.33
3	J	327	LYS	C-N	5.16	1.40	1.33
2	1	125	ILE	C-O	-5.16	1.18	1.24
2	k	27	THR	CA-C	-5.16	1.46	1.52
1	f	97	GLN	C-N	5.16	1.40	1.33
2	3	178	ARG	C-N	5.16	1.40	1.33
3	I	306	ILE	C-N	5.16	1.39	1.33
3	L	293	LEU	N-CA	-5.16	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	102	ARG	CZ-NH2	5.16	1.40	1.33
1	c	51	ASP	N-CA	-5.16	1.39	1.46
2	n	102	ARG	NE-CZ	5.16	1.38	1.33
1	e	74	ILE	CA-C	-5.16	1.46	1.52
3	I	102	PRO	CA-C	5.16	1.58	1.52
3	K	281	VAL	C-N	5.16	1.41	1.33
3	J	67	VAL	N-CA	-5.16	1.40	1.46
1	C	235	ARG	CZ-NH2	5.15	1.40	1.33
2	7	172	ILE	C-O	-5.15	1.18	1.24
1	E	186	ASP	C-N	5.15	1.41	1.34
2	7	85	PRO	N-CA	5.15	1.53	1.47
3	I	364	ARG	CD-NE	5.15	1.53	1.46
3	M	328	MET	CA-C	-5.15	1.45	1.52
1	D	237	ASN	C-O	-5.15	1.17	1.24
2	4	29	LYS	C-N	5.15	1.40	1.33
3	L	61	PRO	CA-CB	5.15	1.61	1.54
1	A	180	ARG	NE-CZ	5.15	1.38	1.33
1	E	241	ARG	NE-CZ	5.15	1.38	1.33
1	f	41	LYS	N-CA	-5.15	1.39	1.46
2	j	182	SER	C-N	5.15	1.41	1.33
3	K	62	PRO	C-N	5.15	1.40	1.33
3	K	317	ARG	NE-CZ	5.15	1.38	1.33
2	2	109	GLN	C-N	5.15	1.41	1.33
3	I	352	LYS	N-CA	-5.15	1.40	1.46
1	C	47	ILE	CA-C	-5.14	1.46	1.52
1	e	68	TYR	N-CA	-5.14	1.39	1.46
1	f	180	ARG	CD-NE	5.14	1.53	1.46
1	b	27	ALA	CA-CB	5.14	1.61	1.53
1	g	140	GLY	C-O	-5.14	1.18	1.23
1	g	235	ARG	CZ-NH2	5.14	1.40	1.33
2	6	28	GLU	C-O	-5.14	1.17	1.23
3	I	228	GLN	CA-C	5.14	1.59	1.52
3	J	69	SER	C-N	5.14	1.39	1.33
2	3	150	VAL	N-CA	-5.14	1.39	1.46
1	e	224	VAL	N-CA	5.14	1.52	1.46
2	5	42	ALA	C-N	5.14	1.40	1.33
3	H	24	ARG	NE-CZ	5.14	1.38	1.33
1	A	203	GLU	N-CA	-5.14	1.39	1.46
1	c	69	LYS	C-N	5.14	1.39	1.33
2	2	106	TYR	CA-CB	5.14	1.62	1.53
3	M	187	GLY	C-N	5.14	1.41	1.33
1	c	13	THR	N-CA	-5.13	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	147	LEU	CA-C	-5.13	1.46	1.52
1	a	11	ALA	CA-C	-5.13	1.46	1.52
1	C	241	ARG	N-CA	-5.13	1.40	1.46
3	I	221	ARG	CZ-NH1	5.13	1.40	1.32
1	E	20	ARG	NE-CZ	5.13	1.38	1.33
1	D	160	LYS	N-CA	-5.13	1.39	1.46
1	d	81	LEU	CA-CB	5.13	1.61	1.53
2	3	170	ARG	NE-CZ	5.13	1.38	1.33
3	I	67	VAL	CA-CB	-5.13	1.48	1.54
1	b	69	LYS	N-CA	-5.13	1.39	1.46
1	C	155	ALA	C-N	5.13	1.41	1.33
1	E	155	ALA	CA-CB	5.13	1.62	1.53
2	j	207	ILE	CA-CB	-5.13	1.47	1.54
3	H	330	LEU	N-CA	-5.12	1.39	1.45
1	E	47	ILE	C-O	-5.12	1.18	1.24
2	n	72	ILE	C-N	5.12	1.41	1.33
3	I	50	ARG	CZ-NH2	5.12	1.40	1.33
3	L	203	PHE	CA-C	-5.12	1.46	1.52
1	f	31	VAL	CA-CB	-5.12	1.47	1.54
2	i	83	ARG	CZ-NH2	5.12	1.40	1.33
3	H	181	TYR	CA-C	-5.12	1.46	1.52
2	1	188	VAL	C-N	5.12	1.40	1.33
2	2	181	ALA	C-O	-5.12	1.17	1.23
2	4	108	VAL	CA-CB	5.12	1.60	1.55
2	5	76	LEU	N-CA	5.12	1.52	1.46
1	C	44	GLU	C-N	5.12	1.40	1.33
1	C	242	GLU	N-CA	-5.11	1.40	1.46
2	m	68	ARG	C-N	5.11	1.40	1.33
3	I	366	GLU	CA-C	-5.11	1.46	1.52
2	h	83	ARG	CD-NE	5.11	1.53	1.46
2	3	144	SER	CA-C	-5.11	1.46	1.52
2	k	52	MET	CA-C	-5.11	1.46	1.52
2	l	21	ASP	CA-CB	5.11	1.62	1.53
2	7	84	LYS	CA-C	-5.11	1.47	1.53
3	K	393	LYS	CA-CB	5.11	1.62	1.53
1	d	145	PRO	N-CA	-5.11	1.40	1.47
1	E	44	GLU	CA-CB	5.11	1.61	1.53
2	1	43	LYS	C-N	5.11	1.43	1.34
1	B	40	ILE	CA-CB	-5.11	1.48	1.54
2	m	176	MET	C-N	5.11	1.41	1.33
3	H	246	ILE	CA-C	-5.11	1.47	1.52
1	c	93	ARG	CA-C	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	ARG	CA-CB	-5.11	1.45	1.53
1	f	128	GLY	C-N	5.11	1.39	1.33
2	2	197	TYR	C-N	5.11	1.40	1.33
2	4	167	LEU	CA-C	-5.11	1.46	1.52
3	I	90	ASN	CA-CB	-5.11	1.46	1.53
3	I	224	ARG	CZ-NH2	5.11	1.40	1.33
3	K	27	TYR	CA-C	-5.11	1.46	1.52
3	K	60	SER	C-N	5.11	1.39	1.33
3	L	384	LYS	CA-C	-5.11	1.46	1.52
1	B	214	VAL	CA-CB	-5.11	1.47	1.54
2	2	198	GLN	CD-NE2	5.11	1.44	1.33
2	4	146	THR	C-N	5.11	1.40	1.33
2	m	29	LYS	C-N	5.11	1.40	1.33
3	M	326	ARG	N-CA	-5.10	1.40	1.46
2	i	106	TYR	N-CA	-5.10	1.40	1.46
3	H	130	PHE	CA-C	-5.10	1.46	1.52
3	I	317	ARG	CZ-NH1	5.10	1.39	1.32
1	d	239	ARG	NE-CZ	5.10	1.38	1.33
1	A	241	ARG	CZ-NH1	5.10	1.39	1.32
1	b	53	ARG	CD-NE	5.10	1.53	1.46
1	d	219	ARG	NE-CZ	5.10	1.38	1.33
3	H	128	TYR	CA-C	-5.10	1.45	1.52
3	L	178	VAL	CA-C	-5.10	1.46	1.52
3	M	224	ARG	CD-NE	5.10	1.53	1.46
1	E	145	PRO	CA-C	-5.10	1.46	1.52
1	F	169	ASN	CA-CB	5.10	1.61	1.53
2	4	164	ALA	C-N	5.10	1.40	1.33
3	H	195	VAL	C-N	5.10	1.40	1.33
3	I	288	ASN	CA-CB	5.10	1.61	1.54
3	L	201	ALA	CA-C	-5.10	1.46	1.52
1	C	10	ARG	CD-NE	5.10	1.53	1.46
2	4	173	TYR	C-N	5.10	1.40	1.33
2	7	149	GLY	C-N	5.09	1.40	1.33
1	B	123	TYR	C-N	5.09	1.40	1.33
1	c	173	GLU	CA-CB	5.09	1.61	1.53
3	K	266	MET	C-N	5.09	1.40	1.33
1	D	35	ALA	C-N	5.09	1.40	1.33
1	f	93	ARG	CZ-NH2	5.09	1.40	1.33
3	M	288	ASN	N-CA	-5.09	1.39	1.46
3	J	55	VAL	CA-C	-5.09	1.46	1.52
2	j	61	GLY	C-N	5.09	1.41	1.33
1	e	229	LEU	N-CA	-5.09	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	296	ALA	CA-CB	5.09	1.61	1.53
1	d	241	ARG	NE-CZ	5.09	1.38	1.33
2	2	51	ARG	CZ-NH1	5.09	1.39	1.32
3	H	98	GLU	N-CA	-5.09	1.39	1.46
3	H	131	GLU	CA-CB	5.09	1.62	1.53
3	I	189	THR	N-CA	-5.09	1.40	1.46
3	K	44	TYR	C-N	5.09	1.40	1.33
3	L	32	ASP	CA-CB	5.09	1.61	1.53
3	J	322	LYS	C-N	5.09	1.40	1.33
1	f	110	LYS	CA-C	5.08	1.59	1.52
2	j	89	ALA	C-N	5.08	1.40	1.33
2	6	105	PRO	N-CA	-5.08	1.41	1.47
3	J	17	GLU	C-N	5.08	1.40	1.33
1	C	39	GLY	CA-C	5.08	1.56	1.51
1	F	71	ASP	CA-CB	5.08	1.62	1.53
2	5	115	ILE	C-O	-5.08	1.18	1.24
3	L	54	GLU	N-CA	-5.08	1.40	1.46
1	B	75	CYS	N-CA	5.08	1.52	1.45
2	1	174	SER	N-CA	-5.08	1.40	1.46
2	3	86	THR	CA-C	-5.08	1.45	1.53
3	I	28	ARG	CD-NE	5.08	1.53	1.46
1	e	118	ASP	N-CA	5.08	1.52	1.46
2	l	30	ARG	C-N	5.08	1.40	1.33
1	A	156	LEU	CA-C	-5.08	1.46	1.52
1	F	139	ALA	C-N	5.08	1.39	1.33
1	g	114	LYS	CA-CB	5.08	1.61	1.53
3	H	168	ALA	N-CA	5.08	1.52	1.46
1	A	204	LEU	CA-C	-5.08	1.46	1.52
2	k	51	ARG	CZ-NH1	5.08	1.39	1.32
2	6	76	LEU	CA-CB	5.08	1.61	1.53
2	7	140	THR	CA-C	-5.08	1.46	1.52
2	7	188	VAL	C-N	5.08	1.40	1.33
3	I	185	GLY	CA-C	-5.08	1.44	1.51
1	F	33	ARG	NE-CZ	5.07	1.38	1.33
1	G	63	THR	CB-OG1	-5.07	1.35	1.43
2	1	185	GLY	CA-C	-5.07	1.44	1.51
2	3	83	ARG	NE-CZ	5.07	1.38	1.33
2	4	186	ILE	N-CA	-5.07	1.40	1.46
2	5	101	TYR	CA-CB	5.07	1.60	1.53
2	l	75	ASN	CG-ND2	5.07	1.44	1.33
3	M	218	GLU	C-N	5.07	1.40	1.33
1	G	136	LEU	CB-CG	5.07	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	248	ALA	CA-C	-5.07	1.46	1.52
3	J	163	LYS	C-O	-5.07	1.18	1.24
1	A	147	LEU	CA-C	-5.07	1.46	1.52
1	b	115	LYS	CA-CB	5.07	1.61	1.53
2	n	133	GLU	CA-C	-5.07	1.46	1.52
1	a	216	VAL	CA-CB	5.07	1.60	1.54
1	B	219	ARG	CD-NE	5.07	1.53	1.46
2	5	155	PHE	C-N	5.07	1.40	1.33
2	l	151	LEU	C-N	5.07	1.40	1.33
3	K	224	ARG	CZ-NH2	5.07	1.40	1.33
3	L	335	ASP	CA-C	-5.07	1.46	1.52
3	M	322	LYS	CA-C	5.07	1.59	1.52
1	c	183	LEU	C-O	-5.06	1.17	1.23
1	F	46	VAL	CA-C	-5.06	1.46	1.52
1	e	152	PRO	N-CD	-5.06	1.40	1.47
2	l	137	ILE	C-N	5.06	1.39	1.33
3	L	162	LEU	N-CA	-5.06	1.39	1.46
1	e	143	GLU	C-N	5.06	1.39	1.33
1	A	118	ASP	C-N	5.06	1.40	1.33
1	a	118	ASP	CA-CB	5.06	1.61	1.53
1	a	171	VAL	N-CA	-5.06	1.40	1.46
1	E	137	LEU	CA-C	-5.06	1.46	1.52
1	E	224	VAL	CA-CB	5.06	1.60	1.54
2	i	33	MET	CA-C	-5.06	1.46	1.52
2	i	128	ILE	CA-CB	-5.06	1.48	1.54
2	7	154	ARG	CZ-NH1	5.06	1.39	1.32
3	I	106	VAL	CA-C	-5.06	1.46	1.52
2	3	145	LEU	CA-C	-5.06	1.46	1.52
1	B	46	VAL	N-CA	-5.05	1.40	1.46
1	f	89	ILE	CA-C	-5.05	1.45	1.52
2	5	133	GLU	C-N	5.05	1.40	1.33
2	n	112	ILE	N-CA	-5.05	1.39	1.46
3	I	52	ARG	CA-C	-5.05	1.46	1.52
3	K	305	ARG	CA-CB	5.05	1.61	1.53
3	M	47	GLU	N-CA	5.05	1.52	1.46
1	B	106	PRO	N-CA	5.05	1.53	1.47
1	D	13	THR	C-N	5.05	1.40	1.33
2	4	85	PRO	N-CA	-5.05	1.41	1.47
1	E	103	TYR	CA-C	-5.05	1.45	1.52
1	G	151	ASP	CA-CB	5.05	1.61	1.53
2	m	100	SER	CA-C	-5.05	1.46	1.52
1	B	45	GLY	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	13	LEU	C-N	5.05	1.40	1.33
3	H	229	LEU	C-N	5.05	1.40	1.33
1	E	203	GLU	CA-CB	5.05	1.61	1.53
2	h	139	ALA	C-O	-5.05	1.18	1.23
1	B	174	PHE	N-CA	-5.04	1.40	1.46
1	a	53	ARG	CZ-NH1	5.04	1.39	1.32
1	F	88	LEU	N-CA	-5.04	1.40	1.46
2	1	134	GLU	CA-C	-5.04	1.46	1.52
2	4	79	ILE	N-CA	-5.04	1.40	1.46
2	1	95	SER	CA-CB	5.04	1.61	1.53
2	j	39	SER	C-O	-5.04	1.17	1.23
2	k	23	VAL	CA-C	-5.04	1.46	1.52
2	m	43	LYS	CA-C	-5.04	1.46	1.52
2	7	134	GLU	N-CA	-5.04	1.39	1.46
2	5	36	PHE	N-CA	-5.04	1.40	1.46
1	D	228	GLU	CA-CB	5.04	1.62	1.53
1	d	235	ARG	CZ-NH1	5.04	1.39	1.32
1	F	54	VAL	C-N	5.04	1.40	1.33
2	h	186	ILE	C-N	5.04	1.40	1.33
2	4	199	TYR	CA-C	-5.04	1.46	1.52
2	5	135	LYS	N-CA	-5.04	1.40	1.46
2	n	120	LYS	CA-C	-5.04	1.46	1.52
3	L	49	ARG	CA-C	-5.04	1.46	1.52
3	L	197	ASN	CA-C	-5.04	1.45	1.52
3	M	249	ARG	CZ-NH1	5.04	1.39	1.32
1	d	132	PHE	CA-CB	5.04	1.61	1.53
2	n	190	LYS	CA-C	-5.04	1.46	1.52
3	H	334	VAL	CA-C	-5.04	1.46	1.52
1	C	81	LEU	CA-C	5.04	1.59	1.52
1	C	205	VAL	N-CA	5.04	1.52	1.46
1	G	214	VAL	CA-CB	-5.04	1.48	1.54
1	g	174	PHE	CA-C	-5.04	1.45	1.52
2	1	102	ARG	CZ-NH1	5.04	1.39	1.32
2	j	59	SER	C-N	5.04	1.40	1.33
2	6	131	ALA	CA-C	-5.04	1.46	1.52
2	6	178	ARG	CZ-NH1	5.04	1.39	1.32
2	7	88	ARG	CA-CB	5.04	1.61	1.53
3	J	201	ALA	CA-CB	5.04	1.60	1.53
2	2	184	ASP	CA-C	-5.03	1.46	1.52
2	j	185	GLY	N-CA	-5.03	1.38	1.45
2	4	102	ARG	N-CA	5.03	1.52	1.46
2	n	51	ARG	N-CA	-5.03	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	GLY	CA-C	-5.03	1.44	1.51
1	a	53	ARG	CZ-NH2	5.03	1.40	1.33
1	c	100	ARG	CZ-NH2	5.03	1.40	1.33
1	d	91	ARG	NE-CZ	5.03	1.38	1.33
2	h	178	ARG	CZ-NH2	5.03	1.40	1.33
2	n	203	GLU	CA-C	-5.03	1.46	1.52
3	H	330	LEU	CA-CB	5.03	1.62	1.53
3	I	105	ARG	CZ-NH1	5.03	1.39	1.32
2	n	71	LYS	CA-C	5.03	1.59	1.52
3	I	35	LYS	CA-CB	5.03	1.61	1.53
1	b	240	ILE	N-CA	5.03	1.52	1.46
1	C	142	ASP	CA-C	-5.03	1.46	1.53
1	d	149	GLU	C-N	5.03	1.40	1.33
1	g	38	ILE	C-N	5.03	1.40	1.33
2	l	59	SER	CA-C	-5.03	1.46	1.52
3	K	299	ARG	CD-NE	5.03	1.53	1.46
3	L	177	GLY	CA-C	-5.03	1.44	1.51
1	e	193	LEU	N-CA	-5.02	1.40	1.46
1	G	43	LYS	C-N	5.02	1.40	1.33
1	C	85	ALA	N-CA	-5.02	1.40	1.46
1	F	60	GLU	N-CA	-5.02	1.39	1.46
2	2	98	LEU	N-CA	-5.02	1.40	1.46
2	j	200	SER	CA-C	-5.02	1.46	1.52
2	l	178	ARG	CZ-NH2	5.02	1.40	1.33
3	I	263	ARG	NE-CZ	5.02	1.38	1.33
2	2	113	GLY	CA-C	-5.02	1.48	1.52
1	B	54	VAL	CA-CB	-5.02	1.49	1.54
1	C	130	ARG	CA-C	5.02	1.59	1.53
1	f	20	ARG	CD-NE	5.02	1.53	1.46
2	4	103	TYR	C-N	5.02	1.41	1.33
2	5	197	TYR	N-CA	-5.02	1.39	1.46
2	6	82	GLU	C-N	5.02	1.40	1.33
3	H	52	ARG	CA-CB	-5.02	1.45	1.53
1	e	100	ARG	N-CA	5.02	1.52	1.46
3	I	189	THR	C-O	-5.02	1.18	1.24
3	K	50	ARG	CZ-NH2	5.02	1.40	1.33
1	g	116	ILE	CA-CB	-5.02	1.48	1.54
2	1	38	ALA	C-O	-5.02	1.18	1.24
1	A	82	VAL	N-CA	5.01	1.52	1.46
1	a	225	SER	CA-CB	5.01	1.60	1.53
2	h	54	MET	CA-C	5.01	1.58	1.52
2	4	51	ARG	CZ-NH1	5.01	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	164	ALA	N-CA	-5.01	1.40	1.46
2	j	38	ALA	N-CA	-5.01	1.40	1.46
2	4	107	LEU	N-CA	-5.01	1.40	1.46
2	m	198	GLN	CA-C	-5.01	1.46	1.52
2	7	172	ILE	CA-CB	5.01	1.60	1.54
3	I	269	LEU	C-N	5.01	1.40	1.33
1	A	113	ALA	C-N	5.01	1.40	1.33
2	1	132	ILE	CA-CB	-5.01	1.46	1.54
2	i	109	GLN	N-CA	-5.01	1.40	1.46
2	k	174	SER	N-CA	5.01	1.52	1.46
3	K	268	LEU	CA-CB	5.01	1.61	1.53
3	M	46	ARG	NE-CZ	5.01	1.38	1.33
1	B	121	GLN	CA-C	-5.01	1.45	1.52
1	g	180	ARG	CZ-NH2	5.01	1.40	1.33
2	k	81	ARG	CZ-NH1	5.01	1.39	1.32
2	7	31	ALA	N-CA	-5.01	1.40	1.46
2	n	118	GLU	N-CA	-5.01	1.40	1.46
2	n	167	LEU	CA-CB	5.01	1.61	1.53
3	H	369	LYS	C-O	-5.01	1.17	1.23
1	c	10	ARG	NE-CZ	5.00	1.38	1.33
1	e	180	ARG	CD-NE	5.00	1.53	1.46
1	A	155	ALA	C-O	-5.00	1.17	1.23
1	E	104	ASP	CA-CB	5.00	1.60	1.53
2	4	164	ALA	CA-C	-5.00	1.46	1.52
3	H	289	ARG	NE-CZ	5.00	1.38	1.33
3	H	330	LEU	C-N	5.00	1.40	1.33
1	E	193	LEU	N-CA	-5.00	1.40	1.46
3	L	91	THR	C-N	5.00	1.40	1.33

All (4603) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	l	170	ARG	NE-CZ-NH2	-24.36	97.27	119.20
2	5	170	ARG	NE-CZ-NH2	-19.31	101.82	119.20
1	D	70	ILE	N-CA-C	-16.02	98.66	112.12
1	a	144	VAL	N-CA-C	-15.11	96.80	109.19
2	5	128	ILE	N-CA-C	-13.43	100.07	112.43
1	b	70	ILE	N-CA-C	-13.13	100.66	113.53
2	m	135	LYS	N-CA-C	-12.88	97.48	113.97
2	l	65	PHE	CA-CB-CG	-11.70	102.10	113.80
1	F	205	VAL	CA-C-N	11.62	134.37	119.84
1	F	205	VAL	C-N-CA	11.62	134.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	63	THR	N-CA-C	-11.37	99.94	114.04
3	M	60	SER	CA-C-N	11.29	132.01	120.38
3	M	60	SER	C-N-CA	11.29	132.01	120.38
3	H	77	VAL	N-CA-C	-11.27	91.72	108.17
3	I	123	LYS	CA-C-N	11.19	141.84	121.70
3	I	123	LYS	C-N-CA	11.19	141.84	121.70
3	L	23	LEU	CA-C-N	11.19	135.27	120.28
3	L	23	LEU	C-N-CA	11.19	135.27	120.28
3	M	324	HIS	CA-C-N	11.18	135.26	120.28
3	M	324	HIS	C-N-CA	11.18	135.26	120.28
2	6	88	ARG	NE-CZ-NH2	11.16	129.25	119.20
3	L	101	LYS	N-CA-C	-11.09	98.24	108.22
1	c	20	ARG	CA-C-N	11.00	136.33	120.71
1	c	20	ARG	C-N-CA	11.00	136.33	120.71
3	J	302	ARG	N-CA-C	-10.95	102.14	114.62
1	b	144	VAL	N-CA-C	-10.94	96.64	109.01
1	c	181	ASP	CA-CB-CG	-10.91	101.69	112.60
2	7	192	THR	N-CA-C	-10.66	99.13	112.88
3	J	280	ASP	CA-CB-CG	-10.60	102.00	112.60
2	n	163	GLU	CA-C-N	10.59	135.32	120.29
2	n	163	GLU	C-N-CA	10.59	135.32	120.29
3	I	281	VAL	O-C-N	-10.58	111.83	123.26
3	I	146	LEU	CA-C-N	10.58	134.82	120.54
3	I	146	LEU	C-N-CA	10.58	134.82	120.54
3	M	290	ILE	N-CA-C	-10.55	101.92	113.43
1	a	39	GLY	CA-C-O	-10.51	112.74	120.94
2	1	129	GLY	N-CA-C	-10.49	101.34	112.04
1	C	144	VAL	N-CA-C	-10.48	100.60	109.19
1	A	105	GLU	O-C-N	-10.44	114.54	121.85
3	I	294	ASP	CA-C-O	-10.41	109.96	119.75
3	M	227	PHE	CA-CB-CG	-10.39	103.41	113.80
2	1	128	ILE	N-CA-C	-10.31	103.00	112.90
3	I	290	ILE	N-CA-C	-10.21	103.40	113.20
3	J	303	PHE	CA-CB-CG	-10.20	103.60	113.80
2	m	159	ILE	CA-C-N	10.19	132.80	122.30
2	m	159	ILE	C-N-CA	10.19	132.80	122.30
2	6	156	THR	O-C-N	-10.17	113.05	121.80
3	K	188	LYS	N-CA-C	-10.11	99.77	112.72
2	5	60	VAL	CA-C-N	10.11	131.16	119.94
2	5	60	VAL	C-N-CA	10.11	131.16	119.94
2	m	102	ARG	NE-CZ-NH1	-10.07	111.43	121.50
1	a	163	ALA	CA-C-N	10.06	136.98	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	163	ALA	C-N-CA	10.06	136.98	122.69
3	M	174	PRO	CA-C-N	10.04	129.97	120.03
3	M	174	PRO	C-N-CA	10.04	129.97	120.03
1	G	10	ARG	N-CA-C	-10.03	100.53	113.17
1	E	194	VAL	CA-C-N	10.01	134.05	120.44
1	E	194	VAL	C-N-CA	10.01	134.05	120.44
3	L	198	GLN	CA-C-N	10.01	133.45	120.44
3	L	198	GLN	C-N-CA	10.01	133.45	120.44
2	5	23	VAL	N-CA-C	-9.97	95.19	108.35
3	H	90	ASN	CA-CB-CG	9.96	122.56	112.60
2	l	170	ARG	NE-CZ-NH1	9.95	131.45	121.50
2	k	140	THR	N-CA-CB	9.94	128.39	111.50
1	B	181	ASP	N-CA-C	-9.93	101.40	112.72
1	E	129	VAL	N-CA-C	-9.88	95.31	108.35
1	g	144	VAL	CA-C-O	-9.77	112.73	119.38
3	L	120	PRO	N-CA-CB	9.75	112.45	103.19
1	f	144	VAL	CA-C-N	9.74	130.35	119.83
1	f	144	VAL	C-N-CA	9.74	130.35	119.83
2	l	87	VAL	CA-C-N	9.73	133.32	120.28
2	l	87	VAL	C-N-CA	9.73	133.32	120.28
3	K	391	ASP	CA-CB-CG	9.72	122.32	112.60
2	3	178	ARG	N-CA-C	-9.71	100.94	113.17
3	L	15	LYS	O-C-N	9.71	132.07	122.07
1	b	205	VAL	N-CA-C	-9.70	98.05	109.01
3	J	292	ILE	N-CA-C	-9.69	103.24	112.83
3	M	281	VAL	CA-C-N	9.67	139.10	121.70
3	M	281	VAL	C-N-CA	9.67	139.10	121.70
3	J	290	ILE	N-CA-C	-9.67	103.62	112.90
1	B	100	ARG	NE-CZ-NH2	9.64	127.88	119.20
2	j	189	VAL	N-CA-C	-9.60	94.30	108.12
3	M	361	PHE	CA-C-N	9.60	132.92	120.44
3	M	361	PHE	C-N-CA	9.60	132.92	120.44
2	1	116	ASP	CA-C-N	9.59	133.14	120.28
2	1	116	ASP	C-N-CA	9.59	133.14	120.28
1	G	240	ILE	N-CA-CB	9.59	122.84	110.57
3	M	294	ASP	CA-C-N	9.57	129.20	119.82
3	M	294	ASP	C-N-CA	9.57	129.20	119.82
2	k	128	ILE	N-CA-C	-9.54	103.39	112.83
2	l	29	LYS	N-CA-C	-9.50	94.97	109.41
3	M	124	ASP	CA-CB-CG	9.49	122.09	112.60
2	k	77	TYR	CA-C-N	9.48	132.99	120.28
2	k	77	TYR	C-N-CA	9.48	132.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	172	THR	CA-C-N	9.47	133.74	120.29
1	b	172	THR	C-N-CA	9.47	133.74	120.29
1	G	151	ASP	CA-CB-CG	-9.43	103.17	112.60
3	L	101	LYS	N-CA-CB	9.43	121.00	111.10
3	H	101	LYS	CA-C-N	9.43	129.47	119.76
3	H	101	LYS	C-N-CA	9.43	129.47	119.76
1	f	205	VAL	CA-C-O	-9.41	111.88	119.98
3	L	61	PRO	N-CA-C	-9.41	99.22	110.70
2	7	131	ALA	N-CA-C	-9.38	92.72	108.75
3	L	304	ASP	CA-CB-CG	-9.37	103.23	112.60
3	H	288	ASN	N-CA-C	-9.36	101.64	113.43
3	K	125	PRO	CA-C-N	9.34	133.18	120.38
3	K	125	PRO	C-N-CA	9.34	133.18	120.38
1	F	106	PRO	O-C-N	9.28	133.69	123.01
2	i	23	VAL	N-CA-C	-9.28	96.10	108.35
2	m	21	ASP	CA-CB-CG	-9.27	103.33	112.60
2	5	148	TYR	CA-C-N	9.25	130.44	119.99
2	5	148	TYR	C-N-CA	9.25	130.44	119.99
3	K	323	ILE	N-CA-C	9.21	120.03	110.72
2	l	170	ARG	NH1-CZ-NH2	9.20	131.26	119.30
3	K	95	ILE	N-CA-C	-9.20	95.23	108.11
3	K	146	LEU	CA-C-N	9.20	138.27	121.70
3	K	146	LEU	C-N-CA	9.20	138.27	121.70
3	K	186	THR	N-CA-C	-9.20	101.58	113.17
3	M	301	GLY	N-CA-C	-9.18	100.95	116.01
2	n	200	SER	CA-C-N	9.17	128.78	119.24
2	n	200	SER	C-N-CA	9.17	128.78	119.24
1	D	245	LYS	N-CA-C	-9.15	99.88	113.61
3	K	397	PHE	CA-CB-CG	-9.14	104.66	113.80
3	M	273	ASP	N-CA-C	-9.14	100.42	113.21
3	I	273	ASP	CA-C-N	9.13	129.89	119.94
3	I	273	ASP	C-N-CA	9.13	129.89	119.94
3	J	372	MET	N-CA-C	-9.13	102.27	113.41
1	C	214	VAL	CA-C-O	9.13	129.25	120.31
2	m	98	LEU	CA-C-N	9.12	132.50	120.28
2	m	98	LEU	C-N-CA	9.12	132.50	120.28
2	l	64	GLN	OE1-CD-NE2	9.12	131.72	122.60
3	K	254	ASP	N-CA-C	-9.12	101.87	113.72
2	n	48	ILE	N-CA-C	-9.10	102.98	111.45
1	c	236	ALA	CA-C-N	9.09	132.46	120.28
1	c	236	ALA	C-N-CA	9.09	132.46	120.28
2	m	126	ASP	CA-C-O	-9.09	111.06	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	26	TYR	N-CA-C	-9.07	102.22	113.38
1	g	171	VAL	CA-C-O	-9.04	111.27	120.85
3	K	241	ASP	N-CA-C	-9.04	103.37	114.75
2	m	79	ILE	N-CA-C	9.03	119.09	110.42
1	d	205	VAL	N-CA-C	-9.03	98.81	109.01
3	H	24	ARG	CA-C-N	9.02	132.37	120.28
3	H	24	ARG	C-N-CA	9.02	132.37	120.28
1	B	87	VAL	N-CA-CB	9.01	122.10	110.57
1	E	144	VAL	CA-C-N	8.99	129.06	119.89
1	E	144	VAL	C-N-CA	8.99	129.06	119.89
3	K	131	GLU	CA-C-O	-8.99	110.92	120.99
2	7	194	ASP	N-CA-C	-8.99	103.42	114.75
2	2	175	ALA	CA-C-N	8.92	132.58	120.44
2	2	175	ALA	C-N-CA	8.92	132.58	120.44
1	e	46	VAL	N-CA-C	-8.91	95.29	108.12
2	3	34	GLY	N-CA-C	-8.91	102.36	115.63
1	F	187	ASP	CA-CB-CG	8.91	121.51	112.60
3	M	257	GLY	CA-C-N	8.90	137.72	121.70
3	M	257	GLY	C-N-CA	8.90	137.72	121.70
1	b	132	PHE	CA-CB-CG	-8.90	104.90	113.80
2	j	202	GLU	N-CA-C	8.89	121.77	111.11
1	D	173	GLU	CA-C-N	8.87	131.97	120.44
1	D	173	GLU	C-N-CA	8.87	131.97	120.44
3	I	212	VAL	N-CA-CB	8.86	125.86	111.23
2	i	104	PHE	CA-CB-CG	8.86	122.66	113.80
3	H	273	ASP	N-CA-C	-8.85	93.07	108.20
3	K	386	THR	N-CA-C	-8.81	101.11	114.16
1	D	64	ILE	CA-C-N	8.80	137.55	121.70
1	D	64	ILE	C-N-CA	8.80	137.55	121.70
2	1	93	LEU	CA-C-N	8.80	132.07	120.28
2	1	93	LEU	C-N-CA	8.80	132.07	120.28
2	m	96	ASN	CA-CB-CG	-8.80	103.80	112.60
3	K	10	LEU	CA-C-N	8.79	132.05	120.28
3	K	10	LEU	C-N-CA	8.79	132.05	120.28
2	4	112	ILE	O-C-N	-8.78	114.18	123.14
2	2	142	SER	N-CA-C	-8.78	103.41	114.56
2	5	112	ILE	N-CA-CB	8.77	123.74	111.82
1	F	67	ILE	N-CA-CB	8.75	120.98	111.00
2	3	201	PRO	CA-C-N	8.75	132.00	120.28
2	3	201	PRO	C-N-CA	8.75	132.00	120.28
3	H	20	TYR	CB-CG-CD2	-8.74	107.68	120.80
3	J	358	ALA	N-CA-C	-8.74	101.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	111	LEU	N-CA-C	-8.73	94.17	108.41
2	6	49	ALA	CA-C-N	8.73	132.35	120.38
2	6	49	ALA	C-N-CA	8.73	132.35	120.38
3	J	253	SER	N-CA-C	-8.73	102.79	113.97
3	H	287	THR	N-CA-C	-8.73	96.59	108.38
2	6	44	LYS	N-CA-C	-8.73	99.70	110.61
2	l	194	ASP	CA-CB-CG	-8.72	103.88	112.60
3	J	284	ILE	N-CA-C	-8.71	94.88	107.77
1	B	203	GLU	N-CA-C	-8.70	97.65	110.52
1	b	239	ARG	NE-CZ-NH2	8.70	127.03	119.20
3	K	133	GLU	CA-C-N	8.69	135.00	122.40
3	K	133	GLU	C-N-CA	8.69	135.00	122.40
2	h	35	ASN	N-CA-C	-8.68	101.67	113.30
3	I	67	VAL	N-CA-C	-8.67	95.51	108.17
3	H	260	GLU	N-CA-C	-8.66	102.88	113.97
2	i	203	GLU	CA-C-O	-8.66	111.24	120.42
1	f	151	ASP	CA-C-N	8.65	128.30	119.56
1	f	151	ASP	C-N-CA	8.65	128.30	119.56
1	f	73	HIS	CA-CB-CG	8.65	122.45	113.80
2	7	174	SER	CA-C-N	8.65	131.87	120.28
2	7	174	SER	C-N-CA	8.65	131.87	120.28
1	f	99	ASN	CA-C-N	8.64	132.72	120.28
1	f	99	ASN	C-N-CA	8.64	132.72	120.28
3	K	379	ILE	N-CA-C	-8.64	101.99	110.72
2	3	144	SER	N-CA-C	8.64	120.31	111.07
3	M	182	GLY	CA-C-N	8.63	129.27	120.38
3	M	182	GLY	C-N-CA	8.63	129.27	120.38
3	J	389	ILE	CA-C-N	8.62	128.27	119.56
3	J	389	ILE	C-N-CA	8.62	128.27	119.56
3	M	132	VAL	CA-C-O	8.62	129.35	120.39
3	I	137	GLU	N-CA-C	-8.60	99.87	110.88
1	E	70	ILE	N-CA-C	-8.59	104.83	111.62
2	5	35	ASN	N-CA-C	-8.59	101.45	114.16
1	E	241	ARG	NE-CZ-NH2	8.58	126.92	119.20
3	L	261	VAL	N-CA-C	-8.58	102.49	111.58
1	d	186	ASP	CA-CB-CG	-8.56	104.04	112.60
3	L	174	PRO	CA-C-N	8.56	128.63	119.90
3	L	174	PRO	C-N-CA	8.56	128.63	119.90
3	I	167	PHE	CA-CB-CG	-8.56	105.24	113.80
1	e	11	ALA	CA-C-N	8.55	132.29	120.49
1	e	11	ALA	C-N-CA	8.55	132.29	120.49
3	L	294	ASP	CA-C-N	8.55	129.38	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	294	ASP	C-N-CA	8.55	129.38	119.47
3	M	288	ASN	CA-CB-CG	8.54	121.14	112.60
2	k	104	PHE	N-CA-C	-8.54	96.58	109.30
3	J	147	ASP	CA-CB-CG	-8.52	104.08	112.60
2	k	104	PHE	CA-CB-CG	-8.52	105.28	113.80
1	E	43	LYS	N-CA-C	-8.52	102.33	112.89
1	D	229	LEU	CA-C-N	8.51	133.57	120.97
1	D	229	LEU	C-N-CA	8.51	133.57	120.97
1	C	119	PHE	CA-CB-CG	-8.51	105.29	113.80
2	3	52	MET	N-CA-C	-8.51	95.64	108.99
1	G	130	ARG	CA-C-N	8.49	128.51	119.76
1	G	130	ARG	C-N-CA	8.49	128.51	119.76
3	K	318	ILE	CA-C-O	-8.49	112.17	121.17
3	I	252	ASN	CA-CB-CG	-8.48	104.11	112.60
3	K	197	ASN	CA-CB-CG	-8.48	104.12	112.60
1	E	105	GLU	CA-C-O	-8.47	111.73	119.86
2	5	33	MET	N-CA-C	-8.46	103.81	114.56
2	5	189	VAL	N-CA-CB	8.45	123.86	111.52
1	g	168	ARG	CA-C-N	8.45	131.93	120.44
1	g	168	ARG	C-N-CA	8.45	131.93	120.44
1	g	144	VAL	CA-C-N	8.45	128.77	119.90
1	g	144	VAL	C-N-CA	8.45	128.77	119.90
1	G	230	LYS	CA-C-O	-8.44	110.57	118.33
2	l	37	ILE	O-C-N	-8.44	113.41	122.61
1	F	111	GLU	CA-C-N	8.43	131.58	120.28
1	F	111	GLU	C-N-CA	8.43	131.58	120.28
3	I	34	LYS	CA-C-O	8.43	129.90	119.11
1	E	40	ILE	N-CA-C	-8.43	95.86	108.17
2	4	45	ILE	N-CA-C	-8.43	96.37	108.17
2	i	177	LYS	N-CA-C	8.42	120.46	111.28
1	d	216	VAL	N-CA-C	8.42	118.50	110.42
1	b	173	GLU	CA-C-N	8.42	131.89	120.44
1	b	173	GLU	C-N-CA	8.42	131.89	120.44
3	L	207	VAL	N-CA-C	-8.41	97.24	108.35
1	b	84	ASP	CA-CB-CG	-8.40	104.20	112.60
3	I	155	GLU	O-C-N	8.40	131.02	122.12
1	f	121	GLN	CA-C-N	8.39	132.37	120.28
1	f	121	GLN	C-N-CA	8.39	132.37	120.28
1	e	95	GLU	CA-C-N	8.39	131.35	120.44
1	e	95	GLU	C-N-CA	8.39	131.35	120.44
1	e	26	TYR	CB-CG-CD1	8.39	133.38	120.80
2	1	179	ASP	N-CA-C	-8.37	99.25	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	164	PRO	CA-C-N	8.37	131.50	120.28
3	L	164	PRO	C-N-CA	8.37	131.50	120.28
2	h	153	ASP	N-CA-C	8.37	120.02	111.07
3	K	290	ILE	N-CA-C	-8.36	104.87	112.90
1	b	109	VAL	CA-C-N	8.36	132.16	120.29
1	b	109	VAL	C-N-CA	8.36	132.16	120.29
1	G	144	VAL	CA-C-N	8.36	128.12	119.76
1	G	144	VAL	C-N-CA	8.36	128.12	119.76
3	I	246	ILE	N-CA-C	-8.36	104.99	113.10
3	K	41	ARG	CA-C-N	8.36	132.29	120.42
3	K	41	ARG	C-N-CA	8.36	132.29	120.42
2	3	139	ALA	CA-C-N	8.35	136.73	121.70
2	3	139	ALA	C-N-CA	8.35	136.73	121.70
2	4	18	VAL	CA-C-O	8.35	129.47	120.53
2	5	129	GLY	CA-C-N	8.35	132.20	121.85
2	5	129	GLY	C-N-CA	8.35	132.20	121.85
3	I	317	ARG	NE-CZ-NH2	8.35	126.71	119.20
2	3	154	ARG	NE-CZ-NH2	8.33	126.70	119.20
3	K	122	SER	CA-C-O	-8.33	111.70	121.44
1	d	12	ILE	CA-C-N	8.32	134.67	122.86
1	d	12	ILE	C-N-CA	8.32	134.67	122.86
1	a	218	ASP	N-CA-C	-8.31	105.14	114.62
3	L	389	ILE	CA-C-N	8.30	128.37	119.90
3	L	389	ILE	C-N-CA	8.30	128.37	119.90
2	5	178	ARG	N-CA-C	-8.30	100.66	113.02
3	I	147	ASP	CA-CB-CG	-8.30	104.30	112.60
3	I	167	PHE	CA-C-N	8.30	131.40	120.28
3	I	167	PHE	C-N-CA	8.30	131.40	120.28
3	I	357	GLU	CA-C-N	8.29	131.39	120.28
3	I	357	GLU	C-N-CA	8.29	131.39	120.28
3	L	223	VAL	CA-C-N	8.29	131.39	120.28
3	L	223	VAL	C-N-CA	8.29	131.39	120.28
2	3	150	VAL	CA-C-N	8.29	131.39	120.28
2	3	150	VAL	C-N-CA	8.29	131.39	120.28
2	j	75	ASN	CA-C-N	8.27	132.89	120.31
2	j	75	ASN	C-N-CA	8.27	132.89	120.31
2	3	210	LYS	N-CA-C	-8.27	102.97	113.72
2	m	168	ALA	N-CA-C	8.27	120.29	111.28
3	I	19	ASP	O-C-N	8.27	131.57	122.15
2	n	134	GLU	N-CA-C	-8.26	95.94	109.40
3	M	95	ILE	N-CA-CB	8.26	122.06	112.40
2	4	170	ARG	CA-C-N	8.25	131.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4	170	ARG	C-N-CA	8.25	131.17	120.44
3	I	384	LYS	O-C-N	8.25	130.87	122.12
2	k	57	ALA	CA-C-O	-8.24	112.09	121.40
3	J	333	ASP	N-CA-C	-8.24	103.24	113.38
1	E	210	GLU	N-CA-C	-8.23	94.85	108.76
3	I	338	GLU	CA-C-N	8.23	131.98	120.29
3	I	338	GLU	C-N-CA	8.23	131.98	120.29
3	M	43	ARG	O-C-N	8.23	131.53	122.15
3	M	95	ILE	N-CA-C	-8.23	94.93	106.53
1	E	12	ILE	N-CA-C	-8.22	104.69	112.83
3	H	178	VAL	N-CA-C	-8.22	96.17	108.17
1	b	205	VAL	CA-C-N	8.21	127.89	119.19
1	b	205	VAL	C-N-CA	8.21	127.89	119.19
3	K	96	ASN	CA-CB-CG	-8.21	104.39	112.60
3	H	350	ASP	CA-C-N	8.21	131.70	120.46
3	H	350	ASP	C-N-CA	8.21	131.70	120.46
2	4	147	ALA	CA-C-N	8.20	131.27	120.28
2	4	147	ALA	C-N-CA	8.20	131.27	120.28
3	L	259	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	G	150	THR	CA-CB-OG1	-8.20	97.31	109.60
3	K	32	ASP	N-CA-CB	8.18	122.27	110.16
2	i	198	GLN	CA-C-N	8.17	131.06	120.44
2	i	198	GLN	C-N-CA	8.17	131.06	120.44
2	4	20	LYS	N-CA-C	-8.17	103.03	113.16
3	M	167	PHE	CA-CB-CG	-8.15	105.65	113.80
3	J	164	PRO	CA-C-N	8.14	132.69	120.31
3	J	164	PRO	C-N-CA	8.14	132.69	120.31
1	e	155	ALA	N-CA-C	-8.14	96.64	109.50
2	k	199	TYR	CA-C-O	-8.13	109.38	119.38
3	I	337	LYS	CA-C-N	8.13	131.01	120.44
3	I	337	LYS	C-N-CA	8.13	131.01	120.44
3	L	288	ASN	O-C-N	8.13	130.45	122.07
3	M	374	ASP	O-C-N	8.12	130.43	122.07
2	3	188	VAL	O-C-N	-8.11	114.04	123.04
3	K	382	VAL	CA-C-N	8.11	131.14	120.28
3	K	382	VAL	C-N-CA	8.11	131.14	120.28
1	F	144	VAL	CA-C-N	8.10	127.86	119.76
1	F	144	VAL	C-N-CA	8.10	127.86	119.76
1	d	185	PHE	CA-C-N	8.10	131.13	120.28
1	d	185	PHE	C-N-CA	8.10	131.13	120.28
2	5	203	GLU	CA-C-N	8.10	131.92	120.42
2	5	203	GLU	C-N-CA	8.10	131.92	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	200	SER	CA-C-N	8.09	129.95	119.84
2	6	200	SER	C-N-CA	8.09	129.95	119.84
1	C	80	GLY	N-CA-C	-8.08	103.40	111.56
1	C	196	MET	CA-C-N	8.08	128.95	119.98
1	C	196	MET	C-N-CA	8.08	128.95	119.98
1	E	195	ALA	N-CA-C	-8.08	102.41	111.14
3	I	12	LYS	N-CA-C	8.08	119.72	111.07
1	B	169	ASN	CA-C-N	8.08	131.10	120.28
1	B	169	ASN	C-N-CA	8.08	131.10	120.28
1	F	37	ALA	O-C-N	8.07	132.85	123.41
3	L	282	LYS	N-CA-CB	8.06	124.21	110.50
2	j	72	ILE	N-CA-C	8.06	118.16	110.42
1	c	31	VAL	N-CA-C	-8.06	104.85	112.83
1	d	190	VAL	CA-C-N	8.06	131.42	120.38
1	d	190	VAL	C-N-CA	8.06	131.42	120.38
2	j	204	VAL	CA-C-N	8.05	131.88	120.28
2	j	204	VAL	C-N-CA	8.05	131.88	120.28
3	L	131	GLU	O-C-N	-8.05	114.81	123.26
1	D	33	ARG	NE-CZ-NH2	-8.04	111.97	119.20
2	m	69	ILE	CA-C-O	8.04	129.97	121.05
3	I	379	ILE	O-C-N	8.04	129.79	121.91
3	L	283	VAL	N-CA-CB	8.04	120.16	111.00
3	L	355	CYS	CA-C-N	8.03	131.69	120.29
3	L	355	CYS	C-N-CA	8.03	131.69	120.29
1	E	103	TYR	N-CA-C	-8.03	104.64	114.75
3	L	309	VAL	CA-C-N	8.03	129.87	119.84
3	L	309	VAL	C-N-CA	8.03	129.87	119.84
1	C	224	VAL	N-CA-CB	8.02	119.94	110.95
1	B	205	VAL	N-CA-C	-8.02	91.56	108.88
2	i	177	LYS	CA-C-N	8.02	131.68	120.29
2	i	177	LYS	C-N-CA	8.02	131.68	120.29
1	F	165	GLY	O-C-N	8.01	130.46	122.85
2	k	25	MET	N-CA-C	-8.01	97.20	109.14
2	l	45	ILE	CA-C-O	8.01	128.85	120.36
3	H	116	VAL	N-CA-C	-8.01	106.10	113.71
2	5	153	ASP	N-CA-C	8.01	119.70	110.97
1	c	23	GLN	OE1-CD-NE2	-8.00	114.60	122.60
1	b	151	ASP	CA-CB-CG	-8.00	104.60	112.60
1	E	51	ASP	N-CA-C	7.98	121.84	109.96
2	2	157	PRO	N-CA-C	-7.97	103.34	114.98
1	G	137	LEU	N-CA-C	-7.97	95.91	108.90
1	F	82	VAL	CA-C-N	7.97	130.80	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	82	VAL	C-N-CA	7.97	130.80	120.44
2	4	89	ALA	CA-C-N	7.97	131.74	120.42
2	4	89	ALA	C-N-CA	7.97	131.74	120.42
1	G	42	CYS	CA-C-O	-7.96	111.96	121.60
1	D	20	ARG	NE-CZ-NH1	7.95	129.45	121.50
1	g	142	ASP	N-CA-C	-7.95	103.60	113.38
3	H	303	PHE	CA-C-N	7.95	130.93	120.28
3	H	303	PHE	C-N-CA	7.95	130.93	120.28
1	D	241	ARG	NE-CZ-NH2	7.94	126.34	119.20
2	4	102	ARG	NE-CZ-NH2	7.94	126.34	119.20
3	H	20	TYR	CB-CG-CD1	7.94	132.71	120.80
1	C	200	ILE	CA-C-N	7.94	134.17	122.74
1	C	200	ILE	C-N-CA	7.94	134.17	122.74
3	H	302	ARG	N-CA-C	-7.93	93.90	110.80
3	K	111	GLN	CA-C-N	7.93	134.12	122.86
3	K	111	GLN	C-N-CA	7.93	134.12	122.86
2	m	184	ASP	CA-CB-CG	-7.93	104.67	112.60
3	I	121	THR	CA-C-N	7.93	135.97	121.70
3	I	121	THR	C-N-CA	7.93	135.97	121.70
1	a	131	PRO	CA-C-N	7.92	133.11	121.31
1	a	131	PRO	C-N-CA	7.92	133.11	121.31
2	k	30	ARG	N-CA-CB	7.91	123.86	110.49
1	A	172	THR	CA-C-N	7.91	130.72	120.44
1	A	172	THR	C-N-CA	7.91	130.72	120.44
2	4	49	ALA	N-CA-C	-7.91	97.71	108.38
1	C	214	VAL	O-C-N	-7.89	115.37	123.03
3	K	258	ASP	CA-CB-CG	-7.89	104.71	112.60
3	L	287	THR	CA-C-N	7.88	130.69	120.44
3	L	287	THR	C-N-CA	7.88	130.69	120.44
2	i	162	ASP	O-C-N	-7.88	113.77	122.12
3	H	316	GLY	N-CA-C	7.88	122.44	112.83
3	L	295	PRO	CA-C-N	7.87	130.67	120.44
3	L	295	PRO	C-N-CA	7.87	130.67	120.44
1	G	221	PHE	CA-CB-CG	-7.87	105.94	113.80
2	1	184	ASP	CA-CB-CG	7.87	120.47	112.60
1	F	68	TYR	CA-C-N	7.86	131.96	120.95
1	F	68	TYR	C-N-CA	7.86	131.96	120.95
3	H	321	PHE	N-CA-CB	7.86	121.65	109.94
1	f	184	SER	N-CA-C	-7.86	98.18	110.36
1	F	49	ILE	CA-C-O	7.86	128.21	120.27
1	b	112	LEU	CA-C-O	7.85	128.87	120.55
3	L	24	ARG	N-CA-C	-7.84	102.73	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	101	LYS	O-C-N	-7.84	116.32	121.88
3	I	296	ALA	N-CA-C	7.84	119.45	111.07
1	E	142	ASP	CA-CB-CG	-7.83	104.77	112.60
2	4	90	ILE	CA-C-N	7.83	130.62	120.44
2	4	90	ILE	C-N-CA	7.83	130.62	120.44
1	b	239	ARG	NE-CZ-NH1	-7.83	113.67	121.50
2	7	44	LYS	N-CA-C	-7.83	101.52	113.89
3	L	311	LEU	N-CA-CB	7.83	118.82	109.74
3	I	384	LYS	CA-C-O	-7.82	112.26	120.55
3	L	212	VAL	N-CA-CB	7.82	124.13	111.23
2	7	99	ASN	CA-CB-CG	-7.82	104.78	112.60
1	c	99	ASN	CA-CB-CG	7.81	120.41	112.60
1	B	194	VAL	N-CA-CB	7.80	119.17	110.51
1	C	180	ARG	CA-C-O	7.80	130.25	121.51
1	E	93	ARG	CA-C-N	7.80	130.39	120.56
1	E	93	ARG	C-N-CA	7.80	130.39	120.56
1	e	123	TYR	N-CA-C	-7.80	103.58	113.72
2	h	121	SER	CA-C-N	7.80	133.78	122.94
2	h	121	SER	C-N-CA	7.80	133.78	122.94
3	M	189	THR	N-CA-C	-7.80	102.72	111.14
1	A	198	LEU	CA-C-O	7.79	128.81	120.55
1	b	64	ILE	O-C-N	7.79	130.91	122.57
1	e	121	GLN	CA-C-N	7.79	133.73	120.72
1	e	121	GLN	C-N-CA	7.79	133.73	120.72
2	4	198	GLN	N-CA-C	-7.79	95.57	108.34
1	e	186	ASP	CA-CB-CG	-7.79	104.81	112.60
2	7	97	LEU	CA-C-N	7.79	130.71	120.28
2	7	97	LEU	C-N-CA	7.79	130.71	120.28
3	H	389	ILE	CA-C-N	7.78	127.83	119.90
3	H	389	ILE	C-N-CA	7.78	127.83	119.90
2	1	144	SER	CA-C-N	7.77	130.54	120.44
2	1	144	SER	C-N-CA	7.77	130.54	120.44
3	J	319	GLN	OE1-CD-NE2	7.77	130.37	122.60
1	e	71	ASP	CA-C-O	-7.77	113.13	121.36
1	g	141	VAL	N-CA-C	-7.77	96.28	107.77
2	2	209	ALA	N-CA-C	-7.76	103.39	113.17
2	m	65	PHE	CA-CB-CG	7.75	121.56	113.80
3	I	268	LEU	CA-C-N	7.75	130.66	120.28
3	I	268	LEU	C-N-CA	7.75	130.66	120.28
2	1	201	PRO	CA-C-N	7.74	131.55	120.79
2	1	201	PRO	C-N-CA	7.74	131.55	120.79
1	C	113	ALA	N-CA-C	7.74	120.40	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	33	ARG	N-CA-CB	7.74	121.61	110.16
2	i	64	GLN	OE1-CD-NE2	-7.74	114.86	122.60
3	J	11	GLU	CA-C-N	7.73	131.26	120.29
3	J	11	GLU	C-N-CA	7.73	131.26	120.29
2	5	170	ARG	NH1-CZ-NH2	7.72	129.34	119.30
1	c	18	ASP	CA-CB-CG	-7.72	104.88	112.60
1	d	71	ASP	CA-C-N	7.72	131.65	120.38
1	d	71	ASP	C-N-CA	7.72	131.65	120.38
3	H	231	LYS	CA-C-N	7.72	130.62	120.28
3	H	231	LYS	C-N-CA	7.72	130.62	120.28
1	G	90	ASP	CA-C-N	7.72	130.62	120.28
1	G	90	ASP	C-N-CA	7.72	130.62	120.28
2	m	83	ARG	NE-CZ-NH2	7.71	126.14	119.20
2	n	18	VAL	N-CA-CB	7.71	121.20	110.56
1	g	212	GLY	O-C-N	-7.71	116.50	123.36
1	a	96	ALA	N-CA-C	7.70	119.67	111.28
1	F	106	PRO	CA-C-O	-7.69	113.00	121.23
1	a	169	ASN	CA-C-O	-7.69	112.31	120.92
2	3	81	ARG	NE-CZ-NH2	7.69	126.12	119.20
2	n	194	ASP	CA-CB-CG	-7.69	104.91	112.60
3	K	12	LYS	CA-C-N	7.68	131.19	120.29
3	K	12	LYS	C-N-CA	7.68	131.19	120.29
1	C	109	VAL	CA-C-N	7.68	130.42	120.44
1	C	109	VAL	C-N-CA	7.68	130.42	120.44
2	h	118	GLU	N-CA-C	-7.67	103.02	113.30
2	6	198	GLN	OE1-CD-NE2	7.66	130.26	122.60
2	i	148	TYR	N-CA-C	7.66	119.63	111.28
1	D	11	ALA	CA-C-N	7.65	132.68	120.82
1	D	11	ALA	C-N-CA	7.65	132.68	120.82
3	K	376	THR	CA-C-N	7.65	130.53	120.28
3	K	376	THR	C-N-CA	7.65	130.53	120.28
2	i	143	GLY	CA-C-N	7.65	130.86	120.38
2	i	143	GLY	C-N-CA	7.65	130.86	120.38
1	b	221	PHE	CA-C-O	7.65	128.60	120.95
2	k	209	ALA	CA-C-N	7.65	130.53	120.28
2	k	209	ALA	C-N-CA	7.65	130.53	120.28
3	J	252	ASN	CA-C-O	7.65	126.83	118.65
1	a	142	ASP	O-C-N	7.64	132.43	122.03
1	g	153	SER	CA-C-N	7.64	132.32	122.00
1	g	153	SER	C-N-CA	7.64	132.32	122.00
2	m	29	LYS	N-CA-C	-7.64	102.48	112.41
2	m	148	TYR	CA-C-N	7.64	128.62	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	m	148	TYR	C-N-CA	7.64	128.62	119.99
3	J	395	VAL	N-CA-C	-7.63	105.57	112.90
1	G	69	LYS	N-CA-CB	7.63	121.19	109.97
3	K	40	GLU	N-CA-CB	7.63	122.11	110.28
2	4	156	THR	O-C-N	-7.63	112.39	121.39
2	1	153	ASP	CA-C-O	-7.63	112.81	120.82
1	B	136	LEU	N-CA-C	-7.62	97.52	109.72
1	D	197	GLY	CA-C-O	-7.62	112.77	121.00
3	I	55	VAL	CA-C-N	7.62	131.89	120.31
3	I	55	VAL	C-N-CA	7.62	131.89	120.31
1	g	16	SER	CA-C-O	-7.61	111.02	120.23
1	G	26	TYR	N-CA-C	-7.61	102.93	112.90
3	H	278	ARG	N-CA-C	-7.61	94.59	110.80
3	L	225	GLU	N-CA-C	7.61	120.65	111.82
1	f	67	ILE	CA-C-O	7.61	128.38	120.39
2	k	96	ASN	CA-CB-CG	-7.60	105.00	112.60
1	E	181	ASP	CA-CB-CG	-7.60	105.00	112.60
3	M	46	ARG	CA-C-O	7.59	128.60	120.55
3	I	131	GLU	CA-C-N	7.59	130.68	120.50
3	I	131	GLU	C-N-CA	7.59	130.68	120.50
3	I	292	ILE	N-CA-C	-7.59	104.54	113.42
2	k	49	ALA	N-CA-C	-7.58	98.28	108.74
3	M	273	ASP	O-C-N	7.58	128.90	121.85
1	a	119	PHE	CA-CB-CG	-7.58	106.22	113.80
2	2	60	VAL	N-CA-C	7.58	117.66	110.53
3	K	309	VAL	CA-C-N	7.58	127.48	120.21
3	K	309	VAL	C-N-CA	7.58	127.48	120.21
1	E	120	LYS	CA-C-N	7.57	131.19	120.28
1	E	120	LYS	C-N-CA	7.57	131.19	120.28
3	L	123	LYS	N-CA-C	-7.57	101.19	111.87
2	i	69	ILE	CB-CA-C	-7.57	101.78	112.22
2	j	117	SER	N-CA-C	-7.56	103.78	113.16
2	5	47	GLN	O-C-N	-7.56	113.86	122.93
2	k	21	ASP	CA-CB-CG	7.56	120.16	112.60
2	2	60	VAL	CA-C-N	7.55	129.85	120.34
2	2	60	VAL	C-N-CA	7.55	129.85	120.34
2	4	202	GLU	N-CA-C	7.55	120.17	111.11
2	m	154	ARG	CA-C-O	7.55	127.56	119.03
2	n	47	GLN	O-C-N	-7.55	114.62	123.22
3	J	327	LYS	N-CA-C	-7.55	102.99	111.14
1	A	73	HIS	ND1-CE1-NE2	7.54	115.94	108.40
1	g	205	VAL	N-CA-C	-7.54	99.40	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4	68	ARG	NE-CZ-NH2	-7.54	112.41	119.20
3	L	386	THR	N-CA-CB	7.54	123.14	110.69
2	1	33	MET	N-CA-CB	7.54	123.04	110.59
3	K	101	LYS	N-CA-C	-7.54	99.50	108.25
1	b	185	PHE	CA-CB-CG	-7.54	106.26	113.80
2	2	169	VAL	CA-C-N	7.54	130.24	120.44
2	2	169	VAL	C-N-CA	7.54	130.24	120.44
3	H	295	PRO	CA-C-N	7.53	130.99	120.29
3	H	295	PRO	C-N-CA	7.53	130.99	120.29
2	l	41	ALA	O-C-N	7.53	128.85	121.85
2	1	157	PRO	CA-C-N	7.53	133.97	122.37
2	1	157	PRO	C-N-CA	7.53	133.97	122.37
1	a	73	HIS	ND1-CE1-NE2	7.53	115.93	108.40
2	l	148	TYR	CA-C-N	7.52	128.29	119.94
2	l	148	TYR	C-N-CA	7.52	128.29	119.94
1	D	109	VAL	CA-C-N	7.52	130.22	120.44
1	D	109	VAL	C-N-CA	7.52	130.22	120.44
1	f	28	ARG	CA-C-N	7.52	130.36	120.28
1	f	28	ARG	C-N-CA	7.52	130.36	120.28
1	d	180	ARG	NE-CZ-NH1	-7.52	113.98	121.50
3	J	87	PHE	CA-CB-CG	-7.52	106.28	113.80
1	A	16	SER	CA-C-N	7.51	127.19	119.82
1	A	16	SER	C-N-CA	7.51	127.19	119.82
3	K	338	GLU	CA-C-N	7.51	130.34	120.28
3	K	338	GLU	C-N-CA	7.51	130.34	120.28
3	L	46	ARG	CA-C-N	7.50	130.20	120.44
3	L	46	ARG	C-N-CA	7.50	130.20	120.44
3	L	288	ASN	CA-C-O	-7.50	112.94	120.82
1	c	73	HIS	CB-CG-CD2	-7.50	121.45	131.20
1	D	74	ILE	O-C-N	-7.50	115.08	123.10
2	7	37	ILE	N-CA-C	-7.49	96.04	107.73
2	h	200	SER	CA-C-N	7.49	127.86	119.32
2	h	200	SER	C-N-CA	7.49	127.86	119.32
2	l	162	ASP	CA-CB-CG	-7.48	105.12	112.60
1	E	180	ARG	NE-CZ-NH2	7.48	125.93	119.20
2	1	84	LYS	CA-C-O	-7.48	112.39	120.17
2	j	139	ALA	N-CA-C	-7.48	94.87	110.80
1	a	73	HIS	CE1-NE2-CD2	-7.48	101.52	109.00
1	g	118	ASP	CA-C-N	7.48	130.30	120.28
1	g	118	ASP	C-N-CA	7.48	130.30	120.28
3	K	195	VAL	CA-C-N	7.47	130.30	120.28
3	K	195	VAL	C-N-CA	7.47	130.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	182	ASP	CA-CB-CG	-7.47	105.13	112.60
3	L	80	LYS	CA-C-N	7.47	132.67	120.94
3	L	80	LYS	C-N-CA	7.47	132.67	120.94
3	H	35	LYS	CA-C-N	7.47	130.29	120.28
3	H	35	LYS	C-N-CA	7.47	130.29	120.28
1	d	16	SER	CA-C-O	-7.47	112.82	120.96
1	A	184	SER	CA-C-N	7.46	130.14	120.44
1	A	184	SER	C-N-CA	7.46	130.14	120.44
1	D	65	GLU	N-CA-CB	7.46	123.19	110.50
2	j	83	ARG	CA-C-N	7.46	130.67	120.67
2	j	83	ARG	C-N-CA	7.46	130.67	120.67
3	J	130	PHE	CA-C-O	-7.46	113.43	121.56
1	e	83	ALA	CA-C-N	7.46	130.88	120.29
1	e	83	ALA	C-N-CA	7.46	130.88	120.29
2	k	192	THR	O-C-N	7.46	130.92	122.27
2	j	81	ARG	CA-C-O	7.46	126.95	118.97
2	j	204	VAL	N-CA-CB	7.45	121.76	110.58
1	c	230	LYS	CA-C-N	7.45	127.32	119.05
1	c	230	LYS	C-N-CA	7.45	127.32	119.05
1	g	139	ALA	O-C-N	7.45	132.02	123.31
2	6	158	GLU	N-CA-C	-7.45	102.43	112.26
1	d	188	ALA	CA-C-N	7.44	130.11	120.44
1	d	188	ALA	C-N-CA	7.44	130.11	120.44
2	4	155	PHE	CA-CB-CG	-7.44	106.36	113.80
1	E	218	ASP	N-CA-C	-7.44	103.29	113.18
2	k	102	ARG	NE-CZ-NH2	7.44	125.89	119.20
3	I	58	LEU	N-CA-C	7.44	119.39	111.28
1	G	207	GLU	N-CA-C	-7.43	104.21	113.28
2	1	84	LYS	CA-C-N	7.43	127.36	119.85
2	1	84	LYS	C-N-CA	7.43	127.36	119.85
3	L	24	ARG	CA-C-O	-7.43	112.67	120.55
2	1	33	MET	CB-CA-C	-7.43	99.39	110.24
1	D	118	ASP	N-CA-CB	7.43	121.15	110.16
3	M	294	ASP	CA-C-O	-7.43	112.56	120.88
1	A	168	ARG	CD-NE-CZ	-7.43	114.00	124.40
2	1	112	ILE	N-CA-C	-7.42	97.78	108.17
1	a	228	GLU	N-CA-C	-7.42	103.80	114.12
1	g	202	SER	CA-C-N	7.42	132.31	122.30
1	g	202	SER	C-N-CA	7.42	132.31	122.30
1	g	31	VAL	CB-CA-C	-7.42	101.98	112.22
1	e	33	ARG	NE-CZ-NH2	7.41	125.87	119.20
1	b	201	GLU	N-CA-CB	7.41	123.18	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	214	VAL	N-CA-C	-7.41	96.80	107.77
2	m	212	ARG	CB-CA-C	-7.41	98.73	110.14
2	6	150	VAL	O-C-N	7.40	129.16	121.91
3	K	333	ASP	CA-C-N	7.40	131.91	122.37
3	K	333	ASP	C-N-CA	7.40	131.91	122.37
3	J	361	PHE	N-CA-C	-7.40	103.22	111.28
2	j	176	MET	CA-C-O	-7.39	112.71	120.55
1	d	142	ASP	N-CA-C	-7.39	104.79	113.88
1	e	98	ILE	CA-C-O	-7.39	112.49	120.47
2	4	95	SER	CA-C-O	-7.39	112.72	120.55
1	D	153	SER	N-CA-C	7.39	120.27	111.33
2	m	135	LYS	N-CA-CB	7.39	120.94	110.67
1	G	112	LEU	CA-C-N	7.38	130.18	120.28
1	G	112	LEU	C-N-CA	7.38	130.18	120.28
3	K	222	LEU	CA-C-N	7.38	129.86	120.56
3	K	222	LEU	C-N-CA	7.38	129.86	120.56
3	I	311	LEU	CA-C-N	7.38	127.42	119.89
3	I	311	LEU	C-N-CA	7.38	127.42	119.89
1	B	210	GLU	CA-C-O	7.38	128.67	120.70
2	k	177	LYS	N-CA-CB	7.38	121.09	110.16
1	e	181	ASP	CA-CB-CG	-7.38	105.22	112.60
1	d	110	LYS	N-CA-C	7.38	119.32	111.28
2	3	129	GLY	O-C-N	7.37	129.91	122.91
3	I	283	VAL	O-C-N	-7.37	115.51	123.18
2	5	75	ASN	CB-CA-C	-7.37	98.56	110.79
1	G	229	LEU	CA-C-N	7.36	130.30	120.58
1	G	229	LEU	C-N-CA	7.36	130.30	120.58
1	a	104	ASP	N-CA-CB	7.36	123.28	111.65
1	A	185	PHE	CA-CB-CG	-7.35	106.45	113.80
1	f	105	GLU	CA-C-N	7.35	127.80	119.93
1	f	105	GLU	C-N-CA	7.35	127.80	119.93
2	1	171	ALA	N-CA-C	7.35	119.37	111.36
2	n	200	SER	N-CA-CB	7.34	123.44	110.37
1	c	242	GLU	CA-C-N	7.34	132.98	120.72
1	c	242	GLU	C-N-CA	7.34	132.98	120.72
3	L	394	GLY	N-CA-C	7.34	123.74	112.51
2	4	58	GLY	CA-C-N	7.34	131.17	120.82
2	4	58	GLY	C-N-CA	7.34	131.17	120.82
3	I	130	PHE	CA-CB-CG	-7.34	106.46	113.80
1	c	70	ILE	N-CA-C	-7.33	106.34	113.53
2	j	57	ALA	N-CA-C	-7.33	97.99	109.72
3	I	111	GLN	CA-C-O	-7.33	112.78	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	375	PHE	CA-C-O	-7.33	113.12	120.82
3	K	109	ASN	CA-CB-CG	-7.33	105.27	112.60
2	3	200	SER	N-CA-C	-7.32	99.09	110.14
2	4	144	SER	CA-C-N	7.32	129.95	120.44
2	4	144	SER	C-N-CA	7.32	129.95	120.44
2	4	59	SER	CA-C-N	7.31	131.20	120.74
2	4	59	SER	C-N-CA	7.31	131.20	120.74
1	c	18	ASP	N-CA-CB	7.31	120.98	110.16
2	4	116	ASP	CA-CB-CG	7.31	119.91	112.60
2	l	185	GLY	N-CA-C	-7.31	95.86	113.18
1	c	187	ASP	CA-CB-CG	-7.31	105.29	112.60
1	B	159	TYR	CA-C-N	7.30	133.81	122.49
1	B	159	TYR	C-N-CA	7.30	133.81	122.49
1	E	124	THR	N-CA-C	-7.30	102.30	112.45
3	H	363	ILE	O-C-N	-7.29	114.31	121.90
2	7	165	VAL	CA-CB-CG1	-7.29	98.01	110.40
1	A	36	THR	CA-CB-OG1	7.29	120.53	109.60
2	h	149	GLY	CA-C-N	7.29	130.44	120.46
2	h	149	GLY	C-N-CA	7.29	130.44	120.46
1	G	40	ILE	CA-CB-CG1	7.28	122.78	110.40
2	2	41	ALA	N-CA-C	-7.28	103.38	114.16
2	n	193	GLU	CB-CA-C	7.28	117.04	109.83
1	D	127	GLY	CA-C-O	-7.28	115.03	121.58
1	G	186	ASP	CA-C-O	-7.28	113.20	120.70
3	I	100	LEU	N-CA-CB	7.28	120.67	109.97
3	H	196	ALA	N-CA-C	7.28	119.21	111.28
2	4	80	ARG	NE-CZ-NH2	7.27	125.74	119.20
1	e	181	ASP	N-CA-C	-7.26	103.51	112.88
3	I	297	ILE	CA-C-N	7.26	130.61	120.29
3	I	297	ILE	C-N-CA	7.26	130.61	120.29
3	K	134	GLU	N-CA-C	-7.26	102.94	112.24
3	K	317	ARG	CA-C-N	7.26	129.71	120.56
3	K	317	ARG	C-N-CA	7.26	129.71	120.56
3	M	56	GLU	CA-C-N	7.26	130.60	120.29
3	M	56	GLU	C-N-CA	7.26	130.60	120.29
1	c	205	VAL	CA-C-O	-7.26	115.01	119.51
2	n	42	ALA	CA-C-O	7.26	128.38	120.32
1	e	200	ILE	O-C-N	7.26	129.34	122.23
1	B	44	GLU	N-CA-C	-7.26	103.58	113.30
3	J	326	ARG	CA-C-N	7.25	130.30	120.44
3	J	326	ARG	C-N-CA	7.25	130.30	120.44
1	F	172	THR	CA-C-O	-7.25	112.87	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	219	GLY	O-C-N	7.25	129.31	122.13
3	J	262	GLN	N-CA-C	7.25	120.22	111.82
1	E	91	ARG	NE-CZ-NH2	7.24	125.71	119.20
2	6	108	VAL	CA-C-O	-7.23	115.16	121.09
3	K	120	PRO	CA-C-N	7.22	129.96	120.28
3	K	120	PRO	C-N-CA	7.22	129.96	120.28
2	h	143	GLY	CA-C-N	7.22	129.95	120.28
2	h	143	GLY	C-N-CA	7.22	129.95	120.28
1	B	185	PHE	CA-CB-CG	-7.21	106.59	113.80
1	c	67	ILE	CA-C-O	7.21	128.00	120.36
2	2	35	ASN	N-CA-C	-7.21	102.05	111.71
2	2	112	ILE	N-CA-C	-7.20	97.11	107.77
2	j	160	GLY	CA-C-O	-7.20	114.70	122.76
3	M	135	LYS	CA-C-O	-7.20	110.30	120.16
2	4	126	ASP	N-CA-C	-7.19	100.72	110.36
2	6	88	ARG	NE-CZ-NH1	-7.19	114.31	121.50
2	5	170	ARG	NE-CZ-NH1	7.19	128.69	121.50
3	K	280	ASP	N-CA-C	-7.19	95.49	110.80
3	H	319	GLN	N-CA-C	7.18	119.11	111.28
1	G	189	MET	O-C-N	7.18	129.47	122.07
2	k	192	THR	CA-C-O	-7.18	111.00	118.90
1	E	115	LYS	O-C-N	-7.18	113.97	122.15
2	h	50	ASP	CA-CB-CG	-7.18	105.42	112.60
1	C	107	ILE	CA-C-N	7.17	131.00	120.95
1	C	107	ILE	C-N-CA	7.17	131.00	120.95
3	H	218	GLU	N-CA-CB	7.17	121.40	110.28
3	I	280	ASP	CA-CB-CG	-7.17	105.43	112.60
1	E	108	THR	CA-C-N	7.17	130.28	120.46
1	E	108	THR	C-N-CA	7.17	130.28	120.46
3	I	155	GLU	CA-C-O	-7.17	112.95	120.55
2	6	59	SER	CA-C-N	7.16	130.27	120.46
2	6	59	SER	C-N-CA	7.16	130.27	120.46
3	J	147	ASP	CA-C-O	-7.16	112.96	120.55
2	4	29	LYS	O-C-N	-7.16	114.90	123.13
1	d	21	LEU	CA-C-N	7.15	131.18	120.31
1	d	21	LEU	C-N-CA	7.15	131.18	120.31
1	d	71	ASP	N-CA-C	-7.15	98.78	108.86
1	G	52	LYS	CA-C-N	7.15	130.45	120.29
1	G	52	LYS	C-N-CA	7.15	130.45	120.29
2	h	111	LEU	N-CA-C	-7.15	96.75	108.41
2	h	158	GLU	N-CA-C	-7.15	101.75	111.55
2	m	186	ILE	CA-C-O	7.15	129.19	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	e	218	ASP	CA-CB-CG	7.15	119.75	112.60
1	f	214	VAL	N-CA-C	-7.14	97.74	108.17
2	h	173	TYR	O-C-N	-7.14	114.55	122.12
2	7	163	GLU	N-CA-C	-7.14	104.59	113.38
2	n	36	PHE	CA-C-N	7.14	131.81	122.95
2	n	36	PHE	C-N-CA	7.14	131.81	122.95
1	c	214	VAL	N-CA-C	-7.14	97.84	108.12
1	f	94	ILE	CA-C-N	7.14	129.85	120.28
1	f	94	ILE	C-N-CA	7.14	129.85	120.28
1	G	71	ASP	N-CA-C	-7.14	98.79	108.86
2	5	140	THR	O-C-N	-7.14	115.26	123.33
2	5	191	ILE	N-CA-C	-7.14	94.49	109.34
2	5	191	ILE	N-CA-CB	7.14	123.00	111.23
3	M	245	ALA	CA-C-O	7.14	128.18	119.97
1	b	218	ASP	CA-CB-CG	-7.13	105.47	112.60
1	b	21	LEU	N-CA-C	7.13	119.53	110.33
1	G	131	PRO	N-CA-CB	7.13	109.66	103.31
2	j	141	GLY	N-CA-C	-7.13	102.75	112.52
2	2	191	ILE	N-CA-C	-7.13	94.52	109.34
2	l	103	TYR	N-CA-C	-7.13	103.59	111.36
2	h	140	THR	N-CA-CB	7.12	122.53	110.49
3	I	24	ARG	N-CA-C	7.12	118.69	111.07
1	C	205	VAL	N-CA-C	-7.12	93.50	108.88
2	5	170	ARG	CA-C-N	7.12	129.82	120.28
2	5	170	ARG	C-N-CA	7.12	129.82	120.28
3	M	281	VAL	O-C-N	-7.12	115.57	123.26
1	a	32	LYS	CA-C-N	7.12	130.40	120.29
1	a	32	LYS	C-N-CA	7.12	130.40	120.29
1	F	122	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	d	230	LYS	CA-C-O	-7.11	111.44	118.34
2	m	126	ASP	CA-C-N	7.11	127.27	119.87
2	m	126	ASP	C-N-CA	7.11	127.27	119.87
1	F	67	ILE	CB-CA-C	-7.11	102.36	110.96
3	J	355	CYS	N-CA-C	7.11	119.11	111.36
1	b	118	ASP	CA-C-N	7.11	129.68	120.44
1	b	118	ASP	C-N-CA	7.11	129.68	120.44
2	6	193	GLU	N-CA-CB	7.11	122.50	110.49
3	M	252	ASN	CA-CB-CG	-7.10	105.50	112.60
2	l	86	THR	CA-C-N	7.10	130.19	120.46
2	l	86	THR	C-N-CA	7.10	130.19	120.46
2	l	121	SER	N-CA-C	-7.10	97.49	108.42
3	J	393	LYS	N-CA-C	-7.10	104.36	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	168	ALA	N-CA-C	7.09	119.09	111.36
3	M	131	GLU	N-CA-CB	7.09	122.48	110.49
2	n	134	GLU	N-CA-CB	7.09	123.17	110.83
1	G	172	THR	CA-C-N	7.09	129.78	120.28
1	G	172	THR	C-N-CA	7.09	129.78	120.28
2	l	199	TYR	N-CA-C	7.09	119.86	111.71
1	a	80	GLY	N-CA-C	-7.08	103.84	111.21
1	C	231	PRO	N-CA-CB	7.08	110.81	103.23
1	E	66	LYS	N-CA-C	-7.08	104.90	113.97
3	I	173	GLU	CA-C-N	7.08	127.67	120.38
3	I	173	GLU	C-N-CA	7.08	127.67	120.38
3	M	296	ALA	N-CA-C	-7.08	103.95	112.59
2	i	135	LYS	N-CA-C	-7.08	103.75	112.88
3	K	41	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	F	235	ARG	NE-CZ-NH2	7.07	125.56	119.20
2	l	45	ILE	O-C-N	-7.07	115.56	123.20
3	L	372	MET	N-CA-C	-7.07	103.32	112.23
1	F	196	MET	CA-C-N	7.07	127.83	119.98
1	F	196	MET	C-N-CA	7.07	127.83	119.98
2	5	112	ILE	N-CA-C	-7.07	97.31	107.77
2	i	81	ARG	N-CA-C	-7.07	103.01	113.61
3	M	12	LYS	CA-C-O	-7.07	112.93	120.42
1	C	67	ILE	N-CA-CB	7.06	122.89	111.23
3	I	71	ILE	N-CA-C	-7.06	98.22	108.11
3	J	32	ASP	CA-CB-CG	7.06	119.66	112.60
2	7	81	ARG	NH1-CZ-NH2	7.06	128.47	119.30
1	D	220	THR	N-CA-C	-7.05	97.40	108.90
2	k	135	LYS	N-CA-C	-7.05	103.34	113.21
1	A	65	GLU	O-C-N	-7.05	111.73	123.00
2	l	170	ARG	CD-NE-CZ	7.04	134.25	124.40
3	L	15	LYS	N-CA-C	7.04	118.60	111.07
1	e	151	ASP	CA-C-N	7.03	127.02	119.28
1	e	151	ASP	C-N-CA	7.03	127.02	119.28
3	H	38	GLU	CA-C-O	-7.03	113.44	120.82
3	K	175	PRO	CA-C-N	7.03	129.58	120.44
3	K	175	PRO	C-N-CA	7.03	129.58	120.44
3	L	240	ILE	N-CA-C	-7.03	97.60	107.80
1	E	84	ASP	CA-CB-CG	7.03	119.63	112.60
1	f	67	ILE	N-CA-CB	7.03	121.11	111.41
1	G	190	VAL	CA-C-N	7.03	130.27	120.29
1	G	190	VAL	C-N-CA	7.03	130.27	120.29
3	K	316	GLY	O-C-N	7.03	129.01	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	128	GLY	O-C-N	-7.03	113.56	122.70
1	A	43	LYS	N-CA-C	-7.03	104.71	112.72
3	J	272	LEU	N-CA-C	-7.02	103.62	111.28
1	e	14	VAL	N-CA-CB	7.02	122.81	111.23
3	H	17	GLU	CA-C-N	7.02	129.57	120.44
3	H	17	GLU	C-N-CA	7.02	129.57	120.44
2	j	55	THR	N-CA-CB	7.02	123.04	110.83
3	H	339	LEU	N-CA-C	7.02	119.01	111.36
2	j	98	LEU	N-CA-CB	7.02	120.54	110.16
3	M	396	MET	N-CA-C	-7.01	104.60	113.72
1	a	71	ASP	CA-C-N	7.01	130.37	120.28
1	a	71	ASP	C-N-CA	7.01	130.37	120.28
1	B	187	ASP	CA-C-N	7.00	129.55	120.44
1	B	187	ASP	C-N-CA	7.00	129.55	120.44
2	h	30	ARG	NE-CZ-NH2	7.00	125.50	119.20
2	3	62	ASP	CA-C-N	7.00	129.54	120.44
2	3	62	ASP	C-N-CA	7.00	129.54	120.44
1	B	149	GLU	CB-CG-CD	-7.00	100.70	112.60
1	e	240	ILE	CB-CA-C	-7.00	102.69	112.14
2	3	30	ARG	NE-CZ-NH2	7.00	125.50	119.20
3	H	304	ASP	CA-CB-CG	-7.00	105.60	112.60
3	J	182	GLY	O-C-N	-7.00	114.77	121.77
3	I	218	GLU	CA-C-O	7.00	127.83	120.42
2	n	117	SER	CA-C-N	6.99	129.98	120.54
2	n	117	SER	C-N-CA	6.99	129.98	120.54
3	M	351	ILE	CA-C-N	6.99	129.65	120.28
3	M	351	ILE	C-N-CA	6.99	129.65	120.28
1	d	173	GLU	CA-C-N	6.99	129.52	120.44
1	d	173	GLU	C-N-CA	6.99	129.52	120.44
1	e	197	GLY	O-C-N	-6.99	114.84	122.24
3	I	16	LEU	N-CA-C	-6.99	103.43	112.23
3	L	302	ARG	N-CA-C	-6.99	105.30	114.31
1	g	90	ASP	CA-C-N	6.98	129.52	120.44
1	g	90	ASP	C-N-CA	6.98	129.52	120.44
2	m	79	ILE	O-C-N	6.98	128.75	121.91
2	4	103	TYR	N-CA-CB	6.98	120.48	110.16
1	C	84	ASP	CA-C-N	6.97	129.50	120.44
1	C	84	ASP	C-N-CA	6.97	129.50	120.44
1	d	46	VAL	N-CA-C	-6.97	98.00	108.17
3	K	229	LEU	CA-C-N	6.96	129.49	120.44
3	K	229	LEU	C-N-CA	6.96	129.49	120.44
2	6	98	LEU	N-CA-C	6.96	119.72	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	312	PRO	N-CA-CB	6.96	109.81	103.34
1	g	145	PRO	CB-CA-C	6.96	119.88	111.46
1	E	80	GLY	CA-C-N	6.96	132.51	121.66
1	E	80	GLY	C-N-CA	6.96	132.51	121.66
1	f	103	TYR	CB-CA-C	-6.96	100.03	109.28
1	B	230	LYS	CA-C-O	-6.96	112.23	118.63
2	k	139	ALA	CA-C-N	6.95	134.22	121.70
2	k	139	ALA	C-N-CA	6.95	134.22	121.70
1	B	100	ARG	NE-CZ-NH1	-6.95	114.55	121.50
3	H	395	VAL	CB-CA-C	-6.95	102.58	111.20
1	g	64	ILE	CA-C-N	6.95	131.24	120.75
1	g	64	ILE	C-N-CA	6.95	131.24	120.75
1	B	187	ASP	CB-CA-C	-6.95	99.04	110.85
2	6	175	ALA	CA-C-N	6.95	129.90	120.38
2	6	175	ALA	C-N-CA	6.95	129.90	120.38
1	c	117	CYS	N-CA-CB	6.94	120.14	110.07
3	H	347	SER	CA-C-N	6.94	128.82	120.14
3	H	347	SER	C-N-CA	6.94	128.82	120.14
1	D	27	ALA	N-CA-C	-6.94	104.28	112.89
2	m	204	VAL	CB-CA-C	-6.94	102.64	112.22
1	B	53	ARG	CA-C-N	6.94	130.06	120.49
1	B	53	ARG	C-N-CA	6.94	130.06	120.49
1	d	236	ALA	CA-C-N	6.94	129.58	120.28
1	d	236	ALA	C-N-CA	6.94	129.58	120.28
2	1	144	SER	N-CA-C	6.94	118.84	111.28
1	b	98	ILE	N-CA-CB	6.93	120.98	110.58
2	6	140	THR	N-CA-CB	6.93	123.29	111.50
2	k	162	ASP	CA-CB-CG	-6.93	105.67	112.60
1	C	6	MET	N-CA-C	-6.93	97.33	108.55
3	H	355	CYS	N-CA-C	6.93	118.91	111.36
3	J	357	GLU	CA-C-N	6.93	130.13	120.29
3	J	357	GLU	C-N-CA	6.93	130.13	120.29
3	L	394	GLY	CA-C-N	6.93	134.17	121.70
3	L	394	GLY	C-N-CA	6.93	134.17	121.70
3	K	240	ILE	CA-C-N	-6.92	109.47	121.52
3	K	240	ILE	C-N-CA	-6.92	109.47	121.52
3	M	114	ALA	CA-C-N	6.92	129.84	120.63
3	M	114	ALA	C-N-CA	6.92	129.84	120.63
1	b	181	ASP	CA-CB-CG	-6.92	105.68	112.60
1	A	60	GLU	CA-C-O	-6.92	113.03	120.92
1	d	218	ASP	N-CA-C	-6.91	106.04	114.75
2	l	96	ASN	N-CA-C	6.91	118.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	51	ASP	CA-C-N	6.91	129.42	120.44
1	d	51	ASP	C-N-CA	6.91	129.42	120.44
2	7	147	ALA	CA-C-O	-6.91	113.57	120.82
1	c	65	GLU	N-CA-CB	6.90	121.18	110.21
1	b	53	ARG	CA-C-O	6.90	128.79	120.92
1	g	16	SER	O-C-N	6.90	128.48	121.72
2	l	83	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	f	71	ASP	N-CA-C	-6.89	99.22	108.74
2	n	37	ILE	N-CA-CB	6.89	119.87	111.60
3	L	351	ILE	CA-C-N	6.89	130.08	120.29
3	L	351	ILE	C-N-CA	6.89	130.08	120.29
1	f	138	ILE	N-CA-CB	6.89	119.27	111.21
3	I	149	GLN	CA-C-O	-6.89	113.25	120.55
1	F	13	THR	N-CA-C	-6.89	103.99	112.88
1	F	172	THR	O-C-N	6.89	129.42	122.12
1	E	79	SER	N-CA-C	-6.89	98.18	108.99
1	A	59	LEU	N-CA-CB	6.89	120.21	110.36
1	A	189	MET	CA-C-N	6.89	130.20	120.42
1	A	189	MET	C-N-CA	6.89	130.20	120.42
1	D	38	ILE	CA-C-N	6.88	127.36	122.33
1	D	38	ILE	C-N-CA	6.88	127.36	122.33
3	M	143	ILE	CA-C-O	-6.88	113.10	119.91
2	3	187	ASP	CA-CB-CG	6.88	119.48	112.60
3	M	57	ARG	CA-C-N	6.88	130.05	120.29
3	M	57	ARG	C-N-CA	6.88	130.05	120.29
1	B	13	THR	CA-C-N	6.87	131.07	122.48
1	B	13	THR	C-N-CA	6.87	131.07	122.48
1	E	14	VAL	N-CA-CB	6.87	121.55	111.52
3	L	377	LYS	CA-C-N	6.87	129.49	120.28
3	L	377	LYS	C-N-CA	6.87	129.49	120.28
1	d	103	TYR	O-C-N	6.87	130.09	121.64
3	M	143	ILE	O-C-N	6.87	129.26	122.05
3	L	128	TYR	N-CA-C	-6.87	105.43	113.88
3	M	73	GLU	CB-CG-CD	-6.87	100.93	112.60
2	6	99	ASN	CA-C-O	-6.87	113.14	120.42
3	H	336	PHE	CA-CB-CG	-6.87	106.94	113.80
3	K	102	PRO	N-CA-CB	6.87	109.28	103.17
2	5	101	TYR	CB-CG-CD2	6.86	131.09	120.80
1	E	98	ILE	CA-C-O	6.86	127.91	120.57
2	h	206	GLN	OE1-CD-NE2	6.86	129.46	122.60
3	I	39	SER	O-C-N	6.86	129.39	122.12
1	g	28	ARG	N-CA-C	-6.86	103.86	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	212	GLY	CA-C-O	-6.86	113.61	121.49
1	d	193	LEU	CA-C-O	-6.85	113.16	120.42
1	f	200	ILE	CA-CB-CG2	-6.85	98.86	110.50
1	b	240	ILE	O-C-N	6.85	128.51	121.87
1	a	235	ARG	CA-C-N	6.84	129.34	120.44
1	a	235	ARG	C-N-CA	6.84	129.34	120.44
1	E	241	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	e	105	GLU	O-C-N	6.84	127.17	121.83
3	H	98	GLU	N-CA-C	-6.84	104.05	112.88
3	M	126	MET	CG-SD-CE	-6.84	85.85	100.90
2	l	76	LEU	CA-C-N	6.84	129.44	120.28
2	l	76	LEU	C-N-CA	6.84	129.44	120.28
2	3	87	VAL	CA-C-N	6.84	129.44	120.28
2	3	87	VAL	C-N-CA	6.84	129.44	120.28
2	4	139	ALA	N-CA-C	-6.84	99.15	108.38
2	7	104	PHE	N-CA-C	-6.83	100.63	110.40
1	C	92	ALA	CA-C-N	6.83	129.99	120.29
1	C	92	ALA	C-N-CA	6.83	129.99	120.29
1	F	37	ALA	CA-C-O	-6.83	112.14	120.54
3	K	303	PHE	CA-CB-CG	-6.83	106.97	113.80
3	L	48	VAL	CA-C-O	-6.83	113.85	120.95
1	D	202	SER	CA-C-N	6.82	130.44	120.82
1	D	202	SER	C-N-CA	6.82	130.44	120.82
2	1	85	PRO	N-CA-CB	6.82	109.67	103.33
2	j	179	ASP	CA-CB-CG	-6.82	105.78	112.60
3	L	320	ILE	O-C-N	6.82	128.49	121.87
1	b	120	LYS	CA-C-N	6.82	129.42	120.28
1	b	120	LYS	C-N-CA	6.82	129.42	120.28
1	G	60	GLU	CA-C-N	6.82	129.97	120.29
1	G	60	GLU	C-N-CA	6.82	129.97	120.29
3	I	310	PRO	CA-C-N	6.82	131.03	120.60
3	I	310	PRO	C-N-CA	6.82	131.03	120.60
2	2	190	LYS	N-CA-CB	6.82	121.76	110.85
2	j	167	LEU	CA-C-N	6.82	129.97	120.29
2	j	167	LEU	C-N-CA	6.82	129.97	120.29
3	M	283	VAL	N-CA-C	-6.82	97.92	107.80
1	A	85	ALA	CA-C-N	6.81	129.74	120.54
1	A	85	ALA	C-N-CA	6.81	129.74	120.54
1	b	189	MET	CA-C-O	-6.81	113.67	120.82
2	j	163	GLU	N-CA-C	-6.81	103.98	112.90
3	I	305	ARG	CA-C-O	6.81	129.15	120.57
2	4	39	SER	N-CA-C	-6.81	99.19	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	180	ARG	N-CA-C	-6.81	99.07	109.41
2	1	191	ILE	N-CA-CB	6.80	122.46	111.23
2	3	48	ILE	N-CA-C	-6.80	105.21	111.67
3	H	261	VAL	CA-C-O	-6.80	111.00	119.43
1	C	64	ILE	CB-CA-C	6.80	119.34	110.91
2	k	148	TYR	CA-C-O	-6.80	113.29	120.63
1	F	95	GLU	N-CA-CB	6.80	119.87	110.01
2	i	172	ILE	CA-C-N	6.80	129.39	120.28
2	i	172	ILE	C-N-CA	6.80	129.39	120.28
3	H	120	PRO	N-CA-CB	-6.80	96.11	103.25
3	J	61	PRO	CA-C-N	6.79	126.56	119.76
3	J	61	PRO	C-N-CA	6.79	126.56	119.76
1	d	26	TYR	CA-C-N	6.79	130.63	120.31
1	d	26	TYR	C-N-CA	6.79	130.63	120.31
1	C	87	VAL	O-C-N	6.79	128.82	121.83
2	6	209	ALA	CA-C-N	6.79	133.61	121.66
2	6	209	ALA	C-N-CA	6.79	133.61	121.66
3	I	331	ALA	N-CA-C	-6.79	99.61	110.14
1	D	194	VAL	CA-C-O	-6.79	113.89	120.95
2	m	211	PHE	CA-CB-CG	-6.79	107.01	113.80
2	4	103	TYR	CA-C-O	6.79	127.61	120.42
1	A	216	VAL	N-CA-C	-6.79	106.52	113.10
2	3	27	THR	CA-CB-OG1	6.79	119.78	109.60
3	I	244	ASP	N-CA-C	-6.78	103.02	112.45
3	K	267	GLN	CA-C-N	6.78	129.26	120.44
3	K	267	GLN	C-N-CA	6.78	129.26	120.44
2	l	187	ASP	CA-CB-CG	6.78	119.38	112.60
1	d	239	ARG	NE-CZ-NH2	6.78	125.30	119.20
3	J	211	PHE	CA-CB-CG	6.78	120.58	113.80
1	A	52	LYS	N-CA-C	-6.78	104.14	112.88
1	B	231	PRO	CA-C-N	6.78	130.61	120.31
1	B	231	PRO	C-N-CA	6.78	130.61	120.31
2	5	126	ASP	O-C-N	-6.78	115.00	121.57
1	d	64	ILE	N-CA-CB	6.77	118.54	110.95
2	2	19	CYS	N-CA-C	-6.77	99.64	110.14
2	l	128	ILE	CA-CB-CG1	6.77	121.91	110.40
1	F	15	PHE	CA-CB-CG	-6.77	107.03	113.80
1	c	73	HIS	CB-CG-ND1	6.77	132.85	122.70
3	K	354	ILE	CA-C-N	6.77	129.24	120.44
3	K	354	ILE	C-N-CA	6.77	129.24	120.44
2	5	143	GLY	CA-C-N	6.77	129.35	120.28
2	5	143	GLY	C-N-CA	6.77	129.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	104	ALA	CB-CA-C	-6.76	99.20	110.29
1	E	10	ARG	NE-CZ-NH2	-6.76	113.11	119.20
3	K	263	ARG	NE-CZ-NH2	-6.76	113.11	119.20
3	L	397	PHE	CA-CB-CG	-6.76	107.04	113.80
2	2	126	ASP	CA-CB-CG	-6.76	105.84	112.60
3	I	339	LEU	CA-C-N	6.76	129.34	120.28
3	I	339	LEU	C-N-CA	6.76	129.34	120.28
2	h	29	LYS	N-CA-C	-6.75	105.07	113.38
1	f	169	ASN	CA-CB-CG	-6.75	105.85	112.60
2	6	161	VAL	N-CA-C	6.75	119.53	111.09
3	H	280	ASP	CA-CB-CG	-6.75	105.85	112.60
3	I	85	PRO	O-C-N	6.75	131.20	123.10
1	b	200	ILE	CA-C-N	6.75	131.72	122.34
1	b	200	ILE	C-N-CA	6.75	131.72	122.34
2	n	78	GLU	CA-C-N	6.75	129.20	120.56
2	n	78	GLU	C-N-CA	6.75	129.20	120.56
2	n	85	PRO	N-CA-CB	6.75	109.18	103.17
3	H	12	LYS	CA-C-N	6.75	129.32	120.28
3	H	12	LYS	C-N-CA	6.75	129.32	120.28
3	J	259	ARG	CA-C-O	-6.75	113.34	120.63
3	H	374	ASP	N-CA-CB	6.74	120.03	110.12
3	M	235	PRO	N-CA-CB	6.74	110.02	102.60
1	B	5	GLN	CB-CA-C	6.74	122.91	110.10
1	B	85	ALA	CA-C-N	6.74	129.20	120.44
1	B	85	ALA	C-N-CA	6.74	129.20	120.44
1	C	47	ILE	N-CA-C	-6.74	98.77	108.48
1	f	20	ARG	NE-CZ-NH2	-6.74	113.13	119.20
2	3	103	TYR	N-CA-C	-6.74	104.01	111.36
1	G	95	GLU	CA-C-N	6.74	129.86	120.29
1	G	95	GLU	C-N-CA	6.74	129.86	120.29
1	G	240	ILE	CB-CA-C	-6.74	103.19	112.02
2	m	163	GLU	N-CA-C	-6.74	105.21	113.50
1	b	84	ASP	CA-C-N	6.73	129.30	120.28
1	b	84	ASP	C-N-CA	6.73	129.30	120.28
2	6	134	GLU	N-CA-CB	6.73	121.88	110.71
3	K	124	ASP	CA-C-N	6.73	126.68	119.28
3	K	124	ASP	C-N-CA	6.73	126.68	119.28
1	D	190	VAL	CA-CB-CG2	-6.72	98.97	110.40
3	M	59	ARG	CA-C-N	6.72	130.26	120.51
3	M	59	ARG	C-N-CA	6.72	130.26	120.51
2	n	25	MET	N-CA-C	-6.72	97.63	109.06
1	F	161	ALA	O-C-N	-6.72	115.76	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	197	GLY	CA-C-O	-6.72	112.91	120.30
2	h	191	ILE	N-CA-C	-6.72	95.37	109.34
2	5	111	LEU	N-CA-C	-6.72	97.41	108.76
2	4	77	TYR	N-CA-C	-6.71	103.96	111.28
3	L	383	LEU	CA-C-N	6.71	129.28	120.28
3	L	383	LEU	C-N-CA	6.71	129.28	120.28
1	B	52	LYS	CG-CD-CE	6.71	126.73	111.30
1	b	148	TYR	CA-C-N	6.71	132.45	122.99
1	b	148	TYR	C-N-CA	6.71	132.45	122.99
3	M	217	GLY	CA-C-N	6.71	129.28	120.28
3	M	217	GLY	C-N-CA	6.71	129.28	120.28
1	A	116	ILE	CA-C-N	6.71	129.27	120.28
1	A	116	ILE	C-N-CA	6.71	129.27	120.28
2	i	33	MET	N-CA-C	-6.71	96.40	108.48
1	b	182	ASP	N-CA-C	-6.71	103.69	112.41
1	d	170	ALA	N-CA-C	6.71	118.39	111.14
2	h	17	LEU	N-CA-CB	6.71	124.00	111.52
3	I	41	ARG	CA-C-N	6.71	129.94	120.42
3	I	41	ARG	C-N-CA	6.71	129.94	120.42
2	2	60	VAL	CA-C-O	-6.71	113.61	121.05
1	D	33	ARG	CB-CA-C	-6.70	100.35	111.41
1	e	59	LEU	N-CA-C	-6.70	99.91	109.96
2	n	123	TYR	O-C-N	6.70	131.94	123.23
3	L	73	GLU	N-CA-C	-6.70	104.68	112.92
3	K	76	ARG	N-CA-C	-6.70	98.98	108.96
3	L	11	GLU	CA-C-N	6.70	129.15	120.44
3	L	11	GLU	C-N-CA	6.70	129.15	120.44
2	i	118	GLU	CB-CA-C	-6.70	99.12	110.64
2	k	90	ILE	CA-C-N	6.70	129.25	120.28
2	k	90	ILE	C-N-CA	6.70	129.25	120.28
2	n	175	ALA	N-CA-C	6.70	118.58	111.28
1	G	218	ASP	CA-CB-CG	6.69	119.29	112.60
3	H	360	MET	CA-C-N	6.69	129.80	120.29
3	H	360	MET	C-N-CA	6.69	129.80	120.29
2	6	125	ILE	N-CA-C	-6.69	98.80	108.17
3	I	27	TYR	N-CA-C	6.69	119.58	111.82
2	l	195	GLU	N-CA-C	-6.69	99.17	109.14
1	f	46	VAL	CB-CA-C	6.69	120.09	110.33
1	b	235	ARG	N-CA-CB	6.68	121.49	110.39
3	J	258	ASP	O-C-N	6.68	129.21	122.12
2	7	204	VAL	CB-CA-C	-6.68	103.00	112.22
3	J	192	ALA	O-C-N	-6.68	115.04	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	VAL	CA-C-N	6.68	129.23	120.28
1	A	31	VAL	C-N-CA	6.68	129.23	120.28
2	1	112	ILE	CA-C-O	6.68	127.56	120.48
3	I	147	ASP	O-C-N	6.68	129.04	122.09
1	b	220	THR	CA-CB-OG1	6.68	119.62	109.60
1	e	202	SER	N-CA-C	-6.68	98.85	108.60
1	d	212	GLY	O-C-N	-6.68	117.78	123.59
1	e	203	GLU	O-C-N	-6.68	114.98	122.86
3	K	226	VAL	N-CA-CB	6.68	119.62	110.54
2	i	39	SER	CA-C-N	6.67	131.87	120.72
2	i	39	SER	C-N-CA	6.67	131.87	120.72
1	D	180	ARG	N-CA-C	-6.67	99.18	109.52
1	d	55	GLY	CA-C-N	6.67	134.28	121.54
1	d	55	GLY	C-N-CA	6.67	134.28	121.54
1	e	26	TYR	CB-CG-CD2	-6.67	110.80	120.80
2	h	28	GLU	CA-C-O	-6.67	113.42	121.28
1	A	97	GLN	CA-C-N	6.66	129.88	120.42
1	A	97	GLN	C-N-CA	6.66	129.88	120.42
2	n	70	ILE	CA-C-N	6.66	129.21	120.28
2	n	70	ILE	C-N-CA	6.66	129.21	120.28
1	C	191	LEU	CA-C-N	6.66	127.33	120.00
1	C	191	LEU	C-N-CA	6.66	127.33	120.00
2	6	118	GLU	CA-C-O	6.66	127.10	119.18
3	I	60	SER	O-C-N	-6.66	114.21	121.53
3	M	143	ILE	N-CA-C	-6.66	105.85	112.17
3	K	26	LEU	CA-C-O	-6.65	113.85	120.70
1	a	206	PRO	O-C-N	6.65	131.48	122.37
1	E	231	PRO	N-CA-CB	6.65	110.40	103.15
3	I	137	GLU	CA-C-N	6.65	131.44	123.19
3	I	137	GLU	C-N-CA	6.65	131.44	123.19
1	D	44	GLU	N-CA-C	-6.65	105.08	113.72
2	k	83	ARG	N-CA-CB	6.65	122.76	110.99
1	a	112	LEU	CA-C-N	6.65	129.19	120.28
1	a	112	LEU	C-N-CA	6.65	129.19	120.28
1	d	196	MET	N-CA-CB	6.65	119.89	110.12
1	f	130	ARG	CA-C-N	6.65	126.68	119.90
1	f	130	ARG	C-N-CA	6.65	126.68	119.90
2	m	203	GLU	O-C-N	6.65	129.73	122.15
1	a	210	GLU	CB-CA-C	6.65	122.87	109.38
2	3	128	ILE	N-CA-C	-6.65	106.04	112.29
3	M	104	ALA	N-CA-CB	6.64	120.09	110.06
1	g	125	GLN	N-CA-C	-6.64	104.20	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	65	PHE	CA-C-O	-6.64	113.84	120.82
3	J	128	TYR	CA-CB-CG	-6.64	101.94	113.90
2	3	156	THR	N-CA-C	-6.64	98.19	108.55
1	A	227	GLU	CA-C-N	6.64	129.18	120.28
1	A	227	GLU	C-N-CA	6.64	129.18	120.28
1	d	122	GLN	N-CA-CB	6.64	119.99	110.16
1	f	232	TYR	CA-C-N	6.64	128.93	120.56
1	f	232	TYR	C-N-CA	6.64	128.93	120.56
3	H	60	SER	CA-C-O	-6.64	114.13	119.71
1	B	236	ALA	N-CA-CB	6.64	119.64	110.01
2	1	161	VAL	CA-C-N	6.64	129.18	120.28
2	1	161	VAL	C-N-CA	6.64	129.18	120.28
3	H	309	VAL	O-C-N	-6.64	114.59	120.96
2	k	166	GLU	O-C-N	6.64	129.26	122.09
2	7	211	PHE	N-CA-C	-6.63	104.41	113.30
1	C	73	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
2	5	173	TYR	CA-C-N	6.63	129.16	120.28
2	5	173	TYR	C-N-CA	6.63	129.16	120.28
3	I	377	LYS	CA-C-O	-6.63	112.34	119.97
3	K	227	PHE	N-CA-C	6.63	120.58	112.23
1	A	54	VAL	CA-C-O	-6.63	115.66	121.09
3	L	95	ILE	CA-CB-CG1	6.63	121.67	110.40
1	b	24	VAL	N-CA-C	-6.63	104.03	110.72
2	3	161	VAL	CA-C-N	6.63	129.70	120.29
2	3	161	VAL	C-N-CA	6.63	129.70	120.29
3	K	305	ARG	CA-C-O	6.63	127.49	120.33
2	n	162	ASP	CA-CB-CG	-6.62	105.97	112.60
3	K	168	ALA	CA-C-N	6.62	129.16	120.28
3	K	168	ALA	C-N-CA	6.62	129.16	120.28
2	h	42	ALA	N-CA-CB	6.62	119.71	110.17
3	I	156	ALA	CA-C-N	-6.62	116.39	123.08
3	I	156	ALA	C-N-CA	-6.62	116.39	123.08
1	c	52	LYS	CA-C-O	6.62	126.33	119.05
1	E	16	SER	CA-C-O	-6.62	113.59	120.87
3	I	86	LYS	N-CA-C	-6.62	98.84	109.96
3	J	94	TYR	N-CA-C	-6.62	103.88	112.68
1	f	30	ALA	N-CA-C	6.62	119.32	111.71
1	f	217	ASP	CA-CB-CG	6.62	119.22	112.60
2	l	80	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	a	67	ILE	O-C-N	-6.61	116.30	123.18
1	F	160	LYS	N-CA-C	-6.61	105.78	114.31
1	D	229	LEU	O-C-N	6.61	129.23	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	240	ILE	CA-C-O	-6.61	114.08	120.95
3	K	144	GLY	N-CA-C	-6.61	103.70	112.82
1	B	27	ALA	N-CA-C	-6.60	104.70	112.89
1	b	50	ALA	N-CA-C	-6.60	99.38	109.41
1	f	237	ASN	N-CA-C	-6.60	104.17	111.36
3	J	276	ASP	CA-C-O	-6.60	114.66	120.60
3	H	380	GLU	CA-C-N	6.60	129.36	120.65
3	H	380	GLU	C-N-CA	6.60	129.36	120.65
1	a	142	ASP	N-CA-C	-6.59	104.16	112.93
1	g	177	LYS	N-CA-C	-6.59	104.88	113.12
1	C	108	THR	N-CA-CB	6.59	119.67	109.85
1	g	242	GLU	N-CA-C	6.59	118.47	111.28
3	L	381	LYS	CA-C-N	6.59	129.78	120.42
3	L	381	LYS	C-N-CA	6.59	129.78	120.42
1	C	180	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	e	30	ALA	N-CA-C	-6.59	103.59	111.69
1	g	152	PRO	N-CA-C	-6.59	105.27	113.84
1	g	170	ALA	N-CA-C	6.59	118.26	111.14
2	1	48	ILE	N-CA-C	-6.59	106.14	111.81
1	g	108	THR	CA-CB-OG1	6.59	119.48	109.60
2	7	189	VAL	CA-CB-CG2	-6.59	99.20	110.40
2	l	175	ALA	N-CA-C	6.58	118.46	111.28
2	i	47	GLN	O-C-N	6.58	130.70	123.13
1	D	55	GLY	CA-C-N	6.58	134.10	121.54
1	D	55	GLY	C-N-CA	6.58	134.10	121.54
1	e	73	HIS	ND1-CE1-NE2	6.58	114.98	108.40
2	i	57	ALA	N-CA-C	-6.58	98.18	108.90
3	K	90	ASN	CA-CB-CG	6.58	119.18	112.60
1	D	118	ASP	CA-CB-CG	6.57	119.17	112.60
1	D	205	VAL	CA-C-N	6.57	128.06	119.84
1	D	205	VAL	C-N-CA	6.57	128.06	119.84
3	J	38	GLU	CA-C-N	6.57	129.09	120.28
3	J	38	GLU	C-N-CA	6.57	129.09	120.28
1	A	151	ASP	CA-CB-CG	-6.57	106.03	112.60
1	e	238	GLU	N-CA-CB	6.57	119.73	109.94
2	i	190	LYS	N-CA-C	-6.57	97.70	108.41
3	K	124	ASP	O-C-N	-6.57	113.29	121.64
1	D	182	ASP	CA-CB-CG	-6.57	106.03	112.60
1	G	200	ILE	CA-C-N	6.57	131.47	122.07
1	G	200	ILE	C-N-CA	6.57	131.47	122.07
2	7	159	ILE	CA-C-N	6.57	128.78	122.27
2	7	159	ILE	C-N-CA	6.57	128.78	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ARG	CA-C-N	6.57	131.06	120.55
1	A	86	ARG	C-N-CA	6.57	131.06	120.55
1	f	241	ARG	NE-CZ-NH1	-6.57	114.94	121.50
3	I	332	GLU	CA-C-N	6.57	131.19	120.23
3	I	332	GLU	C-N-CA	6.57	131.19	120.23
2	7	152	GLU	N-CA-CB	6.56	119.87	110.16
1	A	76	ALA	CA-C-N	6.56	135.26	122.07
1	A	76	ALA	C-N-CA	6.56	135.26	122.07
1	f	160	LYS	N-CA-C	-6.56	103.39	111.40
1	g	73	HIS	CA-CB-CG	6.56	120.36	113.80
2	m	44	LYS	O-C-N	6.56	130.06	122.25
2	7	33	MET	CG-SD-CE	-6.56	86.47	100.90
2	7	54	MET	CB-CA-C	6.56	120.24	110.14
2	n	63	ALA	O-C-N	6.56	128.83	122.07
1	B	140	GLY	N-CA-C	-6.56	99.95	110.18
2	i	211	PHE	CA-CB-CG	-6.56	107.24	113.80
2	j	143	GLY	CA-C-N	6.56	129.96	120.38
2	j	143	GLY	C-N-CA	6.56	129.96	120.38
2	6	95	SER	N-CA-C	6.55	118.08	111.07
3	H	222	LEU	CA-C-N	6.55	128.82	120.56
3	H	222	LEU	C-N-CA	6.55	128.82	120.56
2	n	104	PHE	CA-C-N	6.55	126.51	119.76
2	n	104	PHE	C-N-CA	6.55	126.51	119.76
3	K	31	GLU	CA-C-N	6.55	129.59	120.29
3	K	31	GLU	C-N-CA	6.55	129.59	120.29
3	J	358	ALA	N-CA-CB	6.55	119.86	110.16
1	d	50	ALA	CA-C-O	-6.55	114.25	121.33
2	5	152	GLU	O-C-N	-6.55	113.42	122.46
2	4	146	THR	CA-C-N	6.55	129.59	120.29
2	4	146	THR	C-N-CA	6.55	129.59	120.29
2	l	207	ILE	N-CA-C	-6.55	103.40	112.50
1	E	238	GLU	CA-C-N	6.55	129.59	120.29
1	E	238	GLU	C-N-CA	6.55	129.59	120.29
2	1	147	ALA	CA-C-N	6.55	129.35	120.38
2	1	147	ALA	C-N-CA	6.55	129.35	120.38
3	J	238	ILE	CA-C-O	6.54	128.33	120.74
3	M	116	VAL	CA-C-O	-6.54	113.09	118.98
1	a	175	PHE	N-CA-C	-6.54	105.27	113.18
1	E	220	THR	N-CA-C	-6.54	96.87	110.80
1	G	184	SER	O-C-N	6.54	130.33	122.68
3	L	390	PRO	N-CA-CB	6.54	109.00	103.25
2	2	166	GLU	CA-C-N	6.54	129.57	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	166	GLU	C-N-CA	6.54	129.57	120.29
2	n	126	ASP	N-CA-C	-6.54	101.05	110.40
3	I	146	LEU	N-CA-C	-6.54	102.67	112.54
3	J	225	GLU	N-CA-C	6.54	118.95	111.11
1	c	214	VAL	N-CA-CB	6.54	121.06	111.52
2	4	38	ALA	N-CA-C	-6.54	103.96	114.09
1	D	78	THR	CA-CB-OG1	6.53	119.40	109.60
1	d	225	SER	CA-C-N	6.53	128.01	119.84
1	d	225	SER	C-N-CA	6.53	128.01	119.84
1	f	131	PRO	N-CA-CB	6.53	109.00	103.25
1	C	190	VAL	N-CA-C	-6.53	104.39	110.53
2	5	87	VAL	CA-C-N	6.53	129.03	120.28
2	5	87	VAL	C-N-CA	6.53	129.03	120.28
1	B	224	VAL	CA-CB-CG2	6.53	121.50	110.40
3	L	189	THR	N-CA-C	-6.53	104.00	112.23
1	a	128	GLY	N-CA-C	-6.53	106.77	115.32
1	E	232	TYR	CA-C-O	-6.53	113.50	120.42
1	F	184	SER	CA-C-N	6.53	128.93	120.44
1	F	184	SER	C-N-CA	6.53	128.93	120.44
3	I	77	VAL	N-CA-C	-6.53	99.08	108.48
1	F	110	LYS	CA-C-O	6.53	127.34	120.42
2	1	199	TYR	N-CA-CB	6.53	119.79	110.13
3	I	328	MET	CB-CA-C	-6.53	106.24	114.40
2	l	200	SER	CA-C-N	6.52	127.99	119.84
2	l	200	SER	C-N-CA	6.52	127.99	119.84
3	K	84	GLY	O-C-N	-6.52	115.25	121.77
3	M	276	ASP	CA-C-O	-6.52	114.50	120.50
2	2	163	GLU	CA-C-O	6.52	126.94	119.18
2	5	134	GLU	N-CA-CB	6.52	121.12	110.17
3	H	94	TYR	N-CA-C	-6.52	105.33	113.28
3	M	321	PHE	CA-CB-CG	-6.52	107.28	113.80
2	5	103	TYR	N-CA-C	-6.52	104.91	112.92
3	M	246	ILE	CA-C-N	6.52	130.37	121.05
3	M	246	ILE	C-N-CA	6.52	130.37	121.05
1	G	144	VAL	CA-C-O	-6.51	115.47	119.51
1	B	27	ALA	CA-C-N	6.51	128.91	120.44
1	B	27	ALA	C-N-CA	6.51	128.91	120.44
1	b	124	THR	N-CA-C	-6.51	103.68	111.69
1	F	73	HIS	CE1-NE2-CD2	-6.51	102.49	109.00
1	B	188	ALA	CA-C-N	6.51	129.00	120.28
1	B	188	ALA	C-N-CA	6.51	129.00	120.28
3	I	125	PRO	N-CA-C	-6.51	103.69	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	129	GLY	CA-C-O	6.51	126.28	118.86
2	n	98	LEU	N-CA-C	6.51	118.37	111.28
3	M	337	LYS	N-CA-C	6.51	118.37	111.28
2	7	189	VAL	N-CA-C	-6.50	99.12	108.48
1	b	84	ASP	N-CA-C	-6.50	103.69	111.69
1	D	212	GLY	N-CA-C	-6.50	100.79	111.38
3	H	55	VAL	N-CA-C	-6.50	104.18	110.42
3	K	324	HIS	CE1-NE2-CD2	-6.50	102.50	109.00
3	L	83	THR	CA-CB-OG1	6.50	119.34	109.60
1	d	200	ILE	N-CA-C	-6.49	105.33	112.80
2	2	200	SER	CA-C-N	6.49	126.72	119.32
2	2	200	SER	C-N-CA	6.49	126.72	119.32
3	H	167	PHE	CA-C-N	6.49	128.88	120.44
3	H	167	PHE	C-N-CA	6.49	128.88	120.44
2	i	70	ILE	CA-C-N	6.49	128.88	120.44
2	i	70	ILE	C-N-CA	6.49	128.88	120.44
1	g	199	SER	N-CA-C	6.49	118.36	111.28
2	l	147	ALA	CA-C-N	6.49	128.98	120.28
2	l	147	ALA	C-N-CA	6.49	128.98	120.28
3	J	283	VAL	O-C-N	-6.49	115.69	123.02
2	i	185	GLY	N-CA-C	-6.49	97.80	113.18
2	n	135	LYS	N-CA-C	-6.49	104.84	112.89
3	K	79	VAL	CA-C-N	6.49	131.66	121.99
3	K	79	VAL	C-N-CA	6.49	131.66	121.99
1	B	22	PHE	CA-C-N	6.49	129.50	120.29
1	B	22	PHE	C-N-CA	6.49	129.50	120.29
1	E	135	SER	N-CA-C	-6.49	98.83	109.40
2	6	20	LYS	N-CA-C	-6.49	104.56	114.16
1	g	194	VAL	O-C-N	6.48	128.16	121.87
2	h	176	MET	N-CA-C	-6.48	105.12	113.16
1	e	74	ILE	N-CA-CB	6.48	120.98	111.52
2	k	127	PRO	CA-C-N	6.48	131.75	122.09
2	k	127	PRO	C-N-CA	6.48	131.75	122.09
2	6	210	LYS	CA-C-O	6.48	126.85	119.27
1	B	131	PRO	CB-CA-C	6.47	119.43	110.95
2	7	177	LYS	N-CA-C	-6.47	105.34	112.72
3	I	299	ARG	O-C-N	-6.47	114.18	121.43
1	d	67	ILE	CA-C-N	6.47	132.31	122.93
1	d	67	ILE	C-N-CA	6.47	132.31	122.93
1	D	51	ASP	CA-C-O	-6.47	114.37	121.87
1	D	67	ILE	CB-CA-C	-6.47	105.31	112.68
2	2	126	ASP	N-CA-CB	6.47	118.64	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	251	THR	N-CA-C	-6.47	97.83	108.76
1	d	136	LEU	N-CA-CB	6.46	122.80	111.55
1	e	79	SER	N-CA-C	-6.46	97.70	108.75
1	f	198	LEU	N-CA-CB	6.46	119.62	110.12
1	d	24	VAL	CA-C-O	-6.46	113.88	121.05
3	M	151	GLU	CA-C-N	6.46	128.94	120.28
3	M	151	GLU	C-N-CA	6.46	128.94	120.28
1	B	112	LEU	N-CA-C	-6.46	104.32	111.36
3	I	367	ARG	CA-C-N	6.46	131.57	122.08
3	I	367	ARG	C-N-CA	6.46	131.57	122.08
3	M	27	TYR	CB-CG-CD2	6.46	130.49	120.80
1	c	53	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	D	83	ALA	N-CA-C	6.46	118.32	111.28
3	I	313	THR	CA-C-N	6.46	128.83	120.44
3	I	313	THR	C-N-CA	6.46	128.83	120.44
1	E	120	LYS	CB-CG-CD	6.45	126.14	111.30
2	5	208	LEU	N-CA-C	6.45	121.16	113.16
1	a	127	GLY	CA-C-O	6.44	127.05	119.45
2	4	49	ALA	N-CA-CB	6.44	121.42	111.24
2	h	190	LYS	N-CA-C	-6.44	100.16	110.14
3	I	262	GLN	N-CA-CB	6.44	119.59	110.12
3	H	330	LEU	CA-C-O	6.44	128.28	121.33
1	G	224	VAL	O-C-N	-6.43	115.60	122.61
3	I	364	ARG	CA-C-N	6.43	130.09	120.31
3	I	364	ARG	C-N-CA	6.43	130.09	120.31
1	A	238	GLU	N-CA-C	6.43	118.29	111.28
1	C	188	ALA	N-CA-C	6.43	118.29	111.28
1	D	211	VAL	CA-C-N	6.43	126.56	121.61
1	D	211	VAL	C-N-CA	6.43	126.56	121.61
1	f	237	ASN	N-CA-CB	6.43	119.68	110.16
1	g	169	ASN	CB-CA-C	-6.43	100.74	110.90
1	g	230	LYS	N-CA-C	6.43	122.26	113.77
2	3	72	ILE	CA-C-N	6.43	130.08	120.31
2	3	72	ILE	C-N-CA	6.43	130.08	120.31
2	7	72	ILE	CA-C-O	-6.43	114.04	120.85
2	i	129	GLY	CA-C-O	6.43	127.83	122.24
2	l	150	VAL	CA-C-N	6.42	129.41	120.29
2	l	150	VAL	C-N-CA	6.42	129.41	120.29
3	J	146	LEU	CA-C-N	6.42	128.89	120.28
3	J	146	LEU	C-N-CA	6.42	128.89	120.28
1	b	45	GLY	N-CA-C	-6.42	101.45	110.63
1	A	223	GLU	CB-CG-CD	-6.42	101.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	311	LEU	N-CA-CB	6.42	119.19	110.14
1	D	218	ASP	CA-CB-CG	6.42	119.02	112.60
2	3	165	VAL	CA-CB-CG2	6.42	121.31	110.40
1	g	230	LYS	CA-C-N	6.41	126.04	119.56
1	g	230	LYS	C-N-CA	6.41	126.04	119.56
2	i	100	SER	CB-CA-C	-6.41	100.14	110.79
2	3	162	ASP	CB-CA-C	-6.41	99.95	110.85
3	H	202	THR	O-C-N	-6.41	114.06	122.59
2	m	91	ALA	CA-C-N	6.41	128.77	120.44
2	m	91	ALA	C-N-CA	6.41	128.77	120.44
1	f	197	GLY	CA-C-N	6.41	128.86	120.28
1	f	197	GLY	C-N-CA	6.41	128.86	120.28
2	i	128	ILE	N-CA-C	-6.41	106.75	112.90
3	K	295	PRO	N-CA-CB	6.41	109.97	103.25
2	3	27	THR	O-C-N	-6.40	115.36	123.24
2	n	22	GLY	O-C-N	-6.40	115.62	123.56
3	J	117	ASN	CA-CB-CG	-6.40	106.20	112.60
1	D	240	ILE	CA-C-O	-6.40	114.38	121.17
2	n	170	ARG	CD-NE-CZ	-6.40	115.44	124.40
3	K	45	GLU	CA-C-O	-6.40	113.76	120.55
3	M	62	PRO	N-CA-CB	6.40	109.64	102.60
1	e	169	ASN	CA-C-N	6.40	128.76	120.44
1	e	169	ASN	C-N-CA	6.40	128.76	120.44
3	L	230	ALA	CA-C-N	6.40	129.38	120.29
3	L	230	ALA	C-N-CA	6.40	129.38	120.29
2	k	194	ASP	CB-CA-C	-6.40	97.69	110.42
2	m	64	GLN	CB-CA-C	-6.40	99.97	110.85
3	K	278	ARG	N-CA-C	-6.40	100.73	110.14
3	K	272	LEU	CA-C-N	6.40	128.85	120.28
3	K	272	LEU	C-N-CA	6.40	128.85	120.28
1	B	18	ASP	CA-CB-CG	-6.39	106.20	112.60
2	4	33	MET	N-CA-CB	6.39	121.30	110.49
2	7	40	LYS	CA-C-O	6.39	127.53	120.82
3	H	19	ASP	O-C-N	-6.39	114.41	122.27
3	I	22	LYS	CA-C-N	6.39	128.85	120.28
3	I	22	LYS	C-N-CA	6.39	128.85	120.28
2	k	158	GLU	N-CA-C	-6.39	104.80	112.59
2	n	47	GLN	N-CA-CB	6.39	120.83	110.42
2	7	80	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	c	222	LYS	CA-C-O	6.38	128.61	121.40
3	I	294	ASP	CB-CA-C	-6.38	99.60	109.62
3	L	147	ASP	CA-CB-CG	6.38	118.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	233	LYS	N-CA-C	-6.38	105.44	112.72
1	a	170	ALA	CA-C-N	6.38	129.48	120.42
1	a	170	ALA	C-N-CA	6.38	129.48	120.42
2	4	125	ILE	N-CA-C	-6.38	99.18	108.11
1	d	130	ARG	CA-C-N	6.38	126.75	119.92
1	d	130	ARG	C-N-CA	6.38	126.75	119.92
3	H	124	ASP	CA-C-O	-6.38	114.20	120.26
3	L	87	PHE	CA-C-O	-6.38	114.19	121.40
3	M	27	TYR	CB-CG-CD1	-6.38	111.23	120.80
1	g	217	ASP	O-C-N	6.38	131.07	122.59
3	H	69	SER	CB-CA-C	-6.38	97.69	109.29
1	e	82	VAL	CA-C-N	6.37	129.11	120.44
1	e	82	VAL	C-N-CA	6.37	129.11	120.44
1	f	59	LEU	CA-C-N	6.37	130.91	122.30
1	f	59	LEU	C-N-CA	6.37	130.91	122.30
2	l	112	ILE	N-CA-C	-6.37	97.15	107.28
1	d	43	LYS	N-CA-C	-6.37	105.14	113.17
3	I	330	LEU	N-CA-CB	6.37	121.25	110.49
1	A	46	VAL	N-CA-C	-6.37	99.55	108.27
1	F	100	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	3	145	LEU	CA-C-N	6.37	129.33	120.29
2	3	145	LEU	C-N-CA	6.37	129.33	120.29
2	7	147	ALA	N-CA-CB	6.37	119.24	110.01
3	I	51	LEU	CA-C-N	6.36	129.98	120.31
3	I	51	LEU	C-N-CA	6.36	129.98	120.31
1	g	221	PHE	CA-CB-CG	-6.36	107.44	113.80
1	B	33	ARG	N-CA-C	-6.36	104.57	112.90
1	C	194	VAL	CA-C-O	-6.36	114.33	120.95
2	k	112	ILE	N-CA-C	-6.36	99.20	108.11
3	K	318	ILE	O-C-N	6.36	128.14	121.91
3	M	157	VAL	CA-C-O	-6.36	112.83	120.78
1	a	157	LEU	CA-C-N	6.36	131.15	122.19
1	a	157	LEU	C-N-CA	6.36	131.15	122.19
2	i	199	TYR	O-C-N	6.36	128.62	122.07
2	l	192	THR	CA-C-N	6.36	133.68	121.54
2	l	192	THR	C-N-CA	6.36	133.68	121.54
3	L	379	ILE	CA-C-N	6.36	129.43	120.28
3	L	379	ILE	C-N-CA	6.36	129.43	120.28
2	6	72	ILE	CB-CA-C	6.35	120.99	112.22
2	h	166	GLU	N-CA-CB	6.35	119.46	110.12
2	2	129	GLY	O-C-N	6.35	127.97	122.64
2	m	111	LEU	N-CA-C	-6.35	98.06	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	275	PHE	N-CA-C	-6.35	104.28	111.14
3	J	32	ASP	CA-C-N	6.35	128.79	120.28
3	J	32	ASP	C-N-CA	6.35	128.79	120.28
1	f	138	ILE	CA-CB-CG1	-6.35	99.61	110.40
3	J	289	ARG	CA-C-O	-6.35	114.47	121.33
1	A	8	TYR	CA-C-O	-6.35	110.01	120.80
1	c	75	CYS	N-CA-C	-6.35	99.68	109.14
2	n	112	ILE	N-CA-C	-6.35	98.48	107.75
3	J	252	ASN	N-CA-C	-6.35	103.03	113.50
2	k	79	ILE	CA-C-N	6.35	128.78	120.28
2	k	79	ILE	C-N-CA	6.35	128.78	120.28
3	M	253	SER	CA-C-N	6.35	133.12	121.70
3	M	253	SER	C-N-CA	6.35	133.12	121.70
1	d	125	GLN	OE1-CD-NE2	6.34	128.94	122.60
1	G	136	LEU	CA-C-N	6.34	131.94	122.99
1	G	136	LEU	C-N-CA	6.34	131.94	122.99
2	1	155	PHE	CA-CB-CG	-6.34	107.45	113.80
1	E	41	LYS	N-CA-C	-6.34	99.38	109.59
2	7	80	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	c	63	THR	N-CA-C	-6.34	107.39	114.62
2	1	94	THR	N-CA-C	-6.34	104.37	111.28
2	h	203	GLU	CA-C-O	6.34	127.14	120.42
2	i	71	LYS	CA-C-N	6.34	129.42	120.42
2	i	71	LYS	C-N-CA	6.34	129.42	120.42
3	I	178	VAL	CA-CB-CG1	-6.34	99.62	110.40
1	d	195	ALA	CA-C-N	6.34	128.78	120.28
1	d	195	ALA	C-N-CA	6.34	128.78	120.28
1	d	226	PRO	CA-C-N	6.34	129.41	120.28
1	d	226	PRO	C-N-CA	6.34	129.41	120.28
3	J	304	ASP	CA-C-N	6.34	132.50	122.36
3	J	304	ASP	C-N-CA	6.34	132.50	122.36
1	F	77	ALA	N-CA-C	-6.33	99.78	109.41
3	H	207	VAL	N-CA-C	-6.33	99.08	108.45
2	h	109	GLN	CB-CA-C	6.33	120.57	110.19
2	j	69	ILE	CA-C-N	6.33	129.41	120.42
2	j	69	ILE	C-N-CA	6.33	129.41	120.42
3	M	182	GLY	CA-C-O	-6.33	112.47	121.52
1	C	23	GLN	CA-C-N	6.33	129.41	120.42
1	C	23	GLN	C-N-CA	6.33	129.41	120.42
2	1	150	VAL	CA-C-O	6.33	127.53	120.95
2	4	61	GLY	N-CA-C	6.33	120.87	112.77
1	f	151	ASP	CA-CB-CG	-6.33	106.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	83	THR	N-CA-C	-6.33	103.68	111.40
3	H	41	ARG	NE-CZ-NH2	6.33	124.89	119.20
1	a	207	GLU	N-CA-C	-6.32	105.60	113.38
1	g	241	ARG	CA-C-N	6.32	128.75	120.28
1	g	241	ARG	C-N-CA	6.32	128.75	120.28
2	6	203	GLU	N-CA-CB	6.32	119.41	110.12
3	H	309	VAL	N-CA-C	-6.32	101.89	108.15
2	k	81	ARG	N-CA-C	-6.32	104.83	113.30
1	b	205	VAL	CA-CB-CG2	6.32	121.14	110.40
3	I	99	GLU	CA-C-N	6.32	129.84	120.87
3	I	99	GLU	C-N-CA	6.32	129.84	120.87
3	I	351	ILE	CA-C-O	-6.32	114.15	120.85
1	D	60	GLU	N-CA-C	-6.31	100.31	109.59
2	4	88	ARG	CA-C-N	6.31	128.65	120.44
2	4	88	ARG	C-N-CA	6.31	128.65	120.44
2	7	169	VAL	CA-C-N	6.31	128.74	120.28
2	7	169	VAL	C-N-CA	6.31	128.74	120.28
3	H	203	PHE	N-CA-C	-6.31	96.82	107.99
3	K	13	LEU	N-CA-CB	6.31	119.49	110.16
1	D	132	PHE	CA-C-O	-6.31	114.25	121.19
1	B	241	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	d	38	ILE	N-CA-C	-6.30	99.12	108.45
3	L	277	PRO	CA-C-O	-6.30	114.07	121.95
2	7	207	ILE	N-CA-C	-6.30	102.99	111.44
1	D	18	ASP	CA-CB-CG	-6.30	106.30	112.60
1	f	28	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	G	228	GLU	CA-C-N	6.30	131.39	120.68
1	G	228	GLU	C-N-CA	6.30	131.39	120.68
3	K	336	PHE	N-CA-CB	6.30	120.05	110.28
1	C	190	VAL	CA-C-N	6.30	129.23	120.29
1	C	190	VAL	C-N-CA	6.30	129.23	120.29
1	d	106	PRO	CA-C-O	-6.30	114.25	121.56
2	h	32	THR	CA-C-N	6.30	133.02	121.94
2	h	32	THR	C-N-CA	6.30	133.02	121.94
1	C	228	GLU	N-CA-C	-6.29	105.64	113.38
3	I	78	VAL	CA-C-N	6.29	131.92	122.98
3	I	78	VAL	C-N-CA	6.29	131.92	122.98
1	D	129	VAL	N-CA-C	-6.29	99.14	108.45
1	e	175	PHE	CA-CB-CG	6.29	120.09	113.80
2	5	99	ASN	CA-C-N	6.29	128.71	120.28
2	5	99	ASN	C-N-CA	6.29	128.71	120.28
3	I	13	LEU	N-CA-CB	6.29	119.91	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	389	ILE	N-CA-C	-6.29	97.77	107.71
2	3	147	ALA	N-CA-C	6.29	118.13	111.28
3	M	88	VAL	N-CA-CB	6.29	119.59	111.67
1	b	99	ASN	CA-C-N	6.29	129.33	120.28
1	b	99	ASN	C-N-CA	6.29	129.33	120.28
1	d	241	ARG	CA-C-N	6.29	128.61	120.44
1	d	241	ARG	C-N-CA	6.29	128.61	120.44
2	h	61	GLY	CA-C-O	6.29	127.94	120.90
1	b	44	GLU	CB-CG-CD	-6.28	101.92	112.60
1	c	44	GLU	N-CA-C	-6.28	104.19	113.61
3	L	51	LEU	N-CA-CB	6.28	119.18	110.07
1	g	56	SER	N-CA-CB	6.28	119.05	110.38
2	5	39	SER	N-CA-C	-6.28	99.43	108.60
2	l	119	GLY	CA-C-O	-6.28	113.39	121.05
1	E	5	GLN	CA-C-N	6.28	133.53	121.54
1	E	5	GLN	C-N-CA	6.28	133.53	121.54
1	C	113	ALA	CA-C-N	6.28	128.60	120.44
1	C	113	ALA	C-N-CA	6.28	128.60	120.44
1	E	83	ALA	O-C-N	6.28	128.54	122.07
1	e	10	ARG	NE-CZ-NH1	-6.28	115.22	121.50
1	g	241	ARG	NE-CZ-NH2	6.27	124.85	119.20
2	l	165	VAL	N-CA-CB	6.27	119.07	110.54
2	6	142	SER	N-CA-C	-6.27	105.66	113.38
1	a	18	ASP	CA-CB-CG	-6.27	106.33	112.60
1	F	189	MET	CG-SD-CE	-6.27	87.10	100.90
2	i	80	ARG	N-CA-CB	6.27	119.44	110.16
1	g	103	TYR	O-C-N	6.27	128.75	122.10
2	m	60	VAL	CA-C-N	6.27	126.94	119.98
2	m	60	VAL	C-N-CA	6.27	126.94	119.98
3	H	149	GLN	O-C-N	6.27	128.77	122.12
1	B	14	VAL	CB-CA-C	-6.27	103.79	111.88
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
2	3	28	GLU	N-CA-C	-6.27	98.17	108.76
2	h	68	ARG	NE-CZ-NH2	6.27	124.84	119.20
3	J	238	ILE	O-C-N	-6.27	113.55	122.76
3	L	113	LEU	CA-C-N	6.27	132.40	122.62
3	L	113	LEU	C-N-CA	6.27	132.40	122.62
1	a	100	ARG	NE-CZ-NH1	-6.26	115.23	121.50
1	d	180	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	G	147	LEU	N-CA-C	-6.26	97.20	108.48
1	g	196	MET	CA-C-N	6.26	127.07	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	196	MET	C-N-CA	6.26	127.07	119.99
2	i	48	ILE	N-CA-C	-6.26	105.62	111.45
3	H	153	ILE	CA-C-N	6.26	129.00	120.54
3	H	153	ILE	C-N-CA	6.26	129.00	120.54
3	L	262	GLN	CA-C-N	6.26	128.58	120.44
3	L	262	GLN	C-N-CA	6.26	128.58	120.44
1	G	220	THR	CA-C-N	6.26	133.50	121.54
1	G	220	THR	C-N-CA	6.26	133.50	121.54
1	A	162	THR	CA-CB-OG1	6.26	118.99	109.60
1	e	237	ASN	CA-CB-CG	-6.26	106.34	112.60
2	k	176	MET	CA-C-N	6.26	129.18	120.29
2	k	176	MET	C-N-CA	6.26	129.18	120.29
3	I	221	ARG	NE-CZ-NH2	6.26	124.83	119.20
3	L	36	PHE	CA-C-N	6.26	129.04	120.46
3	L	36	PHE	C-N-CA	6.26	129.04	120.46
3	J	391	ASP	CA-CB-CG	-6.26	106.34	112.60
2	h	197	TYR	N-CA-C	-6.26	99.45	109.96
1	b	140	GLY	O-C-N	-6.26	117.94	123.76
1	C	241	ARG	CB-CA-C	-6.26	100.21	110.85
2	m	53	ALA	O-C-N	6.26	130.38	123.25
2	1	182	SER	CA-C-N	6.25	129.43	122.55
2	1	182	SER	C-N-CA	6.25	129.43	122.55
2	j	32	THR	N-CA-C	-6.25	99.62	109.50
1	a	182	ASP	N-CA-C	-6.25	104.96	112.59
1	C	84	ASP	CA-CB-CG	-6.25	106.35	112.60
3	J	196	ALA	CA-C-N	6.25	128.57	120.44
3	J	196	ALA	C-N-CA	6.25	128.57	120.44
1	G	243	LEU	N-CA-C	-6.25	105.14	112.89
3	I	111	GLN	CA-C-N	-6.25	111.50	121.44
3	I	111	GLN	C-N-CA	-6.25	111.50	121.44
2	3	27	THR	CA-C-O	6.25	128.42	121.11
1	F	239	ARG	CA-C-O	6.25	127.06	119.31
2	m	62	ASP	CA-C-N	6.25	128.56	120.44
2	m	62	ASP	C-N-CA	6.25	128.56	120.44
3	M	130	PHE	CA-CB-CG	-6.25	107.56	113.80
3	J	45	GLU	CA-C-N	6.25	128.56	120.44
3	J	45	GLU	C-N-CA	6.25	128.56	120.44
2	k	166	GLU	CA-C-N	6.24	128.65	120.28
2	k	166	GLU	C-N-CA	6.24	128.65	120.28
3	L	148	VAL	O-C-N	6.24	127.93	121.87
2	n	109	GLN	OE1-CD-NE2	6.24	128.84	122.60
3	I	308	GLU	N-CA-CB	6.24	119.63	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	195	ALA	CA-C-N	6.24	128.64	120.28
1	G	195	ALA	C-N-CA	6.24	128.64	120.28
1	g	211	VAL	CA-C-N	6.24	127.39	121.46
1	g	211	VAL	C-N-CA	6.24	127.39	121.46
2	k	33	MET	N-CA-C	-6.24	101.14	110.06
2	7	203	GLU	CA-C-O	6.24	127.16	120.55
1	b	209	ILE	N-CA-C	-6.24	100.12	108.35
1	G	151	ASP	N-CA-CB	6.24	116.98	109.74
2	4	16	GLY	N-CA-C	-6.24	98.40	113.18
3	H	251	THR	N-CA-CB	6.24	121.59	110.80
2	5	29	LYS	N-CA-C	6.24	118.16	111.36
3	J	298	LEU	N-CA-C	-6.24	104.94	113.30
1	A	33	ARG	N-CA-C	6.24	118.08	111.28
1	b	33	ARG	N-CA-C	6.24	118.87	111.33
1	F	57	LYS	N-CA-C	-6.24	105.31	113.17
2	h	109	GLN	CA-C-O	6.23	127.18	120.32
2	j	133	GLU	CA-C-N	6.23	130.76	121.72
2	j	133	GLU	C-N-CA	6.23	130.76	121.72
2	k	179	ASP	N-CA-CB	6.23	120.50	110.65
1	E	180	ARG	N-CA-C	-6.23	99.94	109.41
1	c	120	LYS	CA-C-N	6.23	129.25	120.28
1	c	120	LYS	C-N-CA	6.23	129.25	120.28
1	f	237	ASN	CA-C-N	6.23	129.44	120.79
1	f	237	ASN	C-N-CA	6.23	129.44	120.79
3	K	245	ALA	CA-C-O	6.22	125.37	118.52
1	F	241	ARG	N-CA-C	6.22	118.06	111.28
1	b	31	VAL	CA-C-N	6.22	129.12	120.29
1	b	31	VAL	C-N-CA	6.22	129.12	120.29
3	H	299	ARG	CA-C-O	-6.22	113.70	120.17
1	B	232	TYR	CA-C-N	6.22	128.39	120.56
1	B	232	TYR	C-N-CA	6.22	128.39	120.56
1	a	116	ILE	CA-C-N	6.22	128.61	120.28
1	a	116	ILE	C-N-CA	6.22	128.61	120.28
2	l	184	ASP	N-CA-C	-6.22	98.25	108.76
2	5	71	LYS	CA-C-O	-6.21	114.30	120.82
1	A	63	THR	CA-C-N	6.21	133.15	121.97
1	A	63	THR	C-N-CA	6.21	133.15	121.97
3	J	393	LYS	CA-C-O	-6.21	111.76	119.28
1	C	141	VAL	N-CA-C	-6.21	98.58	107.77
2	4	92	THR	N-CA-C	-6.21	105.19	112.89
3	I	346	ALA	N-CA-CB	6.21	121.37	111.56
3	L	324	HIS	CE1-NE2-CD2	-6.21	102.79	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	HIS	CE1-NE2-CD2	-6.21	102.79	109.00
3	L	62	PRO	CB-CA-C	6.21	118.37	111.11
1	D	66	LYS	CA-C-N	-6.21	115.08	122.22
1	D	66	LYS	C-N-CA	-6.21	115.08	122.22
1	f	142	ASP	N-CA-C	-6.21	104.06	111.69
1	g	168	ARG	NE-CZ-NH2	-6.20	113.62	119.20
2	3	25	MET	N-CA-C	-6.20	99.25	108.99
2	5	198	GLN	CB-CG-CD	6.20	123.14	112.60
1	E	53	ARG	NE-CZ-NH2	6.20	124.78	119.20
2	k	142	SER	N-CA-C	-6.20	105.75	113.38
2	m	201	PRO	O-C-N	6.20	131.01	122.64
3	J	15	LYS	N-CA-C	6.20	118.04	111.28
3	J	77	VAL	N-CA-C	-6.20	99.28	108.45
1	a	22	PHE	CA-C-N	6.20	128.58	120.28
1	a	22	PHE	C-N-CA	6.20	128.58	120.28
2	1	156	THR	N-CA-C	-6.20	101.08	110.50
2	3	39	SER	CB-CA-C	-6.20	98.86	110.01
1	E	214	VAL	N-CA-C	-6.20	99.20	108.12
1	G	241	ARG	CA-C-N	6.20	128.58	120.28
1	G	241	ARG	C-N-CA	6.20	128.58	120.28
2	m	78	GLU	CB-CG-CD	-6.20	102.07	112.60
3	K	281	VAL	O-C-N	-6.20	116.63	123.20
2	n	180	SER	O-C-N	6.19	130.55	122.68
1	A	43	LYS	CB-CA-C	-6.19	100.72	110.94
1	f	219	ARG	CD-NE-CZ	-6.19	115.73	124.40
2	4	172	ILE	CA-C-N	6.19	129.08	120.29
2	4	172	ILE	C-N-CA	6.19	129.08	120.29
3	K	210	GLU	CB-CG-CD	-6.19	102.07	112.60
3	K	29	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	f	66	LYS	O-C-N	6.19	128.49	121.93
2	2	182	SER	N-CA-C	-6.19	97.62	110.80
1	C	89	ILE	N-CA-CB	6.19	122.64	110.95
2	5	156	THR	CA-CB-OG1	6.19	118.88	109.60
1	E	60	GLU	CA-C-N	6.18	128.89	120.54
1	E	60	GLU	C-N-CA	6.18	128.89	120.54
1	G	167	GLY	CA-C-N	6.18	130.10	120.82
1	G	167	GLY	C-N-CA	6.18	130.10	120.82
2	5	128	ILE	CA-C-N	6.18	132.54	122.21
2	5	128	ILE	C-N-CA	6.18	132.54	122.21
1	B	144	VAL	O-C-N	-6.18	117.39	121.72
1	F	185	PHE	CA-C-N	6.18	128.84	120.44
1	F	185	PHE	C-N-CA	6.18	128.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	167	LEU	CA-C-N	6.18	128.56	120.28
2	7	167	LEU	C-N-CA	6.18	128.56	120.28
1	b	60	GLU	N-CA-CB	6.18	119.22	109.71
1	C	189	MET	N-CA-C	6.18	118.01	111.28
1	e	158	GLU	CA-C-N	6.18	132.29	122.59
1	e	158	GLU	C-N-CA	6.18	132.29	122.59
2	5	104	PHE	CA-C-O	-6.18	114.82	120.50
1	E	115	LYS	N-CA-CB	6.17	119.30	110.16
3	J	324	HIS	CA-C-N	6.17	129.70	120.31
3	J	324	HIS	C-N-CA	6.17	129.70	120.31
1	b	194	VAL	O-C-N	6.17	127.86	121.87
2	3	104	PHE	O-C-N	6.17	127.03	121.35
2	5	59	SER	N-CA-C	-6.17	100.23	110.17
1	B	81	LEU	CB-CA-C	-6.17	101.00	110.26
1	c	18	ASP	N-CA-C	-6.17	104.63	111.36
2	n	199	TYR	O-C-N	6.17	128.66	122.12
1	D	185	PHE	CA-C-O	6.17	127.06	120.70
2	2	167	LEU	N-CA-C	-6.17	104.63	111.36
3	K	299	ARG	N-CA-CB	6.17	119.77	110.02
3	H	319	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	c	181	ASP	N-CA-C	-6.17	105.70	113.72
2	i	115	ILE	O-C-N	-6.17	116.39	122.93
2	3	63	ALA	CB-CA-C	-6.17	101.20	110.88
1	c	137	LEU	CA-C-O	6.17	126.78	120.24
1	g	100	ARG	CA-C-O	-6.17	113.89	120.42
1	B	73	HIS	CA-CB-CG	6.16	119.96	113.80
3	K	236	SER	CA-C-N	6.16	132.79	121.70
3	K	236	SER	C-N-CA	6.16	132.79	121.70
3	K	329	LYS	O-C-N	6.16	130.54	123.27
1	A	89	ILE	CA-C-O	6.16	126.91	120.25
1	d	164	ILE	O-C-N	-6.16	116.20	123.04
3	K	255	THR	N-CA-CB	6.16	120.90	110.49
3	M	18	GLU	N-CA-CB	6.16	119.83	110.28
1	e	243	LEU	O-C-N	-6.16	115.59	122.12
3	L	319	GLN	CA-C-O	-6.16	112.89	119.97
2	j	206	GLN	CA-C-N	6.16	129.16	120.42
2	j	206	GLN	C-N-CA	6.16	129.16	120.42
2	4	96	ASN	CA-CB-CG	-6.16	106.44	112.60
2	5	162	ASP	CA-CB-CG	-6.16	106.44	112.60
2	6	161	VAL	O-C-N	6.15	128.75	121.80
2	5	165	VAL	CA-C-O	6.15	127.11	120.47
2	m	141	GLY	CA-C-N	6.15	128.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	m	141	GLY	C-N-CA	6.15	128.52	120.28
1	a	41	LYS	N-CA-C	-6.15	99.38	109.40
2	2	210	LYS	O-C-N	6.15	130.47	122.42
3	M	304	ASP	N-CA-CB	6.15	120.88	110.49
1	b	87	VAL	CA-C-N	6.14	129.02	120.29
1	b	87	VAL	C-N-CA	6.14	129.02	120.29
2	h	136	ASP	CA-C-N	6.14	133.03	121.97
2	h	136	ASP	C-N-CA	6.14	133.03	121.97
2	4	45	ILE	N-CA-CB	6.14	119.60	111.25
1	d	40	ILE	CA-CB-CG1	6.14	120.84	110.40
2	i	116	ASP	N-CA-C	-6.14	100.46	109.18
2	j	134	GLU	CB-CG-CD	-6.14	102.16	112.60
2	l	72	ILE	CA-C-N	6.14	128.51	120.28
2	l	72	ILE	C-N-CA	6.14	128.51	120.28
3	I	276	ASP	CA-C-N	6.14	126.15	119.89
3	I	276	ASP	C-N-CA	6.14	126.15	119.89
3	M	227	PHE	N-CA-C	6.14	117.97	111.28
3	K	66	GLY	N-CA-C	-6.14	100.89	111.57
1	B	129	VAL	CA-C-O	-6.14	114.78	121.28
1	b	84	ASP	N-CA-CB	6.14	119.34	110.20
2	4	24	VAL	N-CA-CB	6.14	119.62	111.64
3	J	197	ASN	CA-CB-CG	6.14	118.74	112.60
1	b	33	ARG	CA-C-N	6.13	130.50	121.05
1	b	33	ARG	C-N-CA	6.13	130.50	121.05
2	j	154	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	B	85	ALA	O-C-N	6.13	128.62	122.12
2	i	125	ILE	O-C-N	6.13	129.56	123.18
3	J	335	ASP	CA-C-N	6.13	129.63	120.31
3	J	335	ASP	C-N-CA	6.13	129.63	120.31
1	e	132	PHE	CA-CB-CG	6.13	119.93	113.80
3	I	56	GLU	CA-C-O	-6.13	112.92	119.97
2	j	175	ALA	N-CA-CB	6.13	119.13	110.12
2	k	102	ARG	N-CA-C	-6.13	105.38	112.92
2	5	149	GLY	CA-C-N	6.13	128.85	120.46
2	5	149	GLY	C-N-CA	6.13	128.85	120.46
3	I	119	LEU	CB-CA-C	-6.13	99.19	108.63
1	e	199	SER	N-CA-CB	6.13	119.13	110.12
2	j	174	SER	CA-C-N	6.13	128.49	120.28
2	j	174	SER	C-N-CA	6.13	128.49	120.28
1	a	39	GLY	O-C-N	6.12	128.39	123.49
2	k	212	ARG	N-CA-C	-6.12	105.81	113.28
2	2	89	ALA	CA-C-N	6.12	129.12	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	89	ALA	C-N-CA	6.12	129.12	120.42
2	5	53	ALA	CA-C-N	6.12	132.61	122.33
2	5	53	ALA	C-N-CA	6.12	132.61	122.33
3	I	42	ILE	N-CA-C	-6.12	104.54	110.72
3	I	233	LYS	CA-C-N	6.12	129.97	120.60
3	I	233	LYS	C-N-CA	6.12	129.97	120.60
1	e	169	ASN	N-CA-C	6.12	118.45	111.11
2	7	175	ALA	O-C-N	6.12	128.61	122.12
3	I	79	VAL	N-CA-CB	6.12	120.14	111.82
1	A	95	GLU	CA-C-N	6.12	128.98	120.29
1	A	95	GLU	C-N-CA	6.12	128.98	120.29
1	F	151	ASP	CA-C-N	6.12	125.67	119.19
1	F	151	ASP	C-N-CA	6.12	125.67	119.19
1	G	104	ASP	CB-CA-C	6.12	119.95	111.63
2	n	196	PHE	CB-CA-C	6.12	119.92	111.23
2	j	189	VAL	N-CA-CB	6.12	120.45	111.52
1	C	17	PRO	N-CA-C	-6.12	106.86	114.20
1	F	12	ILE	N-CA-C	-6.12	107.03	112.90
3	L	99	GLU	N-CA-C	-6.12	105.75	112.72
1	F	240	ILE	CB-CA-C	-6.11	103.78	112.22
3	J	59	ARG	N-CA-CB	6.11	120.68	110.41
3	H	243	LEU	N-CA-C	-6.11	105.00	112.88
3	I	317	ARG	CA-C-N	6.11	128.26	120.56
3	I	317	ARG	C-N-CA	6.11	128.26	120.56
3	K	150	ILE	CA-C-N	6.11	128.47	120.28
3	K	150	ILE	C-N-CA	6.11	128.47	120.28
2	l	202	GLU	O-C-N	-6.11	115.54	122.08
3	H	313	THR	CA-C-N	6.11	128.38	120.44
3	H	313	THR	C-N-CA	6.11	128.38	120.44
3	K	320	ILE	O-C-N	-6.11	115.54	121.83
1	E	130	ARG	CA-C-N	6.11	126.30	120.31
1	E	130	ARG	C-N-CA	6.11	126.30	120.31
1	G	23	GLN	CA-CB-CG	6.11	126.32	114.10
2	i	87	VAL	N-CA-CB	6.11	119.74	110.58
3	H	130	PHE	CA-C-N	6.11	133.20	121.54
3	H	130	PHE	C-N-CA	6.11	133.20	121.54
3	M	129	GLY	O-C-N	-6.11	114.76	122.70
1	B	245	LYS	N-CA-CB	6.11	119.82	109.87
2	3	63	ALA	CA-C-O	-6.11	114.41	120.82
2	m	81	ARG	CA-C-N	6.10	131.33	122.36
2	m	81	ARG	C-N-CA	6.10	131.33	122.36
2	5	80	ARG	NE-CZ-NH1	-6.10	115.40	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	74	ASP	CA-CB-CG	6.10	118.70	112.60
1	d	73	HIS	ND1-CE1-NE2	6.10	114.50	108.40
2	7	46	TYR	N-CA-C	-6.10	98.96	108.90
3	L	254	ASP	O-C-N	-6.10	113.81	122.04
2	3	166	GLU	CA-C-O	-6.10	114.09	120.55
2	k	195	GLU	O-C-N	-6.10	116.53	123.48
2	k	200	SER	CA-C-N	6.10	126.27	119.32
2	k	200	SER	C-N-CA	6.10	126.27	119.32
3	H	54	GLU	N-CA-C	6.10	118.89	111.82
3	L	107	ALA	CA-C-N	6.10	132.69	122.87
3	L	107	ALA	C-N-CA	6.10	132.69	122.87
3	L	374	ASP	N-CA-CB	6.10	119.08	110.12
1	g	63	THR	N-CA-C	-6.09	105.14	114.16
1	B	182	ASP	CB-CA-C	-6.09	99.87	110.17
1	B	44	GLU	CB-CA-C	-6.09	99.88	110.17
1	D	141	VAL	CA-C-O	6.09	127.18	120.48
1	D	200	ILE	CA-C-N	6.09	130.78	122.19
1	D	200	ILE	C-N-CA	6.09	130.78	122.19
1	F	83	ALA	CA-C-N	6.09	128.94	120.29
1	F	83	ALA	C-N-CA	6.09	128.94	120.29
3	M	329	LYS	CA-C-N	6.09	131.16	120.87
3	M	329	LYS	C-N-CA	6.09	131.16	120.87
1	E	164	ILE	N-CA-C	-6.09	99.52	108.23
3	H	264	THR	CA-C-N	6.09	128.76	120.54
3	H	264	THR	C-N-CA	6.09	128.76	120.54
3	K	58	LEU	N-CA-C	-6.09	104.56	112.23
3	M	354	ILE	CA-C-N	6.09	128.94	120.29
3	M	354	ILE	C-N-CA	6.09	128.94	120.29
1	a	208	ASN	N-CA-CB	6.09	119.50	110.49
1	B	199	SER	N-CA-CB	6.09	118.83	110.01
1	c	230	LYS	CA-C-O	-6.09	113.03	118.63
1	f	184	SER	N-CA-CB	6.09	119.80	110.49
2	1	106	TYR	N-CA-C	-6.09	99.48	109.40
3	M	189	THR	CA-C-N	6.09	133.16	121.54
3	M	189	THR	C-N-CA	6.09	133.16	121.54
1	g	14	VAL	N-CA-C	-6.08	98.36	107.37
1	E	68	TYR	N-CA-C	-6.08	100.99	110.42
1	a	66	LYS	N-CA-C	-6.08	103.58	113.19
1	C	72	GLU	N-CA-C	-6.08	105.17	112.59
1	b	213	TYR	O-C-N	6.08	129.64	123.26
2	3	141	GLY	O-C-N	-6.08	116.72	123.10
1	E	147	LEU	N-CA-C	-6.08	97.54	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	116	ILE	CA-CB-CG2	-6.08	100.17	110.50
1	G	199	SER	CA-CB-OG	-6.08	98.94	111.10
3	H	56	GLU	CA-C-N	6.08	128.42	120.28
3	H	56	GLU	C-N-CA	6.08	128.42	120.28
1	g	237	ASN	CA-CB-CG	6.08	118.68	112.60
2	4	126	ASP	N-CA-CB	6.08	116.79	109.74
3	L	186	THR	N-CA-C	-6.08	105.63	113.16
2	j	109	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	A	119	PHE	CB-CA-C	-6.07	100.71	110.79
2	3	116	ASP	N-CA-C	-6.07	100.18	109.41
2	5	68	ARG	CA-C-O	-6.07	113.99	120.42
3	H	28	ARG	NE-CZ-NH2	-6.07	113.74	119.20
3	I	315	GLU	CA-C-N	6.07	126.72	119.98
3	I	315	GLU	C-N-CA	6.07	126.72	119.98
1	b	81	LEU	CA-C-N	6.07	130.05	120.47
1	b	81	LEU	C-N-CA	6.07	130.05	120.47
1	F	107	ILE	O-C-N	6.06	128.87	122.62
1	A	150	THR	N-CA-C	-6.06	100.41	110.17
1	C	20	ARG	O-C-N	-6.06	114.53	122.59
1	D	225	SER	CA-C-O	-6.06	114.40	120.64
1	e	183	LEU	N-CA-CB	6.06	119.33	109.69
2	7	201	PRO	CA-C-N	6.06	128.65	120.65
2	7	201	PRO	C-N-CA	6.06	128.65	120.65
1	A	151	ASP	CA-C-O	-6.06	114.42	120.66
1	f	115	LYS	N-CA-C	6.06	117.97	111.36
2	i	118	GLU	CA-C-N	6.06	130.75	121.12
2	i	118	GLU	C-N-CA	6.06	130.75	121.12
1	D	159	TYR	O-C-N	6.06	131.24	122.94
3	H	333	ASP	CA-CB-CG	6.06	118.66	112.60
1	c	112	LEU	CA-C-N	6.06	128.31	120.44
1	c	112	LEU	C-N-CA	6.06	128.31	120.44
3	K	397	PHE	N-CA-CB	6.05	120.01	110.87
3	J	233	LYS	N-CA-C	-6.05	104.06	112.30
2	i	126	ASP	N-CA-CB	-6.05	101.27	110.11
2	3	51	ARG	O-C-N	-6.05	113.78	121.83
2	j	60	VAL	N-CA-CB	-6.05	101.50	110.58
2	k	63	ALA	N-CA-CB	6.05	119.12	110.16
2	2	83	ARG	NE-CZ-NH1	-6.05	115.45	121.50
2	2	99	ASN	O-C-N	6.05	128.53	122.12
3	J	226	VAL	N-CA-CB	6.05	121.72	110.77
1	F	157	LEU	N-CA-C	-6.05	98.54	108.76
1	F	236	ALA	CA-C-N	6.05	129.21	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	236	ALA	C-N-CA	6.05	129.21	120.38
3	H	374	ASP	CB-CA-C	-6.05	100.75	110.79
1	d	66	LYS	N-CA-C	-6.05	106.44	113.88
1	E	204	LEU	CA-C-N	6.05	131.74	121.88
1	E	204	LEU	C-N-CA	6.05	131.74	121.88
1	F	228	GLU	N-CA-C	-6.05	105.90	113.28
1	f	21	LEU	N-CA-CB	6.05	118.94	109.69
1	g	142	ASP	CA-C-N	6.05	133.09	121.54
1	g	142	ASP	C-N-CA	6.05	133.09	121.54
2	6	166	GLU	CA-C-N	6.05	128.88	120.29
2	6	166	GLU	C-N-CA	6.05	128.88	120.29
2	7	198	GLN	OE1-CD-NE2	6.05	128.65	122.60
3	I	269	LEU	CA-C-N	6.05	128.38	120.28
3	I	269	LEU	C-N-CA	6.05	128.38	120.28
1	A	108	THR	CA-C-O	-6.04	114.39	121.16
3	J	258	ASP	CB-CA-C	-6.04	100.76	110.79
1	C	10	ARG	N-CA-C	-6.04	104.55	112.41
1	g	181	ASP	N-CA-C	-6.04	105.22	112.59
2	1	71	LYS	CB-CA-C	-6.04	101.39	110.88
2	l	75	ASN	CA-C-O	6.04	126.96	120.55
3	M	303	PHE	CA-C-N	6.04	133.08	121.54
3	M	303	PHE	C-N-CA	6.04	133.08	121.54
1	D	109	VAL	N-CA-C	-6.04	104.62	110.72
1	F	164	ILE	N-CA-C	-6.04	98.87	108.90
3	H	116	VAL	CB-CA-C	-6.04	104.95	110.63
3	I	39	SER	CA-C-O	-6.04	114.15	120.55
3	L	267	GLN	OE1-CD-NE2	6.04	128.64	122.60
1	E	88	LEU	N-CA-CB	6.04	118.77	110.01
2	j	20	LYS	O-C-N	6.04	129.44	122.25
2	j	75	ASN	N-CA-C	6.04	117.86	111.28
2	5	160	GLY	CA-C-O	-6.04	115.03	122.82
3	I	336	PHE	N-CA-C	-6.04	105.91	113.28
3	K	41	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	B	234	GLU	CA-C-N	6.04	128.86	120.29
1	B	234	GLU	C-N-CA	6.04	128.86	120.29
1	D	168	ARG	NH1-CZ-NH2	-6.04	111.45	119.30
3	J	365	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	15	PHE	N-CA-CB	6.04	119.31	109.95
1	c	149	GLU	CA-C-N	6.04	131.33	123.00
1	c	149	GLU	C-N-CA	6.04	131.33	123.00
3	M	10	LEU	CA-C-N	6.04	128.29	120.44
3	M	10	LEU	C-N-CA	6.04	128.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	219	ARG	CD-NE-CZ	6.04	132.85	124.40
2	j	169	VAL	N-CA-CB	6.04	117.61	110.55
2	7	75	ASN	CA-CB-CG	-6.04	106.56	112.60
1	b	97	GLN	CA-C-N	6.03	128.99	120.42
1	b	97	GLN	C-N-CA	6.03	128.99	120.42
2	i	94	THR	CA-C-N	6.03	128.37	120.28
2	i	94	THR	C-N-CA	6.03	128.37	120.28
2	5	132	ILE	N-CA-C	-6.03	98.44	107.37
3	H	119	LEU	CA-C-N	6.03	127.38	119.84
3	H	119	LEU	C-N-CA	6.03	127.38	119.84
1	A	16	SER	N-CA-CB	6.03	118.18	110.04
1	f	240	ILE	CA-C-N	6.03	128.85	120.29
1	f	240	ILE	C-N-CA	6.03	128.85	120.29
3	L	298	LEU	N-CA-CB	-6.03	101.25	110.12
1	C	118	ASP	N-CA-C	-6.03	104.83	111.82
2	h	67	ALA	CB-CA-C	-6.03	100.78	110.79
2	l	137	ILE	CA-C-O	-6.03	113.24	120.78
3	K	27	TYR	O-C-N	6.03	128.51	122.12
3	K	152	GLU	N-CA-CB	6.03	118.98	110.12
2	6	106	TYR	N-CA-C	-6.03	104.77	113.21
3	L	207	VAL	N-CA-CB	6.03	121.25	111.36
2	2	139	ALA	CA-C-N	6.03	133.05	121.54
2	2	139	ALA	C-N-CA	6.03	133.05	121.54
1	a	21	LEU	CA-C-N	6.02	128.35	120.28
1	a	21	LEU	C-N-CA	6.02	128.35	120.28
2	n	102	ARG	CD-NE-CZ	-6.02	115.97	124.40
2	j	116	ASP	CA-CB-CG	6.02	118.62	112.60
2	k	37	ILE	O-C-N	-6.02	116.53	122.97
3	K	88	VAL	CA-C-N	6.02	131.59	122.92
3	K	88	VAL	C-N-CA	6.02	131.59	122.92
2	1	153	ASP	CA-CB-CG	6.02	118.62	112.60
3	M	154	ARG	CA-C-N	6.02	128.35	120.28
3	M	154	ARG	C-N-CA	6.02	128.35	120.28
2	5	152	GLU	N-CA-C	-6.02	105.43	112.89
2	h	30	ARG	O-C-N	6.02	130.31	123.27
2	7	43	LYS	N-CA-C	-6.02	99.47	109.46
3	I	75	GLY	O-C-N	6.02	129.36	122.38
3	H	383	LEU	CA-C-N	6.02	128.34	120.28
3	H	383	LEU	C-N-CA	6.02	128.34	120.28
1	a	120	LYS	CA-C-O	-6.01	114.05	120.42
1	c	40	ILE	N-CA-C	-6.01	99.50	108.46
2	2	96	ASN	CA-CB-CG	-6.01	106.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	109	GLN	N-CA-CB	6.01	119.99	110.55
3	I	214	LYS	N-CA-C	-6.01	105.71	113.16
3	K	205	ARG	N-CA-CB	6.01	120.03	110.65
3	K	392	LEU	N-CA-CB	6.01	120.65	110.49
3	L	252	ASN	N-CA-CB	6.01	120.88	111.56
3	M	32	ASP	CA-C-O	-6.01	113.31	120.10
1	B	168	ARG	NE-CZ-NH1	6.01	127.51	121.50
2	j	91	ALA	CA-C-N	6.01	128.33	120.28
2	j	91	ALA	C-N-CA	6.01	128.33	120.28
1	c	21	LEU	CA-C-N	6.01	128.33	120.28
1	c	21	LEU	C-N-CA	6.01	128.33	120.28
2	7	181	ALA	CB-CA-C	-6.01	100.02	110.17
3	K	352	LYS	O-C-N	6.01	128.49	122.12
2	n	104	PHE	O-C-N	-6.00	114.30	121.39
1	B	22	PHE	N-CA-CB	6.00	120.19	110.40
1	C	83	ALA	N-CA-C	6.00	118.34	111.02
3	J	61	PRO	N-CA-CB	-6.00	97.26	103.08
2	3	22	GLY	CA-C-N	6.00	131.35	122.71
2	3	22	GLY	C-N-CA	6.00	131.35	122.71
1	B	28	ARG	CA-C-O	6.00	127.12	120.82
1	f	106	PRO	N-CA-CB	6.00	108.59	103.19
1	d	185	PHE	CA-C-O	-6.00	114.52	120.70
2	1	169	VAL	CA-C-O	-6.00	114.49	120.85
3	K	306	ILE	N-CA-C	-6.00	98.99	107.75
3	J	336	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	175	PHE	O-C-N	-6.00	114.57	122.42
1	B	88	LEU	CA-C-N	6.00	128.94	120.42
1	B	88	LEU	C-N-CA	6.00	128.94	120.42
2	h	170	ARG	CA-C-O	6.00	126.87	119.97
2	3	112	ILE	N-CA-C	-6.00	99.00	107.75
2	5	174	SER	CB-CA-C	-6.00	100.84	110.79
3	K	141	GLU	N-CA-C	-5.99	104.67	111.14
1	c	109	VAL	CA-C-N	5.99	128.31	120.28
1	c	109	VAL	C-N-CA	5.99	128.31	120.28
1	e	61	ALA	N-CA-CB	-5.99	102.04	111.39
2	3	208	LEU	N-CA-CB	-5.99	100.34	110.41
3	J	299	ARG	N-CA-C	5.99	118.31	109.50
1	a	65	GLU	N-CA-CB	5.99	120.19	110.42
2	7	63	ALA	CA-C-N	5.99	128.80	120.29
2	7	63	ALA	C-N-CA	5.99	128.80	120.29
1	E	181	ASP	N-CA-C	-5.99	104.36	112.26
1	G	30	ALA	CA-C-N	5.99	128.93	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	30	ALA	C-N-CA	5.99	128.93	120.42
1	G	218	ASP	N-CA-C	-5.99	104.72	112.68
2	l	181	ALA	CA-C-N	5.99	128.79	120.29
2	l	181	ALA	C-N-CA	5.99	128.79	120.29
1	d	18	ASP	N-CA-C	-5.99	106.11	113.41
2	n	176	MET	O-C-N	5.99	129.22	122.22
2	3	176	MET	N-CA-C	-5.98	105.98	113.28
3	M	281	VAL	N-CA-CB	-5.98	103.15	111.41
1	B	20	ARG	NE-CZ-NH1	-5.98	115.52	121.50
2	1	54	MET	CA-C-N	5.98	131.95	122.74
2	1	54	MET	C-N-CA	5.98	131.95	122.74
2	h	23	VAL	CA-C-O	-5.98	113.91	120.43
2	h	208	LEU	N-CA-C	5.98	120.44	113.20
2	j	145	LEU	CA-C-N	5.98	128.30	120.28
2	j	145	LEU	C-N-CA	5.98	128.30	120.28
1	D	67	ILE	N-CA-CB	5.98	117.86	112.06
1	e	36	THR	N-CA-C	5.98	118.42	110.53
2	2	89	ALA	O-C-N	5.98	128.23	122.07
2	i	197	TYR	N-CA-C	-5.98	99.96	109.59
2	4	156	THR	CA-C-N	5.98	126.09	119.87
2	4	156	THR	C-N-CA	5.98	126.09	119.87
3	I	321	PHE	O-C-N	5.98	128.23	122.07
1	a	196	MET	O-C-N	5.98	128.46	122.12
1	b	83	ALA	CA-C-N	5.98	130.80	120.58
1	b	83	ALA	C-N-CA	5.98	130.80	120.58
1	B	218	ASP	O-C-N	5.98	130.00	122.23
1	G	106	PRO	N-CA-CB	5.98	108.87	103.19
3	H	366	GLU	CB-CG-CD	-5.98	102.44	112.60
1	b	205	VAL	O-C-N	-5.98	117.54	121.72
3	M	37	ILE	CA-C-N	5.98	128.29	120.28
3	M	37	ILE	C-N-CA	5.98	128.29	120.28
1	C	196	MET	CG-SD-CE	-5.97	87.75	100.90
1	f	168	ARG	CA-C-N	5.97	128.57	120.44
1	f	168	ARG	C-N-CA	5.97	128.57	120.44
2	1	64	GLN	OE1-CD-NE2	5.97	128.57	122.60
3	I	19	ASP	CA-CB-CG	5.97	118.57	112.60
1	c	74	ILE	N-CA-C	-5.97	99.12	108.86
1	f	57	LYS	CA-C-N	5.97	128.56	120.44
1	f	57	LYS	C-N-CA	5.97	128.56	120.44
2	i	170	ARG	O-C-N	5.97	128.45	122.12
2	3	53	ALA	N-CA-CB	5.97	122.08	111.69
1	a	104	ASP	CA-CB-CG	-5.97	106.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	h	47	GLN	CA-C-O	5.97	126.85	120.46
2	2	40	LYS	N-CA-C	-5.97	107.23	114.75
2	2	53	ALA	N-CA-C	-5.97	100.25	109.14
3	K	154	ARG	NE-CZ-NH2	-5.97	113.83	119.20
3	L	228	GLN	CB-CA-C	-5.97	100.70	110.85
3	H	262	GLN	N-CA-C	-5.97	105.83	113.23
2	5	140	THR	CA-C-O	5.97	127.67	120.99
3	I	162	LEU	CB-CA-C	-5.97	101.51	110.88
3	K	267	GLN	CA-C-O	5.97	126.75	120.42
1	C	73	HIS	CG-CD2-NE2	5.96	113.16	107.20
1	C	145	PRO	O-C-N	-5.96	115.54	123.06
1	G	75	CYS	N-CA-C	-5.96	100.28	109.52
1	a	44	GLU	N-CA-C	-5.96	103.53	112.54
1	a	122	GLN	N-CA-CB	5.96	118.89	110.12
1	b	29	GLU	CA-C-N	5.96	128.76	120.29
1	b	29	GLU	C-N-CA	5.96	128.76	120.29
1	f	186	ASP	CB-CA-C	-5.96	100.89	110.79
3	K	397	PHE	N-CA-C	-5.96	101.10	109.69
1	B	240	ILE	O-C-N	-5.96	116.07	121.91
1	E	217	ASP	CA-CB-CG	5.96	118.56	112.60
2	i	91	ALA	CA-C-O	5.96	127.08	120.82
2	j	165	VAL	CA-C-N	5.96	128.76	120.29
2	j	165	VAL	C-N-CA	5.96	128.76	120.29
2	l	116	ASP	CA-CB-CG	-5.96	106.64	112.60
3	H	278	ARG	N-CA-CB	5.96	120.56	110.49
1	g	230	LYS	O-C-N	-5.96	114.97	120.51
2	4	108	VAL	N-CA-CB	5.96	119.81	111.05
2	7	106	TYR	CB-CA-C	-5.96	100.42	110.19
1	A	112	LEU	CA-C-O	5.96	126.73	120.42
1	E	51	ASP	CA-C-N	5.96	131.84	122.49
1	E	51	ASP	C-N-CA	5.96	131.84	122.49
2	7	134	GLU	N-CA-CB	5.96	121.91	111.13
1	C	205	VAL	CA-C-N	5.96	126.73	120.12
1	C	205	VAL	C-N-CA	5.96	126.73	120.12
1	B	64	ILE	CA-C-N	5.95	132.42	121.70
1	B	64	ILE	C-N-CA	5.95	132.42	121.70
2	2	178	ARG	N-CA-C	-5.95	106.06	113.38
2	7	36	PHE	CA-CB-CG	-5.95	107.85	113.80
1	c	84	ASP	CB-CA-C	-5.95	100.73	110.85
1	f	29	GLU	N-CA-C	5.95	117.77	111.28
2	k	122	ILE	N-CA-C	-5.95	99.64	108.45
2	6	104	PHE	CA-C-O	-5.95	115.53	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	193	GLU	CB-CG-CD	-5.95	102.48	112.60
3	I	137	GLU	N-CA-CB	5.95	120.32	111.51
1	b	141	VAL	N-CA-C	-5.95	99.07	107.75
3	H	45	GLU	N-CA-CB	5.95	118.86	110.12
2	l	116	ASP	CA-C-O	-5.95	115.06	121.36
3	L	104	ALA	CB-CA-C	-5.95	100.15	109.84
1	a	236	ALA	N-CA-C	5.95	117.43	111.07
2	6	188	VAL	O-C-N	-5.95	116.76	123.18
3	H	42	ILE	CA-C-N	5.95	128.25	120.28
3	H	42	ILE	C-N-CA	5.95	128.25	120.28
3	K	180	LEU	N-CA-C	-5.95	99.50	109.07
2	2	80	ARG	NE-CZ-NH2	5.94	124.55	119.20
2	n	196	PHE	N-CA-C	-5.94	95.97	107.44
1	B	66	LYS	N-CA-C	-5.94	106.07	113.38
2	k	69	ILE	CB-CA-C	-5.94	104.24	112.02
2	m	45	ILE	N-CA-C	-5.94	99.56	108.12
3	M	173	GLU	CA-C-N	5.94	126.50	120.38
3	M	173	GLU	C-N-CA	5.94	126.50	120.38
2	k	102	ARG	N-CA-CB	5.94	119.23	110.56
1	e	25	GLU	CA-C-N	5.94	128.72	120.29
1	e	25	GLU	C-N-CA	5.94	128.72	120.29
2	3	75	ASN	CA-C-N	5.94	128.56	120.54
2	3	75	ASN	C-N-CA	5.94	128.56	120.54
3	H	203	PHE	CB-CA-C	5.94	120.47	110.79
3	M	94	TYR	N-CA-C	-5.94	105.87	113.23
3	M	375	PHE	CB-CA-C	-5.94	101.56	110.88
1	D	176	GLU	N-CA-CB	5.93	118.84	110.12
1	F	105	GLU	CA-C-O	-5.93	114.32	119.72
2	k	202	GLU	CA-C-N	5.93	128.23	120.28
2	k	202	GLU	C-N-CA	5.93	128.23	120.28
2	4	185	GLY	CA-C-N	5.93	131.19	122.94
2	4	185	GLY	C-N-CA	5.93	131.19	122.94
3	K	47	GLU	CA-C-N	5.93	128.59	120.46
3	K	47	GLU	C-N-CA	5.93	128.59	120.46
3	L	19	ASP	N-CA-C	-5.93	104.89	111.36
2	l	15	VAL	N-CA-C	-5.93	99.20	108.81
1	d	90	ASP	CA-C-N	5.93	128.15	120.44
1	d	90	ASP	C-N-CA	5.93	128.15	120.44
1	E	92	ALA	CA-C-O	5.93	126.70	120.42
3	H	71	ILE	N-CA-C	-5.93	100.52	108.35
2	5	209	ALA	N-CA-C	-5.93	104.82	111.28
2	j	103	TYR	CB-CA-C	-5.93	97.61	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	135	LYS	CA-C-N	5.93	126.26	119.92
3	I	135	LYS	C-N-CA	5.93	126.26	119.92
1	e	86	ARG	N-CA-C	5.92	117.41	111.07
1	b	166	MET	N-CA-C	-5.92	104.77	112.23
1	C	48	LEU	N-CA-C	-5.92	98.63	108.34
1	D	29	GLU	N-CA-C	-5.92	105.55	112.89
1	g	143	GLU	N-CA-C	-5.92	98.19	110.80
2	1	198	GLN	CA-C-O	5.92	126.62	120.40
2	5	143	GLY	O-C-N	-5.92	115.52	122.27
3	L	252	ASN	OD1-CG-ND2	5.92	128.52	122.60
3	J	277	PRO	N-CA-C	-5.92	107.87	114.92
2	j	126	ASP	CA-C-O	-5.92	115.81	121.08
2	7	133	GLU	N-CA-C	5.92	123.41	110.80
1	B	119	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	167	GLY	CA-C-N	5.92	128.46	120.65
1	B	167	GLY	C-N-CA	5.92	128.46	120.65
1	b	126	TYR	N-CA-CB	5.92	118.67	109.97
1	f	95	GLU	O-C-N	-5.92	115.85	122.12
2	h	198	GLN	N-CA-C	-5.92	97.49	108.02
3	K	178	VAL	CB-CA-C	-5.92	101.87	110.63
3	M	64	LEU	N-CA-C	-5.92	100.06	109.76
3	J	302	ARG	O-C-N	5.92	129.36	121.67
1	F	225	SER	CA-C-N	5.92	125.79	119.28
1	F	225	SER	C-N-CA	5.92	125.79	119.28
3	M	83	THR	N-CA-C	-5.92	104.41	111.69
2	i	104	PHE	CA-C-N	5.91	125.93	119.90
2	i	104	PHE	C-N-CA	5.91	125.93	119.90
3	I	199	THR	O-C-N	5.91	129.54	122.27
3	M	258	ASP	N-CA-CB	5.91	120.55	110.50
1	B	181	ASP	CA-CB-CG	-5.91	106.69	112.60
1	D	178	GLU	CA-C-N	5.91	129.15	120.82
1	D	178	GLU	C-N-CA	5.91	129.15	120.82
2	h	91	ALA	CA-C-N	5.91	128.68	120.29
2	h	91	ALA	C-N-CA	5.91	128.68	120.29
2	l	198	GLN	N-CA-C	-5.91	98.78	108.41
3	H	241	ASP	CA-CB-CG	-5.91	106.69	112.60
3	K	261	VAL	N-CA-C	-5.91	103.52	111.44
1	B	232	TYR	CA-CB-CG	-5.91	103.26	113.90
2	i	97	LEU	CB-CA-C	-5.91	100.98	110.79
2	m	140	THR	CA-C-O	-5.91	113.86	120.66
2	7	74	ALA	CA-C-O	5.91	126.81	120.55
3	H	297	ILE	N-CA-C	5.91	116.65	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	71	ASP	CA-CB-CG	5.91	118.50	112.60
1	g	225	SER	N-CA-C	-5.90	102.67	110.40
3	L	305	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	a	25	GLU	N-CA-CB	5.90	118.57	110.01
1	f	73	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
2	l	151	LEU	O-C-N	-5.90	115.42	122.15
3	J	56	GLU	CA-C-N	5.90	128.67	120.29
3	J	56	GLU	C-N-CA	5.90	128.67	120.29
1	a	119	PHE	N-CA-C	-5.90	104.93	111.36
1	B	65	GLU	CB-CA-C	5.90	121.31	110.10
3	H	367	ARG	NE-CZ-NH2	5.90	124.51	119.20
3	L	56	GLU	N-CA-C	5.90	117.71	111.28
1	e	16	SER	O-C-N	-5.90	115.35	121.60
1	A	223	GLU	CA-C-N	5.90	131.13	123.11
1	A	223	GLU	C-N-CA	5.90	131.13	123.11
1	E	137	LEU	N-CA-CB	5.90	119.97	110.65
2	3	91	ALA	CA-C-N	5.90	129.27	120.31
2	3	91	ALA	C-N-CA	5.90	129.27	120.31
3	J	213	GLN	N-CA-C	-5.89	100.45	109.65
2	k	90	ILE	N-CA-C	5.89	117.42	111.00
2	l	24	VAL	N-CA-C	-5.89	99.93	108.89
3	I	164	PRO	CA-C-N	5.89	130.03	120.60
3	I	164	PRO	C-N-CA	5.89	130.03	120.60
3	K	285	GLY	CA-C-O	5.89	127.51	121.21
3	K	298	LEU	CA-C-O	5.89	126.41	119.28
1	c	10	ARG	NE-CZ-NH1	-5.89	115.61	121.50
3	I	254	ASP	CA-C-N	5.89	128.65	120.29
3	I	254	ASP	C-N-CA	5.89	128.65	120.29
1	E	236	ALA	CA-C-N	5.89	128.17	120.28
1	E	236	ALA	C-N-CA	5.89	128.17	120.28
1	f	225	SER	CA-C-N	5.89	125.56	119.56
1	f	225	SER	C-N-CA	5.89	125.56	119.56
2	k	97	LEU	N-CA-CB	5.89	118.55	110.01
3	K	111	GLN	CB-CA-C	-5.89	101.60	110.90
2	h	163	GLU	CB-CG-CD	-5.88	102.59	112.60
2	4	158	GLU	N-CA-C	-5.88	104.76	112.41
2	m	151	LEU	N-CA-C	5.88	118.48	111.71
3	H	310	PRO	O-C-N	5.88	130.58	122.64
3	L	111	GLN	N-CA-CB	5.88	118.93	110.40
3	L	262	GLN	CG-CD-OE1	5.88	132.56	120.80
1	C	238	GLU	N-CA-C	5.88	117.69	111.28
1	D	111	GLU	CA-C-O	5.88	126.78	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	335	ASP	CA-C-N	5.88	130.54	120.72
3	H	335	ASP	C-N-CA	5.88	130.54	120.72
1	a	168	ARG	N-CA-C	5.88	117.38	110.97
1	e	232	TYR	CA-C-N	5.88	128.51	120.46
1	e	232	TYR	C-N-CA	5.88	128.51	120.46
1	f	70	ILE	N-CA-C	-5.88	105.35	111.58
1	g	12	ILE	N-CA-C	-5.88	104.40	113.16
2	h	127	PRO	CA-C-N	5.88	132.55	121.97
2	h	127	PRO	C-N-CA	5.88	132.55	121.97
1	A	102	THR	N-CA-C	-5.88	106.08	113.72
2	m	176	MET	N-CA-C	-5.88	104.46	111.69
3	M	292	ILE	CA-C-N	5.88	131.41	122.65
3	M	292	ILE	C-N-CA	5.88	131.41	122.65
3	K	167	PHE	CA-C-N	5.88	128.08	120.44
3	K	167	PHE	C-N-CA	5.88	128.08	120.44
3	L	229	LEU	CA-C-O	-5.88	114.65	120.70
2	m	170	ARG	NE-CZ-NH1	-5.87	115.63	121.50
3	L	355	CYS	N-CA-CB	5.87	118.53	110.01
1	B	97	GLN	CA-C-N	5.87	128.76	120.42
1	B	97	GLN	C-N-CA	5.87	128.76	120.42
2	7	172	ILE	CA-C-N	5.87	128.07	120.44
2	7	172	ILE	C-N-CA	5.87	128.07	120.44
2	4	33	MET	N-CA-C	-5.87	98.30	110.80
2	6	13	THR	CA-CB-OG1	5.87	118.41	109.60
3	J	323	ILE	CA-C-N	5.87	130.66	120.68
3	J	323	ILE	C-N-CA	5.87	130.66	120.68
2	1	206	GLN	CA-C-N	5.87	129.92	120.30
2	1	206	GLN	C-N-CA	5.87	129.92	120.30
2	h	42	ALA	O-C-N	5.87	129.78	122.86
3	J	196	ALA	N-CA-CB	5.87	118.75	110.12
1	F	44	GLU	CA-C-N	5.87	129.67	121.22
1	F	44	GLU	C-N-CA	5.87	129.67	121.22
2	h	103	TYR	N-CA-C	-5.87	105.89	113.16
2	7	189	VAL	CA-C-O	5.87	127.53	120.67
3	K	304	ASP	O-C-N	5.87	128.15	121.93
3	J	172	ILE	CA-C-N	5.87	128.63	120.65
3	J	172	ILE	C-N-CA	5.87	128.63	120.65
3	I	128	TYR	O-C-N	5.86	129.23	122.25
3	J	360	MET	O-C-N	-5.86	115.47	122.15
1	e	22	PHE	N-CA-C	-5.86	104.97	111.36
3	M	29	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	F	48	LEU	O-C-N	-5.86	116.45	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	170	ARG	CG-CD-NE	-5.86	99.11	112.00
2	j	70	ILE	N-CA-C	-5.86	104.80	110.72
3	J	58	LEU	CA-C-O	-5.86	114.21	120.42
3	J	368	ALA	CA-C-N	5.86	130.21	122.30
3	J	368	ALA	C-N-CA	5.86	130.21	122.30
1	G	241	ARG	NE-CZ-NH2	5.86	124.47	119.20
2	2	128	ILE	N-CA-C	-5.86	106.01	113.22
1	F	20	ARG	CA-C-O	-5.86	113.92	120.54
3	J	250	ARG	N-CA-C	-5.86	100.12	109.96
1	c	119	PHE	O-C-N	5.86	128.10	122.07
1	G	87	VAL	O-C-N	-5.86	115.18	121.80
2	n	141	GLY	O-C-N	-5.86	116.22	122.95
1	C	50	ALA	CA-C-O	5.85	127.55	120.99
2	6	168	ALA	CA-C-N	5.85	128.48	120.46
2	6	168	ALA	C-N-CA	5.85	128.48	120.46
2	l	17	LEU	CA-C-N	5.85	129.99	121.80
2	l	17	LEU	C-N-CA	5.85	129.99	121.80
3	H	222	LEU	N-CA-C	5.85	118.41	111.33
1	A	15	PHE	CA-CB-CG	-5.85	107.95	113.80
3	M	19	ASP	CA-CB-CG	-5.85	106.75	112.60
1	a	110	LYS	CA-C-N	5.85	128.60	120.29
1	a	110	LYS	C-N-CA	5.85	128.60	120.29
1	B	130	ARG	CB-CA-C	5.85	117.56	108.61
1	b	169	ASN	CA-C-O	5.85	126.75	120.55
1	b	236	ALA	CA-C-N	5.85	129.20	120.31
1	b	236	ALA	C-N-CA	5.85	129.20	120.31
2	3	69	ILE	CA-C-N	5.85	128.73	120.42
2	3	69	ILE	C-N-CA	5.85	128.73	120.42
1	a	200	ILE	N-CA-C	-5.85	106.79	112.29
2	6	172	ILE	N-CA-C	-5.85	104.63	111.00
1	b	234	GLU	N-CA-C	5.85	117.33	111.07
1	G	142	ASP	CA-CB-CG	-5.85	106.75	112.60
3	M	393	LYS	N-CA-C	-5.85	106.11	113.18
1	A	164	ILE	N-CA-C	-5.84	99.38	108.44
1	E	157	LEU	N-CA-C	-5.84	98.75	108.75
2	i	52	MET	CA-C-O	-5.84	114.28	121.06
2	m	23	VAL	N-CA-C	-5.84	100.64	108.35
3	L	198	GLN	OE1-CD-NE2	5.84	128.44	122.60
3	I	194	ALA	CA-C-N	5.84	128.72	120.42
3	I	194	ALA	C-N-CA	5.84	128.72	120.42
3	L	324	HIS	CG-CD2-NE2	5.84	113.04	107.20
3	L	355	CYS	CA-C-O	-5.84	114.69	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	72	GLU	N-CA-C	-5.84	106.39	112.93
3	K	34	LYS	O-C-N	-5.84	114.60	122.43
1	E	151	ASP	CA-C-O	-5.84	114.84	120.97
3	I	179	LEU	N-CA-C	-5.84	98.89	108.41
2	5	204	VAL	N-CA-C	-5.84	104.83	110.72
3	H	224	ARG	CA-C-N	5.84	128.03	120.44
3	H	224	ARG	C-N-CA	5.84	128.03	120.44
1	A	100	ARG	O-C-N	-5.83	115.09	122.27
2	4	112	ILE	CA-C-O	5.83	127.37	120.72
2	l	176	MET	CA-C-N	5.83	128.68	120.28
2	l	176	MET	C-N-CA	5.83	128.68	120.28
2	7	83	ARG	CA-C-N	5.83	129.53	120.60
2	7	83	ARG	C-N-CA	5.83	129.53	120.60
2	6	139	ALA	N-CA-C	-5.83	98.38	110.80
3	I	138	VAL	O-C-N	-5.83	117.06	123.18
2	k	202	GLU	N-CA-C	5.83	118.11	111.11
1	G	194	VAL	N-CA-C	-5.83	104.67	110.62
3	H	140	TYR	CA-C-O	-5.83	113.51	120.10
2	5	153	ASP	CA-CB-CG	5.83	118.43	112.60
3	K	25	GLU	CA-C-N	5.83	128.36	120.44
3	K	25	GLU	C-N-CA	5.83	128.36	120.44
3	J	353	ALA	CA-C-N	5.83	128.69	120.42
3	J	353	ALA	C-N-CA	5.83	128.69	120.42
1	D	197	GLY	O-C-N	5.82	127.77	122.18
2	3	36	PHE	N-CA-C	-5.82	99.85	108.99
2	5	95	SER	N-CA-CB	5.82	118.68	110.12
2	5	169	VAL	CA-C-N	5.82	128.08	120.28
2	5	169	VAL	C-N-CA	5.82	128.08	120.28
3	M	333	ASP	CA-C-N	5.82	128.90	120.98
3	M	333	ASP	C-N-CA	5.82	128.90	120.98
1	a	31	VAL	CA-C-N	5.82	128.56	120.29
1	a	31	VAL	C-N-CA	5.82	128.56	120.29
1	D	143	GLU	N-CA-C	-5.82	98.40	110.80
1	e	96	ALA	CA-C-N	5.82	128.08	120.28
1	e	96	ALA	C-N-CA	5.82	128.08	120.28
2	2	182	SER	N-CA-CB	5.82	120.33	110.49
3	K	324	HIS	CG-CD2-NE2	5.82	113.02	107.20
3	J	88	VAL	N-CA-C	-5.82	100.20	108.58
1	B	122	GLN	CB-CG-CD	-5.82	102.71	112.60
1	G	204	LEU	N-CA-CB	5.82	118.59	110.04
2	5	59	SER	CA-C-N	5.82	129.86	120.55
2	5	59	SER	C-N-CA	5.82	129.86	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	167	LEU	CA-C-O	5.82	126.70	120.24
3	M	242	GLU	CA-CB-CG	5.82	125.73	114.10
1	A	105	GLU	CA-C-N	5.81	127.11	119.84
1	A	105	GLU	C-N-CA	5.81	127.11	119.84
1	D	137	LEU	CB-CA-C	-5.81	99.66	109.72
2	j	78	GLU	CA-C-N	5.81	127.88	120.56
2	j	78	GLU	C-N-CA	5.81	127.88	120.56
2	j	196	PHE	N-CA-C	-5.81	95.55	107.70
2	5	143	GLY	CA-C-O	5.81	126.42	119.10
3	I	374	ASP	CB-CA-C	-5.81	100.97	110.85
1	d	175	PHE	N-CA-CB	5.81	119.87	110.40
1	G	186	ASP	O-C-N	5.81	128.37	122.09
2	i	112	ILE	N-CA-C	-5.81	99.97	108.11
1	G	187	ASP	CA-C-N	5.81	128.07	120.28
1	G	187	ASP	C-N-CA	5.81	128.07	120.28
2	l	33	MET	CG-SD-CE	-5.81	88.12	100.90
1	C	13	THR	CA-CB-OG1	5.81	118.31	109.60
3	L	180	LEU	CA-C-O	5.81	126.63	120.36
1	c	135	SER	O-C-N	-5.80	116.10	123.24
2	n	194	ASP	CB-CA-C	-5.80	98.73	109.29
3	M	45	GLU	O-C-N	-5.80	115.97	122.12
1	c	193	LEU	CB-CA-C	-5.80	101.16	110.79
2	l	193	GLU	N-CA-CB	5.80	120.30	110.49
3	K	281	VAL	CA-C-O	5.80	126.42	120.39
1	b	61	ALA	N-CA-C	-5.80	104.87	112.41
1	f	216	VAL	CB-CA-C	-5.80	104.55	111.97
2	3	44	LYS	CA-C-N	5.80	131.00	123.11
2	3	44	LYS	C-N-CA	5.80	131.00	123.11
3	J	337	LYS	N-CA-CB	5.80	118.74	110.16
1	D	120	LYS	CB-CG-CD	5.80	124.63	111.30
2	2	83	ARG	CA-C-N	5.80	129.49	120.68
2	2	83	ARG	C-N-CA	5.80	129.49	120.68
2	l	18	VAL	N-CA-CB	5.80	117.44	110.95
3	J	147	ASP	O-C-N	5.80	128.26	122.12
1	B	38	ILE	N-CA-C	-5.79	99.83	108.46
1	A	81	LEU	CA-C-N	5.79	128.40	120.46
1	A	81	LEU	C-N-CA	5.79	128.40	120.46
1	C	116	ILE	N-CA-C	-5.79	104.87	110.72
1	G	103	TYR	N-CA-C	-5.79	108.02	114.62
3	L	63	LEU	CA-C-O	5.79	126.38	120.24
3	I	287	THR	N-CA-C	-5.79	100.56	108.38
1	E	51	ASP	CA-C-O	-5.79	114.04	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	41	LYS	N-CA-CB	5.79	120.41	110.68
1	f	228	GLU	N-CA-C	-5.79	106.56	113.97
2	j	131	ALA	N-CA-C	-5.79	98.17	108.13
3	M	192	ALA	N-CA-C	5.79	117.26	111.07
2	3	142	SER	CA-C-O	5.79	126.33	119.67
1	E	67	ILE	N-CA-CB	5.79	120.55	111.99
2	6	126	ASP	N-CA-C	-5.79	102.31	110.29
3	M	59	ARG	N-CA-CB	5.79	118.72	110.16
3	M	317	ARG	CA-C-N	5.79	128.38	120.46
3	M	317	ARG	C-N-CA	5.79	128.38	120.46
2	5	166	GLU	CA-C-O	5.78	126.55	120.42
3	H	338	GLU	N-CA-C	-5.78	105.06	111.36
3	I	380	GLU	N-CA-C	5.78	117.58	111.28
1	G	109	VAL	N-CA-CB	5.78	117.31	110.55
3	M	317	ARG	NE-CZ-NH2	-5.78	114.00	119.20
2	l	204	VAL	CA-C-O	5.78	126.71	120.47
2	n	163	GLU	CA-C-O	5.78	126.55	120.42
2	7	28	GLU	N-CA-CB	5.78	119.67	110.65
3	I	307	ILE	CA-C-O	-5.78	114.38	120.39
3	L	370	VAL	N-CA-CB	5.78	118.54	110.56
1	f	73	HIS	ND1-CE1-NE2	5.78	114.18	108.40
2	i	132	ILE	CB-CA-C	-5.78	102.22	110.83
2	6	132	ILE	N-CA-C	-5.78	100.36	108.80
1	G	236	ALA	CA-C-N	5.78	128.60	120.28
1	G	236	ALA	C-N-CA	5.78	128.60	120.28
2	m	172	ILE	N-CA-C	-5.78	103.70	111.44
3	L	375	PHE	CA-C-N	5.78	128.02	120.28
3	L	375	PHE	C-N-CA	5.78	128.02	120.28
1	d	118	ASP	CA-C-N	5.77	127.95	120.44
1	d	118	ASP	C-N-CA	5.77	127.95	120.44
2	7	155	PHE	O-C-N	5.77	129.77	123.13
3	H	149	GLN	CA-C-O	-5.77	114.43	120.55
1	c	26	TYR	N-CA-C	-5.77	104.96	112.23
1	G	118	ASP	CA-C-O	-5.77	114.30	120.42
1	D	62	ASP	CA-C-O	5.77	125.39	119.05
2	1	75	ASN	O-C-N	5.77	128.01	122.07
2	5	50	ASP	N-CA-C	5.77	118.31	111.33
3	K	341	ARG	N-CA-CB	5.77	118.60	110.12
1	B	186	ASP	N-CA-C	5.77	117.57	111.28
1	C	132	PHE	CA-CB-CG	-5.77	108.03	113.80
1	E	44	GLU	CA-C-N	-5.77	113.50	121.23
1	E	44	GLU	C-N-CA	-5.77	113.50	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	147	ALA	CA-C-N	5.77	128.48	120.29
2	2	147	ALA	C-N-CA	5.77	128.48	120.29
2	i	137	ILE	CB-CA-C	-5.77	103.09	111.68
1	e	239	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	2	65	PHE	N-CA-C	-5.77	104.60	111.69
3	H	388	PRO	N-CA-C	5.77	119.91	111.03
1	F	91	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	f	126	TYR	CA-C-O	-5.76	114.03	120.54
2	4	45	ILE	CA-C-N	-5.76	113.86	122.39
2	4	45	ILE	C-N-CA	-5.76	113.86	122.39
2	k	181	ALA	CB-CA-C	-5.76	101.50	110.37
1	C	207	GLU	CA-C-O	5.76	126.25	119.28
1	g	241	ARG	NE-CZ-NH1	-5.76	115.74	121.50
2	7	105	PRO	N-CA-CB	5.76	109.30	103.25
3	J	371	THR	N-CA-CB	5.76	116.05	108.96
1	C	173	GLU	CA-C-O	5.76	126.52	120.42
1	f	167	GLY	CA-C-N	5.76	127.93	120.44
1	f	167	GLY	C-N-CA	5.76	127.93	120.44
2	2	109	GLN	OE1-CD-NE2	-5.76	116.84	122.60
2	6	175	ALA	CB-CA-C	-5.76	99.98	110.63
3	I	165	GLU	N-CA-C	5.76	119.41	112.38
1	C	136	LEU	N-CA-C	-5.76	100.80	109.95
1	a	113	ALA	CA-C-N	5.76	128.00	120.28
1	a	113	ALA	C-N-CA	5.76	128.00	120.28
2	i	79	ILE	N-CA-C	5.76	116.49	110.62
2	5	75	ASN	OD1-CG-ND2	-5.76	116.84	122.60
2	5	176	MET	CG-SD-CE	-5.76	88.23	100.90
3	M	179	LEU	N-CA-CB	5.75	119.36	110.21
2	6	151	LEU	O-C-N	5.75	128.71	122.15
1	E	243	LEU	CA-C-O	5.75	126.45	119.38
1	e	23	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	g	145	PRO	CA-C-O	-5.75	114.47	121.03
2	3	93	LEU	CA-C-N	5.75	127.99	120.28
2	3	93	LEU	C-N-CA	5.75	127.99	120.28
3	K	107	ALA	N-CA-CB	5.75	119.58	110.55
1	G	67	ILE	CB-CA-C	5.75	117.47	111.09
2	m	77	TYR	O-C-N	5.75	128.21	122.12
3	K	194	ALA	CA-C-N	5.75	128.34	120.46
3	K	194	ALA	C-N-CA	5.75	128.34	120.46
3	K	304	ASP	N-CA-C	-5.75	105.90	114.64
1	a	51	ASP	N-CA-C	-5.75	99.82	108.96
2	k	136	ASP	O-C-N	5.75	130.23	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	27	TYR	CB-CG-CD2	5.75	129.42	120.80
3	I	86	LYS	N-CA-CB	5.75	119.54	110.23
3	K	186	THR	CA-CB-OG1	5.75	118.22	109.60
3	K	293	LEU	N-CA-CB	5.75	119.54	110.23
2	1	51	ARG	NE-CZ-NH2	5.74	124.37	119.20
2	3	126	ASP	N-CA-C	-5.74	103.53	110.13
1	b	120	LYS	N-CA-C	5.74	117.62	111.36
2	1	144	SER	N-CA-CB	5.74	118.56	110.12
1	e	117	CYS	CB-CA-C	-5.74	101.09	110.85
1	f	69	LYS	O-C-N	-5.74	115.96	123.02
2	j	58	GLY	N-CA-C	-5.74	105.24	111.21
2	4	51	ARG	N-CA-C	-5.74	104.02	111.71
3	I	321	PHE	CA-C-N	5.74	127.97	120.28
3	I	321	PHE	C-N-CA	5.74	127.97	120.28
3	M	303	PHE	N-CA-C	-5.74	98.57	110.80
1	e	108	THR	N-CA-CB	5.74	118.48	110.04
2	2	65	PHE	CA-CB-CG	-5.74	108.06	113.80
2	m	211	PHE	N-CA-C	-5.74	105.95	113.12
2	n	120	LYS	CA-C-N	5.74	132.50	121.54
2	n	120	LYS	C-N-CA	5.74	132.50	121.54
1	B	99	ASN	CA-CB-CG	-5.74	106.86	112.60
3	M	367	ARG	NE-CZ-NH2	-5.74	114.04	119.20
2	i	45	ILE	CA-C-O	-5.73	114.37	120.39
2	5	14	THR	N-CA-CB	5.73	121.67	111.69
2	l	128	ILE	N-CA-C	-5.73	106.72	112.17
1	D	63	THR	CA-CB-OG1	5.73	118.20	109.60
1	g	31	VAL	CA-C-N	5.73	127.96	120.28
1	g	31	VAL	C-N-CA	5.73	127.96	120.28
3	J	28	ARG	CA-C-N	5.73	128.24	120.44
3	J	28	ARG	C-N-CA	5.73	128.24	120.44
3	J	54	GLU	CA-C-N	5.73	128.31	120.46
3	J	54	GLU	C-N-CA	5.73	128.31	120.46
1	d	241	ARG	N-CA-C	5.73	117.61	111.36
2	2	152	GLU	CA-C-N	5.73	128.53	120.28
2	2	152	GLU	C-N-CA	5.73	128.53	120.28
2	j	155	PHE	N-CA-CB	5.73	118.71	110.06
2	j	67	ALA	N-CA-C	5.73	119.37	112.38
2	7	143	GLY	CA-C-N	5.73	127.96	120.28
2	7	143	GLY	C-N-CA	5.73	127.96	120.28
3	L	338	GLU	N-CA-C	-5.73	105.17	111.82
1	e	102	THR	N-CA-C	5.73	120.27	113.28
1	G	130	ARG	NE-CZ-NH2	5.73	124.35	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	275	PHE	CB-CG-CD2	5.73	130.43	120.70
1	B	57	LYS	N-CA-C	-5.72	106.27	113.20
1	d	104	ASP	CA-C-O	-5.72	113.70	120.57
2	k	102	ARG	CD-NE-CZ	-5.72	116.39	124.40
2	6	144	SER	N-CA-C	5.72	118.26	111.33
1	b	73	HIS	CB-CG-CD2	-5.72	123.76	131.20
2	1	182	SER	CA-C-O	-5.72	115.32	121.56
2	6	87	VAL	N-CA-C	-5.72	104.78	110.62
2	n	116	ASP	O-C-N	5.72	129.62	122.92
3	L	160	PRO	N-CA-CB	5.72	109.26	103.25
2	m	18	VAL	N-CA-CB	5.72	116.77	110.53
3	H	355	CYS	CA-C-N	5.72	127.88	120.44
3	H	355	CYS	C-N-CA	5.72	127.88	120.44
3	L	337	LYS	CA-C-O	-5.72	114.81	120.70
2	3	30	ARG	N-CA-CB	5.72	120.16	110.49
3	I	142	ASP	CA-C-O	5.72	125.34	119.05
3	K	112	THR	N-CA-CB	5.72	119.53	110.84
3	L	217	GLY	N-CA-C	-5.72	107.48	114.92
2	6	134	GLU	CA-C-N	5.72	128.26	120.54
2	6	134	GLU	C-N-CA	5.72	128.26	120.54
2	n	17	LEU	N-CA-CB	5.72	122.16	111.52
3	K	183	PRO	CA-C-N	5.72	125.73	119.90
3	K	183	PRO	C-N-CA	5.72	125.73	119.90
2	l	31	ALA	O-C-N	-5.72	116.25	123.17
3	H	302	ARG	N-CA-CB	5.72	120.15	110.49
1	b	214	VAL	O-C-N	-5.71	117.17	122.71
1	E	173	GLU	N-CA-C	5.71	117.59	111.36
2	h	162	ASP	CA-CB-CG	-5.71	106.89	112.60
3	H	324	HIS	CB-CA-C	-5.71	100.24	110.70
3	K	395	VAL	N-CA-C	-5.71	106.14	111.45
3	L	324	HIS	ND1-CE1-NE2	5.71	114.11	108.40
1	E	108	THR	CA-CB-OG1	5.71	118.17	109.60
3	J	223	VAL	CA-C-O	-5.71	115.01	120.95
2	h	162	ASP	CA-C-N	5.71	131.80	121.92
2	h	162	ASP	C-N-CA	5.71	131.80	121.92
2	j	144	SER	N-CA-CB	-5.71	101.11	110.14
3	M	387	THR	CB-CA-C	5.71	117.72	109.09
3	J	297	ILE	N-CA-C	-5.71	107.42	112.90
1	D	245	LYS	N-CA-CB	5.71	119.31	110.80
2	l	137	ILE	N-CA-CB	5.71	120.65	111.23
2	7	204	VAL	N-CA-CB	5.71	119.14	110.58
3	I	213	GLN	N-CA-CB	5.71	119.31	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	h	24	VAL	CA-C-O	5.71	126.38	120.39
3	H	397	PHE	CA-CB-CG	-5.71	108.09	113.80
3	L	231	LYS	CA-C-N	5.71	130.38	120.68
3	L	231	LYS	C-N-CA	5.71	130.38	120.68
2	6	210	LYS	O-C-N	-5.71	114.64	122.46
3	L	222	LEU	CA-C-N	5.71	128.52	120.42
3	L	222	LEU	C-N-CA	5.71	128.52	120.42
3	M	154	ARG	NE-CZ-NH1	-5.71	115.80	121.50
1	c	69	LYS	N-CA-C	-5.70	99.94	109.24
1	c	143	GLU	N-CA-C	-5.70	105.14	111.36
1	F	40	ILE	CB-CA-C	5.70	119.28	110.50
2	3	71	LYS	O-C-N	5.70	128.02	122.09
3	J	177	GLY	CA-C-N	5.70	130.92	122.71
3	J	177	GLY	C-N-CA	5.70	130.92	122.71
1	c	67	ILE	N-CA-C	-5.70	99.92	108.12
2	j	192	THR	CA-CB-OG1	5.70	118.15	109.60
2	l	88	ARG	NE-CZ-NH2	5.70	124.33	119.20
3	K	77	VAL	CA-C-O	-5.70	114.29	120.67
3	L	362	ALA	CA-C-N	5.70	128.27	120.46
3	L	362	ALA	C-N-CA	5.70	128.27	120.46
1	G	109	VAL	O-C-N	5.70	127.49	121.91
3	K	372	MET	N-CA-C	-5.70	105.07	111.28
3	H	281	VAL	CA-C-N	5.70	131.95	121.70
3	H	281	VAL	C-N-CA	5.70	131.95	121.70
1	e	219	ARG	CA-C-N	5.69	130.84	121.39
1	e	219	ARG	C-N-CA	5.69	130.84	121.39
1	C	56	SER	CA-C-N	5.69	131.76	122.65
1	C	56	SER	C-N-CA	5.69	131.76	122.65
1	F	44	GLU	O-C-N	-5.69	115.67	122.27
1	F	66	LYS	N-CA-C	-5.69	106.68	113.97
2	2	153	ASP	N-CA-CB	5.69	118.99	110.22
2	k	104	PHE	CA-C-N	5.69	126.02	119.93
2	k	104	PHE	C-N-CA	5.69	126.02	119.93
3	L	382	VAL	CA-C-N	5.69	128.48	120.28
3	L	382	VAL	C-N-CA	5.69	128.48	120.28
3	J	51	LEU	CA-C-N	5.69	127.84	120.44
3	J	51	LEU	C-N-CA	5.69	127.84	120.44
3	J	137	GLU	N-CA-C	-5.69	105.01	112.41
1	f	99	ASN	CB-CG-ND2	5.69	124.94	116.40
1	G	193	LEU	N-CA-C	-5.69	104.69	111.69
2	k	183	GLY	CA-C-N	5.69	131.81	121.97
2	k	183	GLY	C-N-CA	5.69	131.81	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	l	66	LEU	CA-C-N	5.69	128.47	120.28
2	l	66	LEU	C-N-CA	5.69	128.47	120.28
1	E	211	VAL	CA-C-N	-5.69	117.41	122.47
1	E	211	VAL	C-N-CA	-5.69	117.41	122.47
2	m	187	ASP	CA-CB-CG	5.69	118.29	112.60
3	J	14	LYS	CA-C-O	-5.69	114.39	120.42
1	E	215	LYS	CA-C-N	5.69	132.20	121.97
1	E	215	LYS	C-N-CA	5.69	132.20	121.97
2	7	70	ILE	CA-C-O	5.69	126.88	120.85
1	g	240	ILE	O-C-N	5.68	127.48	121.91
1	a	202	SER	CA-C-N	5.68	129.33	120.75
1	a	202	SER	C-N-CA	5.68	129.33	120.75
1	f	58	LEU	N-CA-CB	5.68	118.31	110.07
1	G	74	ILE	O-C-N	-5.68	116.75	123.05
2	i	146	THR	O-C-N	5.68	128.22	122.09
2	m	47	GLN	OE1-CD-NE2	-5.68	116.92	122.60
3	I	123	LYS	N-CA-CB	5.68	120.09	110.49
3	I	198	GLN	N-CA-C	5.68	117.55	111.36
3	K	369	LYS	CA-C-N	5.68	130.71	121.62
3	K	369	LYS	C-N-CA	5.68	130.71	121.62
2	1	207	ILE	O-C-N	5.68	128.21	121.80
1	B	18	ASP	N-CA-C	-5.67	106.36	113.28
1	B	144	VAL	N-CA-C	-5.67	102.60	109.01
2	6	66	LEU	O-C-N	5.67	128.62	122.15
3	L	118	VAL	N-CA-C	-5.67	100.31	108.48
3	L	225	GLU	O-C-N	5.67	129.25	122.27
3	L	374	ASP	CA-CB-CG	-5.67	106.92	112.60
3	K	149	GLN	CA-C-N	5.67	128.23	120.46
3	K	149	GLN	C-N-CA	5.67	128.23	120.46
2	i	75	ASN	CA-C-N	5.67	127.88	120.28
2	i	75	ASN	C-N-CA	5.67	127.88	120.28
3	K	164	PRO	CA-C-N	5.67	127.81	120.44
3	K	164	PRO	C-N-CA	5.67	127.81	120.44
1	C	58	LEU	N-CA-C	-5.67	106.41	113.38
1	D	139	ALA	O-C-N	-5.67	116.56	123.30
3	M	15	LYS	O-C-N	5.67	128.61	122.15
2	1	108	VAL	O-C-N	-5.67	117.04	123.10
2	2	49	ALA	CA-C-N	5.67	128.14	120.38
2	2	49	ALA	C-N-CA	5.67	128.14	120.38
3	L	305	ARG	CA-C-N	-5.67	115.92	122.95
3	L	305	ARG	C-N-CA	-5.67	115.92	122.95
3	J	78	VAL	N-CA-CB	5.67	116.90	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	83	ALA	CA-C-N	5.67	130.31	120.68
1	G	83	ALA	C-N-CA	5.67	130.31	120.68
3	J	315	GLU	CA-C-N	5.67	126.11	119.94
3	J	315	GLU	C-N-CA	5.67	126.11	119.94
1	F	195	ALA	CB-CA-C	-5.66	101.22	110.85
2	2	22	GLY	CA-C-N	5.66	130.39	122.23
2	2	22	GLY	C-N-CA	5.66	130.39	122.23
2	3	21	ASP	CA-CB-CG	5.66	118.26	112.60
2	3	55	THR	CA-CB-OG1	5.66	118.09	109.60
3	K	379	ILE	CA-C-N	5.66	127.80	120.44
3	K	379	ILE	C-N-CA	5.66	127.80	120.44
1	a	43	LYS	CB-CA-C	-5.66	101.60	110.94
1	B	180	ARG	O-C-N	-5.66	116.32	123.17
2	1	103	TYR	N-CA-C	-5.66	106.21	113.23
2	2	46	TYR	CA-CB-CG	-5.66	103.71	113.90
2	m	114	GLY	CA-C-O	5.66	124.82	120.91
1	c	223	GLU	N-CA-CB	5.66	119.45	110.57
2	1	191	ILE	N-CA-C	-5.66	97.57	109.34
3	I	144	GLY	CA-C-N	5.66	132.00	120.80
3	I	144	GLY	C-N-CA	5.66	132.00	120.80
1	a	169	ASN	CA-CB-CG	-5.66	106.94	112.60
1	f	88	LEU	CA-C-O	5.66	126.42	120.42
2	5	78	GLU	CB-CG-CD	-5.66	102.98	112.60
2	6	81	ARG	CB-CA-C	-5.66	100.05	109.55
1	e	243	LEU	CA-C-O	5.65	126.54	120.55
2	k	83	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	C	15	PHE	CA-C-O	5.65	127.97	121.47
2	k	118	GLU	N-CA-C	-5.65	106.37	113.72
3	L	32	ASP	CA-C-N	5.65	128.32	120.29
3	L	32	ASP	C-N-CA	5.65	128.32	120.29
2	l	159	ILE	N-CA-CB	5.65	116.69	110.53
3	M	141	GLU	CA-C-O	5.65	126.26	119.59
1	c	18	ASP	CA-C-O	-5.65	114.43	120.42
1	F	218	ASP	CA-CB-CG	-5.65	106.95	112.60
1	f	172	THR	CA-C-N	5.65	127.85	120.28
1	f	172	THR	C-N-CA	5.65	127.85	120.28
3	H	390	PRO	N-CA-CB	5.65	108.22	103.25
1	b	117	CYS	CA-C-N	5.64	128.31	120.29
1	b	117	CYS	C-N-CA	5.64	128.31	120.29
2	3	134	GLU	O-C-N	5.64	129.66	123.22
3	K	335	ASP	CA-C-N	5.64	128.89	120.31
3	K	335	ASP	C-N-CA	5.64	128.89	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	325	THR	CA-C-N	5.64	128.16	120.54
3	L	325	THR	C-N-CA	5.64	128.16	120.54
3	J	165	GLU	O-C-N	5.64	129.21	122.27
1	a	21	LEU	N-CA-CB	5.64	119.21	110.46
1	d	136	LEU	CA-C-O	5.64	128.04	121.44
1	g	51	ASP	CA-CB-CG	5.64	118.24	112.60
3	I	257	GLY	CA-C-N	5.64	127.84	120.28
3	I	257	GLY	C-N-CA	5.64	127.84	120.28
2	j	132	ILE	CA-C-N	5.64	129.90	121.72
2	j	132	ILE	C-N-CA	5.64	129.90	121.72
1	g	106	PRO	N-CA-CB	5.64	108.26	103.19
2	i	79	ILE	CA-C-O	5.64	126.81	120.95
2	i	212	ARG	N-CA-C	-5.64	108.19	114.62
2	4	95	SER	CA-C-N	5.64	128.29	120.29
2	4	95	SER	C-N-CA	5.64	128.29	120.29
2	n	25	MET	CG-SD-CE	-5.64	88.50	100.90
3	J	269	LEU	CA-C-N	5.64	127.77	120.44
3	J	269	LEU	C-N-CA	5.64	127.77	120.44
2	6	184	ASP	CA-C-O	5.63	127.16	121.07
2	n	179	ASP	N-CA-C	-5.63	98.72	108.69
1	E	195	ALA	CA-C-N	5.63	128.29	120.29
1	E	195	ALA	C-N-CA	5.63	128.29	120.29
2	5	160	GLY	CA-C-N	5.63	128.18	120.46
2	5	160	GLY	C-N-CA	5.63	128.18	120.46
3	J	167	PHE	N-CA-C	-5.63	106.39	113.20
1	a	126	TYR	N-CA-C	5.63	118.49	110.10
1	e	221	PHE	CA-CB-CG	-5.63	108.17	113.80
2	h	55	THR	CA-C-O	5.63	126.78	120.70
2	6	95	SER	O-C-N	5.63	127.87	122.07
3	M	341	ARG	CA-C-O	-5.63	114.58	120.55
1	f	71	ASP	CA-C-O	5.63	127.33	121.36
2	k	96	ASN	N-CA-CB	5.63	118.49	110.16
3	M	375	PHE	CA-C-N	5.63	128.14	120.54
3	M	375	PHE	C-N-CA	5.63	128.14	120.54
1	b	65	GLU	CB-CG-CD	-5.63	103.04	112.60
1	C	82	VAL	CA-C-N	5.63	128.61	120.79
1	C	82	VAL	C-N-CA	5.63	128.61	120.79
1	F	167	GLY	CA-C-N	5.63	127.75	120.44
1	F	167	GLY	C-N-CA	5.63	127.75	120.44
3	L	350	ASP	N-CA-C	-5.63	105.23	111.36
1	a	115	LYS	O-C-N	5.62	128.08	122.12
1	D	69	LYS	CA-C-N	-5.62	116.86	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	69	LYS	C-N-CA	-5.62	116.86	122.77
1	e	101	LEU	CB-CA-C	-5.62	102.02	110.90
3	H	383	LEU	N-CA-CB	5.62	118.48	110.16
3	I	324	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
3	L	23	LEU	CB-CA-C	-5.62	101.29	110.85
1	c	33	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	c	142	ASP	N-CA-C	-5.62	98.83	110.80
1	G	91	ARG	N-CA-CB	5.62	118.38	110.12
2	1	102	ARG	N-CA-C	-5.62	106.31	114.12
3	I	148	VAL	N-CA-C	5.62	116.40	110.72
3	L	239	PHE	N-CA-CB	5.62	119.42	110.65
1	A	16	SER	CA-C-O	-5.62	114.85	120.64
2	j	35	ASN	OD1-CG-ND2	-5.62	116.98	122.60
2	6	22	GLY	CA-C-N	5.62	130.80	122.99
2	6	22	GLY	C-N-CA	5.62	130.80	122.99
3	I	261	VAL	CA-C-N	5.62	127.81	120.28
3	I	261	VAL	C-N-CA	5.62	127.81	120.28
1	G	55	GLY	O-C-N	5.62	129.02	122.56
1	g	135	SER	N-CA-C	-5.62	100.63	109.50
1	a	73	HIS	CA-CB-CG	5.62	119.42	113.80
1	B	27	ALA	CA-C-O	5.62	126.27	119.31
1	a	173	GLU	CA-C-N	5.61	127.74	120.44
1	a	173	GLU	C-N-CA	5.61	127.74	120.44
1	B	150	THR	N-CA-C	-5.61	100.03	109.07
1	g	100	ARG	N-CA-C	-5.61	105.24	111.36
3	L	239	PHE	N-CA-C	-5.61	99.26	108.41
3	M	11	GLU	CB-CG-CD	-5.61	103.06	112.60
2	2	112	ILE	O-C-N	-5.61	117.34	123.18
2	k	145	LEU	N-CA-CB	5.61	118.15	110.01
3	J	345	GLY	O-C-N	-5.61	116.82	122.54
1	C	8	TYR	N-CA-C	-5.61	103.70	110.88
2	k	67	ALA	CA-C-O	5.61	126.50	120.55
3	I	188	LYS	CA-C-N	5.61	127.80	120.28
3	I	188	LYS	C-N-CA	5.61	127.80	120.28
3	K	270	ALA	CB-CA-C	-5.61	102.07	110.88
3	L	55	VAL	CB-CA-C	-5.61	104.79	111.97
1	A	83	ALA	N-CA-C	5.61	117.07	111.07
1	D	234	GLU	CB-CA-C	-5.61	101.48	110.79
1	D	239	ARG	O-C-N	-5.61	116.29	122.07
1	e	229	LEU	CA-C-N	5.61	130.43	121.62
1	e	229	LEU	C-N-CA	5.61	130.43	121.62
3	L	183	PRO	CB-CA-C	-5.61	104.08	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	GLU	N-CA-CB	5.61	118.36	110.12
1	B	42	CYS	N-CA-C	-5.61	101.22	109.18
1	g	121	GLN	CA-C-O	-5.61	113.52	119.97
2	1	169	VAL	CA-CB-CG2	-5.61	100.87	110.40
2	j	115	ILE	CB-CA-C	5.61	119.33	110.81
3	L	207	VAL	CA-CB-CG1	5.61	119.93	110.40
2	k	70	ILE	CA-C-N	5.60	127.73	120.44
2	k	70	ILE	C-N-CA	5.60	127.73	120.44
3	L	254	ASP	CA-C-N	5.60	131.79	121.70
3	L	254	ASP	C-N-CA	5.60	131.79	121.70
1	e	205	VAL	N-CA-C	-5.60	100.94	107.61
2	k	51	ARG	NE-CZ-NH1	-5.60	115.90	121.50
2	5	204	VAL	CA-C-N	5.60	128.35	120.28
2	5	204	VAL	C-N-CA	5.60	128.35	120.28
2	l	172	ILE	N-CA-C	-5.60	104.71	112.50
1	f	187	ASP	CB-CA-C	-5.60	101.49	110.79
1	d	162	THR	CA-CB-OG1	5.60	118.00	109.60
1	E	168	ARG	CA-C-N	5.60	127.78	120.28
1	E	168	ARG	C-N-CA	5.60	127.78	120.28
1	F	74	ILE	O-C-N	5.60	129.12	123.07
2	h	14	THR	CA-C-O	-5.60	114.72	120.99
2	j	180	SER	N-CA-C	-5.60	106.34	112.72
3	I	207	VAL	O-C-N	5.60	129.10	122.83
2	j	41	ALA	N-CA-C	-5.60	103.98	112.99
2	6	152	GLU	N-CA-C	5.60	117.46	111.36
2	n	76	LEU	N-CA-CB	5.60	118.35	110.12
3	M	282	LYS	N-CA-CB	5.60	120.02	110.50
1	G	47	ILE	CA-C-O	-5.60	113.93	121.32
1	E	188	ALA	CA-C-N	5.59	128.23	120.29
1	E	188	ALA	C-N-CA	5.59	128.23	120.29
1	f	165	GLY	CA-C-N	5.59	127.78	120.28
1	f	165	GLY	C-N-CA	5.59	127.78	120.28
1	f	223	GLU	CA-C-O	5.59	127.09	120.66
2	j	88	ARG	CA-C-N	5.59	128.05	120.44
2	j	88	ARG	C-N-CA	5.59	128.05	120.44
1	f	20	ARG	O-C-N	5.59	129.95	123.41
1	G	190	VAL	N-CA-C	5.59	116.37	110.72
2	1	150	VAL	O-C-N	-5.59	116.45	121.87
1	c	205	VAL	N-CA-CB	5.59	118.30	112.37
2	i	169	VAL	N-CA-CB	-5.59	104.01	110.55
2	4	72	ILE	N-CA-CB	-5.59	104.01	110.55
2	7	88	ARG	NH1-CZ-NH2	5.59	126.57	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	223	VAL	N-CA-CB	5.59	118.14	110.54
2	i	191	ILE	N-CA-CB	5.59	118.70	111.83
1	C	146	LYS	N-CA-C	-5.58	100.81	109.24
2	3	51	ARG	NE-CZ-NH1	-5.58	115.92	121.50
2	k	30	ARG	CA-C-N	5.58	130.87	122.99
2	k	30	ARG	C-N-CA	5.58	130.87	122.99
2	k	187	ASP	CA-CB-CG	5.58	118.19	112.60
3	M	185	GLY	CA-C-N	5.58	128.02	120.65
3	M	185	GLY	C-N-CA	5.58	128.02	120.65
1	G	32	LYS	O-C-N	5.58	128.12	122.09
2	5	201	PRO	CA-C-N	5.58	127.70	120.44
2	5	201	PRO	C-N-CA	5.58	127.70	120.44
2	2	131	ALA	N-CA-CB	5.58	118.77	110.29
2	7	25	MET	N-CA-C	-5.58	100.81	109.24
2	7	111	LEU	N-CA-CB	5.58	119.53	110.77
3	M	358	ALA	N-CA-C	-5.58	105.20	111.28
1	e	91	ARG	NE-CZ-NH2	5.58	124.22	119.20
3	H	88	VAL	CA-C-N	5.58	131.05	122.68
3	H	88	VAL	C-N-CA	5.58	131.05	122.68
1	A	158	GLU	N-CA-CB	5.58	118.60	109.95
2	6	106	TYR	CA-C-N	5.58	129.83	122.30
2	6	106	TYR	C-N-CA	5.58	129.83	122.30
3	I	362	ALA	CA-C-N	5.58	128.10	120.46
3	I	362	ALA	C-N-CA	5.58	128.10	120.46
1	d	15	PHE	CA-CB-CG	-5.58	108.22	113.80
2	5	105	PRO	O-C-N	5.58	130.17	122.64
1	A	100	ARG	CA-C-O	5.58	126.38	119.97
1	c	223	GLU	N-CA-C	-5.58	100.09	109.07
1	D	86	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	d	58	LEU	CA-C-N	5.58	129.47	121.50
1	d	58	LEU	C-N-CA	5.58	129.47	121.50
1	g	235	ARG	CB-CA-C	-5.58	101.37	110.85
2	i	37	ILE	CA-C-N	5.58	128.21	120.29
2	i	37	ILE	C-N-CA	5.58	128.21	120.29
2	k	139	ALA	N-CA-CB	5.58	119.91	110.49
2	n	14	THR	CA-C-O	-5.58	115.10	121.40
1	c	53	ARG	NE-CZ-NH1	-5.57	115.93	121.50
2	k	157	PRO	N-CA-C	-5.57	106.89	114.80
3	M	96	ASN	CA-CB-CG	-5.57	107.03	112.60
1	g	91	ARG	O-C-N	5.57	127.81	122.07
1	g	183	LEU	N-CA-C	5.57	117.73	110.43
2	5	24	VAL	O-C-N	-5.57	117.16	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	196	PHE	N-CA-C	-5.57	96.69	107.44
2	7	66	LEU	CB-CA-C	-5.57	101.38	110.85
3	I	145	GLY	N-CA-C	-5.57	106.32	114.90
2	h	120	LYS	N-CA-C	-5.57	99.33	108.41
2	4	111	LEU	O-C-N	5.57	129.73	123.27
3	L	231	LYS	N-CA-C	-5.57	105.29	111.36
1	D	222	LYS	N-CA-C	-5.57	100.70	109.50
1	d	138	ILE	N-CA-C	-5.57	99.04	107.73
1	G	33	ARG	CA-C-O	-5.57	113.57	119.97
1	D	185	PHE	CA-C-N	5.57	128.19	120.29
1	D	185	PHE	C-N-CA	5.57	128.19	120.29
2	3	87	VAL	O-C-N	5.57	127.27	121.87
2	3	211	PHE	CA-C-N	5.57	132.17	121.54
2	3	211	PHE	C-N-CA	5.57	132.17	121.54
3	I	140	TYR	CB-CG-CD2	5.57	129.15	120.80
1	F	182	ASP	O-C-N	5.56	128.87	122.25
2	i	170	ARG	CA-C-O	-5.56	114.65	120.55
3	M	325	THR	CA-C-N	5.56	127.67	120.44
3	M	325	THR	C-N-CA	5.56	127.67	120.44
1	d	181	ASP	CA-CB-CG	5.56	118.16	112.60
3	M	198	GLN	OE1-CD-NE2	5.56	128.16	122.60
3	M	343	THR	CA-CB-OG1	5.56	117.94	109.60
1	b	237	ASN	O-C-N	-5.56	115.43	122.27
3	H	149	GLN	OE1-CD-NE2	5.56	128.16	122.60
3	L	90	ASN	CA-C-N	5.56	129.15	120.75
3	L	90	ASN	C-N-CA	5.56	129.15	120.75
1	C	211	VAL	CA-C-O	5.56	126.49	120.43
1	f	103	TYR	N-CA-C	-5.56	108.28	114.62
1	G	182	ASP	CA-CB-CG	-5.56	107.04	112.60
1	g	206	PRO	N-CA-CB	-5.56	98.19	103.41
2	1	33	MET	CG-SD-CE	-5.56	88.67	100.90
2	i	139	ALA	N-CA-C	-5.56	99.98	108.76
3	H	192	ALA	CA-C-N	5.56	127.73	120.28
3	H	192	ALA	C-N-CA	5.56	127.73	120.28
1	e	132	PHE	N-CA-CB	5.56	118.93	109.87
1	g	157	LEU	N-CA-CB	5.56	119.94	110.71
2	1	182	SER	O-C-N	5.56	129.42	122.86
3	I	31	GLU	CA-C-N	5.56	127.72	120.28
3	I	31	GLU	C-N-CA	5.56	127.72	120.28
1	E	203	GLU	O-C-N	5.55	129.48	122.65
1	b	117	CYS	N-CA-CB	5.55	118.89	110.28
1	A	159	TYR	CA-C-O	5.55	128.32	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	167	GLY	CA-C-N	5.55	128.51	120.79
1	d	167	GLY	C-N-CA	5.55	128.51	120.79
1	e	28	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	f	124	THR	CA-CB-CG2	5.55	119.94	110.50
2	i	156	THR	N-CA-C	-5.55	100.53	109.58
2	l	78	GLU	CA-C-O	-5.55	114.99	120.82
3	I	281	VAL	N-CA-C	-5.55	100.34	108.11
3	K	367	ARG	CA-C-N	5.55	131.26	122.60
3	K	367	ARG	C-N-CA	5.55	131.26	122.60
3	M	259	ARG	N-CA-C	-5.55	105.38	111.82
1	E	141	VAL	N-CA-C	-5.55	100.13	108.12
1	f	139	ALA	O-C-N	-5.55	116.70	123.30
3	J	99	GLU	CA-C-N	5.55	128.65	120.82
3	J	99	GLU	C-N-CA	5.55	128.65	120.82
2	5	172	ILE	CA-C-O	5.55	125.91	119.36
2	n	213	LYS	CA-CB-CG	5.55	125.19	114.10
2	m	174	SER	N-CA-C	-5.55	105.31	111.36
3	H	337	LYS	CA-C-N	5.55	128.17	120.29
3	H	337	LYS	C-N-CA	5.55	128.17	120.29
3	M	374	ASP	CA-C-O	-5.55	115.00	120.82
1	d	132	PHE	CA-C-O	5.54	127.37	121.16
2	4	79	ILE	CA-C-N	5.54	127.98	120.44
2	4	79	ILE	C-N-CA	5.54	127.98	120.44
2	k	205	GLU	CA-C-O	5.54	126.37	120.10
2	l	19	CYS	N-CA-C	-5.54	102.25	110.46
1	A	47	ILE	CA-CB-CG1	5.54	119.83	110.40
1	A	94	ILE	N-CA-C	-5.54	105.12	110.72
1	E	132	PHE	CB-CG-CD2	-5.54	111.28	120.70
1	e	132	PHE	CA-C-O	-5.54	114.06	120.49
2	4	178	ARG	N-CA-C	-5.54	104.76	113.02
2	n	46	TYR	CA-C-N	5.54	130.14	122.77
2	n	46	TYR	C-N-CA	5.54	130.14	122.77
3	K	14	LYS	CA-CB-CG	5.54	125.18	114.10
3	K	356	THR	CA-C-O	5.54	126.34	119.97
2	h	95	SER	N-CA-CB	5.54	118.26	110.12
2	n	47	GLN	CA-C-O	5.54	126.29	120.36
3	I	133	GLU	CA-C-N	5.54	130.00	122.19
3	I	133	GLU	C-N-CA	5.54	130.00	122.19
3	I	141	GLU	N-CA-C	-5.54	105.88	113.30
1	d	53	ARG	CD-NE-CZ	-5.54	116.65	124.40
1	d	149	GLU	CB-CG-CD	-5.54	103.19	112.60
2	n	106	TYR	N-CA-C	-5.54	99.58	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	155	ALA	O-C-N	-5.54	116.74	122.94
1	c	80	GLY	N-CA-C	-5.54	103.84	111.76
2	4	21	ASP	O-C-N	5.54	128.69	122.27
2	l	199	TYR	O-C-N	5.54	128.70	122.22
3	I	206	VAL	CB-CA-C	5.54	119.03	110.50
1	A	178	GLU	N-CA-CB	5.53	118.45	110.20
1	b	73	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	b	89	ILE	CA-CB-CG2	-5.53	101.09	110.50
1	d	81	LEU	N-CA-CB	5.53	118.16	109.69
1	E	121	GLN	CA-C-N	5.53	128.72	120.31
1	E	121	GLN	C-N-CA	5.53	128.72	120.31
3	M	383	LEU	CA-C-N	5.53	127.70	120.28
3	M	383	LEU	C-N-CA	5.53	127.70	120.28
1	a	28	ARG	N-CA-C	5.53	117.39	111.36
1	B	244	LEU	CB-CA-C	-5.53	100.85	110.09
1	e	103	TYR	N-CA-C	-5.53	107.53	114.56
2	l	145	LEU	CB-CA-C	-5.53	102.19	110.88
1	b	113	ALA	CA-C-O	5.53	126.41	120.55
1	E	197	GLY	O-C-N	5.53	128.31	122.28
2	2	138	VAL	O-C-N	-5.53	116.92	123.00
2	i	44	LYS	CA-C-N	5.53	130.38	123.14
2	i	44	LYS	C-N-CA	5.53	130.38	123.14
2	k	51	ARG	NE-CZ-NH2	5.53	124.18	119.20
3	M	395	VAL	CA-CB-CG2	5.53	119.80	110.40
1	D	120	LYS	CA-C-N	5.53	127.69	120.28
1	D	120	LYS	C-N-CA	5.53	127.69	120.28
2	6	168	ALA	CA-C-O	-5.53	114.69	120.55
3	I	226	VAL	CA-CB-CG2	-5.53	101.00	110.40
2	3	47	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	6	95	SER	CA-C-O	-5.53	115.02	120.82
1	G	168	ARG	NE-CZ-NH1	-5.53	115.97	121.50
2	j	112	ILE	N-CA-CB	5.53	118.82	111.64
2	4	25	MET	CA-C-O	-5.53	114.87	121.11
3	I	338	GLU	N-CA-CB	5.53	118.02	110.01
3	M	147	ASP	CA-C-N	5.53	128.03	120.46
3	M	147	ASP	C-N-CA	5.53	128.03	120.46
3	J	360	MET	N-CA-C	-5.53	105.34	111.36
1	E	44	GLU	N-CA-C	-5.52	105.90	113.30
1	f	45	GLY	CA-C-N	-5.52	115.31	122.99
1	f	45	GLY	C-N-CA	-5.52	115.31	122.99
2	j	105	PRO	O-C-N	5.52	129.67	123.04
2	m	51	ARG	NE-CZ-NH2	5.52	124.17	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	34	LYS	CA-C-N	5.52	128.13	120.29
3	H	34	LYS	C-N-CA	5.52	128.13	120.29
1	e	205	VAL	N-CA-CB	5.52	118.22	112.37
2	7	144	SER	N-CA-C	5.52	117.30	111.28
2	2	104	PHE	CG-CD2-CE2	5.52	130.08	120.70
2	4	169	VAL	CA-C-N	5.52	127.62	120.44
2	4	169	VAL	C-N-CA	5.52	127.62	120.44
2	n	46	TYR	N-CA-C	-5.52	100.90	109.24
3	H	341	ARG	CA-C-N	5.52	128.26	120.42
3	H	341	ARG	C-N-CA	5.52	128.26	120.42
3	M	121	THR	CA-C-O	-5.52	115.12	121.47
3	M	393	LYS	CA-C-O	5.52	126.17	119.11
2	7	101	TYR	N-CA-C	-5.52	106.33	112.57
3	I	20	TYR	CA-C-N	5.52	127.61	120.44
3	I	20	TYR	C-N-CA	5.52	127.61	120.44
3	J	376	THR	CA-C-N	5.52	127.67	120.28
3	J	376	THR	C-N-CA	5.52	127.67	120.28
2	1	127	PRO	N-CA-C	-5.52	107.58	114.20
2	h	122	ILE	O-C-N	5.52	129.00	123.10
2	h	187	ASP	CA-C-N	5.52	131.46	122.69
2	h	187	ASP	C-N-CA	5.52	131.46	122.69
2	7	21	ASP	N-CA-C	-5.52	104.80	113.02
3	L	126	MET	CA-C-N	5.52	128.02	120.46
3	L	126	MET	C-N-CA	5.52	128.02	120.46
1	a	87	VAL	CA-C-N	5.51	128.69	120.31
1	a	87	VAL	C-N-CA	5.51	128.69	120.31
2	5	136	ASP	CA-C-N	-5.51	115.45	123.06
2	5	136	ASP	C-N-CA	-5.51	115.45	123.06
3	I	132	VAL	CA-C-O	5.51	127.42	121.36
2	1	201	PRO	N-CA-C	5.51	123.82	112.47
3	H	19	ASP	CA-C-N	5.51	128.12	120.29
3	H	19	ASP	C-N-CA	5.51	128.12	120.29
3	H	342	ILE	CA-C-O	5.51	126.69	120.85
1	G	111	GLU	CA-C-N	5.51	127.93	120.44
1	G	111	GLU	C-N-CA	5.51	127.93	120.44
1	G	164	ILE	CA-CB-CG1	5.51	119.77	110.40
1	g	109	VAL	CA-C-N	5.51	127.66	120.28
1	g	109	VAL	C-N-CA	5.51	127.66	120.28
3	M	323	ILE	N-CA-C	-5.51	105.00	110.62
2	j	14	THR	N-CA-C	-5.51	100.69	109.23
2	m	209	ALA	O-C-N	5.51	129.42	122.37
3	L	150	ILE	CB-CA-C	-5.51	104.70	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	15	PHE	CB-CA-C	-5.51	101.08	109.89
2	6	165	VAL	N-CA-C	-5.51	105.16	110.72
2	7	68	ARG	N-CA-CB	5.51	118.31	110.16
3	L	167	PHE	CA-CB-CG	-5.51	108.29	113.80
3	M	280	ASP	CA-CB-CG	5.51	118.11	112.60
2	3	205	GLU	CA-C-O	-5.50	114.03	120.20
2	l	61	GLY	CA-C-N	5.50	128.11	120.29
2	l	61	GLY	C-N-CA	5.50	128.11	120.29
2	7	186	ILE	CB-CA-C	5.50	120.28	111.69
1	a	208	ASN	CA-CB-CG	5.50	118.10	112.60
1	g	111	GLU	N-CA-C	5.50	118.20	111.82
2	h	207	ILE	N-CA-C	-5.50	105.00	111.00
2	2	172	ILE	CA-CB-CG2	5.50	119.86	110.50
2	m	46	TYR	CG-CD1-CE1	-5.50	112.94	121.20
2	n	115	ILE	O-C-N	5.50	129.12	123.18
3	I	133	GLU	N-CA-C	-5.50	107.14	112.97
3	L	59	ARG	N-CA-C	-5.50	106.34	113.16
1	b	90	ASP	CA-CB-CG	-5.50	107.10	112.60
1	F	213	TYR	CB-CG-CD1	-5.50	112.55	120.80
2	5	173	TYR	N-CA-C	-5.50	106.07	112.89
2	l	187	ASP	N-CA-C	-5.50	101.31	110.17
3	M	335	ASP	CA-C-N	5.50	128.67	120.31
3	M	335	ASP	C-N-CA	5.50	128.67	120.31
1	g	97	GLN	CA-C-N	5.50	128.23	120.42
1	g	97	GLN	C-N-CA	5.50	128.23	120.42
2	i	196	PHE	N-CA-C	-5.50	96.21	107.70
2	h	98	LEU	CA-C-N	5.50	128.19	120.28
2	h	98	LEU	C-N-CA	5.50	128.19	120.28
2	7	88	ARG	N-CA-C	5.50	117.27	111.28
3	K	205	ARG	CG-CD-NE	-5.50	99.91	112.00
3	K	371	THR	CA-C-N	5.50	127.64	120.28
3	K	371	THR	C-N-CA	5.50	127.64	120.28
3	M	309	VAL	CA-CB-CG2	-5.50	101.06	110.40
1	f	71	ASP	CA-CB-CG	-5.50	107.11	112.60
2	4	118	GLU	CB-CA-C	-5.50	100.32	109.55
3	J	209	SER	CA-C-N	5.49	132.28	122.06
3	J	209	SER	C-N-CA	5.49	132.28	122.06
1	G	122	GLN	CB-CA-C	-5.49	101.51	110.85
2	1	173	TYR	CA-C-N	5.49	127.64	120.28
2	1	173	TYR	C-N-CA	5.49	127.64	120.28
1	e	24	VAL	N-CA-C	-5.49	105.37	110.53
3	H	303	PHE	CA-CB-CG	-5.49	108.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	135	LYS	CA-C-N	5.49	126.70	119.84
3	M	135	LYS	C-N-CA	5.49	126.70	119.84
3	J	325	THR	CA-C-O	-5.49	113.66	119.97
3	M	86	LYS	N-CA-CB	5.49	119.24	110.46
1	g	200	ILE	CA-CB-CG1	5.49	119.73	110.40
2	2	150	VAL	CA-C-O	-5.49	115.25	120.95
2	i	175	ALA	CA-C-N	5.49	128.18	120.28
2	i	175	ALA	C-N-CA	5.49	128.18	120.28
2	j	29	LYS	N-CA-C	-5.49	106.72	113.41
3	I	210	GLU	N-CA-C	-5.49	105.80	112.88
3	K	109	ASN	CA-C-N	5.49	127.89	120.38
3	K	109	ASN	C-N-CA	5.49	127.89	120.38
1	D	71	ASP	CA-C-N	5.48	131.99	122.56
1	D	71	ASP	C-N-CA	5.48	131.99	122.56
2	4	109	GLN	N-CA-C	-5.48	100.24	109.07
1	b	152	PRO	N-CA-C	-5.48	108.98	114.68
1	d	119	PHE	CA-C-N	5.48	128.07	120.29
1	d	119	PHE	C-N-CA	5.48	128.07	120.29
1	E	62	ASP	O-C-N	5.48	129.47	123.22
2	3	153	ASP	N-CA-CB	5.48	118.02	110.07
2	j	99	ASN	CA-C-N	5.48	128.07	120.29
2	j	99	ASN	C-N-CA	5.48	128.07	120.29
1	C	19	GLY	N-CA-C	-5.48	100.19	113.18
1	g	240	ILE	CA-C-N	5.48	127.62	120.28
1	g	240	ILE	C-N-CA	5.48	127.62	120.28
2	m	28	GLU	N-CA-C	-5.48	101.24	109.95
3	K	49	ARG	O-C-N	5.48	127.93	122.12
1	B	159	TYR	N-CA-C	-5.48	101.08	109.41
2	n	36	PHE	N-CA-C	-5.48	101.65	110.14
1	c	81	LEU	CA-C-N	5.48	129.31	120.55
1	c	81	LEU	C-N-CA	5.48	129.31	120.55
2	h	150	VAL	CA-C-N	5.48	127.62	120.28
2	h	150	VAL	C-N-CA	5.48	127.62	120.28
3	H	209	SER	CA-C-N	5.48	128.63	120.31
3	H	209	SER	C-N-CA	5.48	128.63	120.31
1	A	73	HIS	CG-CD2-NE2	5.47	112.67	107.20
1	B	136	LEU	N-CA-CB	5.47	120.44	111.08
1	e	162	THR	O-C-N	5.47	128.76	123.29
1	e	182	ASP	CA-C-N	5.47	128.62	120.90
1	e	182	ASP	C-N-CA	5.47	128.62	120.90
1	F	39	GLY	O-C-N	-5.47	118.55	123.37
2	5	152	GLU	CA-C-N	5.47	127.88	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	152	GLU	C-N-CA	5.47	127.88	120.65
2	m	201	PRO	N-CA-C	5.47	123.75	112.47
3	I	130	PHE	CB-CA-C	-5.47	100.35	109.55
3	J	211	PHE	N-CA-CB	5.47	118.02	109.97
3	J	248	ALA	O-C-N	-5.47	117.51	123.26
2	4	35	ASN	N-CA-CB	5.47	119.74	110.49
3	K	346	ALA	N-CA-CB	5.47	120.76	111.57
3	K	397	PHE	O-C-N	5.47	130.58	122.81
3	L	42	ILE	O-C-N	-5.47	116.56	121.87
1	g	147	LEU	N-CA-C	-5.47	99.39	108.75
1	A	119	PHE	N-CA-CB	5.47	118.16	110.12
2	4	121	SER	O-C-N	5.47	128.88	123.46
2	n	183	GLY	CA-C-N	5.47	131.99	121.54
2	n	183	GLY	C-N-CA	5.47	131.99	121.54
1	F	19	GLY	N-CA-C	-5.47	107.77	115.32
2	7	127	PRO	CA-C-N	5.47	129.31	121.55
2	7	127	PRO	C-N-CA	5.47	129.31	121.55
1	F	222	LYS	N-CA-C	-5.47	101.00	109.14
2	1	167	LEU	CA-C-N	5.47	127.60	120.28
2	1	167	LEU	C-N-CA	5.47	127.60	120.28
2	3	184	ASP	N-CA-CB	5.47	118.09	109.83
2	4	69	ILE	N-CA-C	-5.47	105.04	110.62
2	5	27	THR	N-CA-C	-5.47	100.99	109.14
3	K	32	ASP	CA-C-O	5.47	126.21	120.42
1	B	17	PRO	N-CA-C	-5.46	107.31	114.03
1	c	117	CYS	CA-C-O	-5.46	115.07	120.70
3	H	304	ASP	N-CA-C	-5.46	105.32	111.28
1	a	179	TYR	CA-C-O	5.46	127.28	121.16
1	c	29	GLU	N-CA-C	-5.46	106.57	113.18
2	1	211	PHE	CB-CG-CD2	5.46	129.99	120.70
2	j	194	ASP	CB-CA-C	-5.46	101.00	109.80
1	A	234	GLU	N-CA-C	-5.46	105.41	111.36
3	J	361	PHE	CB-CG-CD1	5.46	129.99	120.70
1	b	71	ASP	CA-CB-CG	5.46	118.06	112.60
1	d	198	LEU	CB-CA-C	5.46	119.45	110.88
1	e	159	TYR	CA-C-O	5.46	127.83	121.44
1	F	179	TYR	N-CA-C	5.46	117.94	110.24
2	2	99	ASN	CA-C-N	5.46	128.04	120.29
2	2	99	ASN	C-N-CA	5.46	128.04	120.29
3	H	44	TYR	O-C-N	5.46	128.98	122.27
3	H	48	VAL	O-C-N	-5.46	116.22	121.90
3	L	313	THR	N-CA-CB	5.46	117.67	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	242	GLU	CA-C-O	5.46	126.33	120.55
2	h	49	ALA	CA-C-O	-5.46	115.58	121.36
3	L	248	ALA	O-C-N	5.46	130.32	123.23
3	J	242	GLU	CA-C-N	5.46	130.63	122.23
3	J	242	GLU	C-N-CA	5.46	130.63	122.23
1	b	73	HIS	CE1-NE2-CD2	-5.45	103.55	109.00
1	G	211	VAL	N-CA-C	-5.45	100.21	108.17
1	g	126	TYR	N-CA-C	-5.45	103.19	110.55
1	g	242	GLU	CB-CG-CD	-5.45	103.33	112.60
2	k	34	GLY	CA-C-N	5.45	127.59	120.28
2	k	34	GLY	C-N-CA	5.45	127.59	120.28
2	5	166	GLU	CA-C-N	5.45	128.03	120.29
2	5	166	GLU	C-N-CA	5.45	128.03	120.29
2	2	129	GLY	N-CA-C	-5.45	104.58	111.72
2	2	143	GLY	CA-C-N	5.45	127.59	120.28
2	2	143	GLY	C-N-CA	5.45	127.59	120.28
1	a	44	GLU	CA-C-O	5.45	125.18	119.51
1	a	189	MET	CG-SD-CE	-5.45	88.91	100.90
1	b	230	LYS	CA-C-O	-5.45	112.69	120.16
1	C	151	ASP	N-CA-C	-5.45	101.76	110.10
1	F	163	ALA	CA-C-N	5.45	130.43	122.69
1	F	163	ALA	C-N-CA	5.45	130.43	122.69
1	g	217	ASP	CA-CB-CG	5.45	118.05	112.60
2	2	125	ILE	CA-C-N	5.45	130.40	121.57
2	2	125	ILE	C-N-CA	5.45	130.40	121.57
2	l	98	LEU	CA-C-O	5.45	126.20	120.42
3	H	347	SER	CA-C-O	-5.45	115.38	121.81
3	L	243	LEU	CB-CA-C	-5.45	101.35	110.56
3	M	375	PHE	N-CA-CB	5.45	117.91	110.01
1	d	155	ALA	N-CA-C	-5.45	100.83	109.76
2	5	115	ILE	CA-C-N	5.45	130.77	122.11
2	5	115	ILE	C-N-CA	5.45	130.77	122.11
2	j	191	ILE	N-CA-C	-5.45	96.92	106.61
3	M	231	LYS	CB-CA-C	-5.45	101.75	110.79
3	K	29	ARG	CA-C-O	-5.45	114.65	120.42
3	L	49	ARG	CA-C-N	5.45	127.52	120.44
3	L	49	ARG	C-N-CA	5.45	127.52	120.44
2	1	166	GLU	N-CA-CB	5.44	117.90	110.01
2	k	123	TYR	N-CA-CB	5.44	119.83	110.68
1	B	207	GLU	CB-CG-CD	-5.44	103.35	112.60
2	1	62	ASP	CA-C-N	5.44	127.52	120.44
2	1	62	ASP	C-N-CA	5.44	127.52	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	191	ILE	N-CA-C	-5.44	99.71	107.77
3	M	86	LYS	N-CA-C	-5.44	102.47	110.52
3	M	159	LEU	CA-C-O	-5.44	113.40	118.73
1	E	187	ASP	CA-C-N	5.44	128.01	120.29
1	E	187	ASP	C-N-CA	5.44	128.01	120.29
2	6	154	ARG	NE-CZ-NH1	-5.44	116.06	121.50
2	n	91	ALA	O-C-N	5.44	127.89	122.12
3	J	31	GLU	CA-C-O	-5.44	115.11	120.82
1	a	86	ARG	N-CA-C	-5.44	105.35	111.28
1	D	103	TYR	N-CA-C	-5.44	107.65	114.56
2	j	18	VAL	N-CA-CB	5.44	116.65	110.72
3	L	218	GLU	CA-C-N	5.44	126.14	119.99
3	L	218	GLU	C-N-CA	5.44	126.14	119.99
1	E	93	ARG	N-CA-CB	5.44	117.89	110.01
2	2	43	LYS	CB-CA-C	-5.44	99.86	109.70
2	3	61	GLY	CA-C-N	5.44	127.57	120.28
2	3	61	GLY	C-N-CA	5.44	127.57	120.28
1	c	49	ILE	CB-CA-C	5.43	118.87	110.50
1	F	44	GLU	CA-C-O	5.43	124.88	118.90
3	I	288	ASN	N-CA-C	-5.43	107.30	114.31
3	L	50	ARG	N-CA-CB	5.43	117.89	110.01
3	J	65	VAL	CA-CB-CG2	-5.43	101.16	110.40
1	b	16	SER	CA-C-N	5.43	125.52	119.87
1	b	16	SER	C-N-CA	5.43	125.52	119.87
1	D	77	ALA	N-CA-C	-5.43	101.72	110.14
1	E	114	LYS	CA-C-N	5.43	128.00	120.29
1	E	114	LYS	C-N-CA	5.43	128.00	120.29
1	F	55	GLY	N-CA-C	5.43	118.80	112.50
2	i	109	GLN	CB-CA-C	-5.43	101.39	110.19
1	b	94	ILE	CA-C-N	5.43	127.56	120.28
1	b	94	ILE	C-N-CA	5.43	127.56	120.28
1	c	96	ALA	CA-C-N	5.43	128.56	120.31
1	c	96	ALA	C-N-CA	5.43	128.56	120.31
1	E	125	GLN	N-CA-CB	5.43	117.88	110.01
1	E	202	SER	N-CA-C	-5.43	100.87	108.96
2	h	165	VAL	N-CA-CB	5.43	119.63	110.56
2	3	192	THR	CA-C-N	5.43	131.91	121.54
2	3	192	THR	C-N-CA	5.43	131.91	121.54
2	4	200	SER	CA-C-N	5.43	126.63	119.84
2	4	200	SER	C-N-CA	5.43	126.63	119.84
3	J	151	GLU	N-CA-CB	5.43	118.10	110.12
1	g	214	VAL	N-CA-CB	5.43	119.20	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	92	THR	O-C-N	-5.43	115.96	122.15
2	6	56	THR	CA-CB-OG1	5.43	117.74	109.60
1	B	201	GLU	N-CA-CB	5.43	120.16	111.91
1	b	44	GLU	CA-C-N	-5.43	113.96	121.23
1	b	44	GLU	C-N-CA	-5.43	113.96	121.23
1	c	201	GLU	CA-C-O	-5.43	114.25	120.98
1	F	137	LEU	N-CA-C	-5.43	99.44	108.34
1	C	194	VAL	CA-C-N	5.42	127.55	120.28
1	C	194	VAL	C-N-CA	5.42	127.55	120.28
1	a	149	GLU	N-CA-C	-5.42	99.59	108.76
1	b	98	ILE	CA-C-N	5.42	127.99	120.29
1	b	98	ILE	C-N-CA	5.42	127.99	120.29
1	E	67	ILE	N-CA-C	-5.42	99.70	107.78
2	7	115	ILE	O-C-N	-5.42	117.30	123.10
1	c	191	LEU	CA-C-N	5.42	127.17	120.34
1	c	191	LEU	C-N-CA	5.42	127.17	120.34
2	m	109	GLN	N-CA-CB	5.42	119.79	110.68
3	I	27	TYR	CB-CG-CD1	-5.42	112.67	120.80
3	J	371	THR	CA-CB-OG1	5.42	117.73	109.60
1	b	178	GLU	CA-C-O	-5.42	112.76	120.51
1	g	225	SER	CA-C-N	5.42	125.76	119.47
1	g	225	SER	C-N-CA	5.42	125.76	119.47
3	H	210	GLU	CA-C-N	5.42	128.57	120.87
3	H	210	GLU	C-N-CA	5.42	128.57	120.87
3	L	371	THR	CA-C-N	5.42	129.89	120.68
3	L	371	THR	C-N-CA	5.42	129.89	120.68
2	1	73	GLU	CA-C-N	5.42	127.48	120.44
2	1	73	GLU	C-N-CA	5.42	127.48	120.44
2	h	24	VAL	N-CA-C	-5.42	100.52	108.11
2	6	169	VAL	CB-CA-C	-5.42	104.82	112.14
1	A	77	ALA	N-CA-C	-5.42	102.50	110.52
1	E	100	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	f	129	VAL	O-C-N	-5.42	117.46	123.20
2	4	212	ARG	CD-NE-CZ	-5.42	116.82	124.40
2	k	43	LYS	CA-C-O	-5.42	114.99	121.11
3	I	94	TYR	CA-C-N	5.42	130.25	122.45
3	I	94	TYR	C-N-CA	5.42	130.25	122.45
3	I	263	ARG	CA-C-N	5.42	127.54	120.28
3	I	263	ARG	C-N-CA	5.42	127.54	120.28
1	D	126	TYR	CA-C-N	5.42	125.83	120.31
1	D	126	TYR	C-N-CA	5.42	125.83	120.31
2	3	109	GLN	N-CA-C	-5.42	100.57	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	83	ARG	CA-C-N	5.42	128.88	120.60
2	6	83	ARG	C-N-CA	5.42	128.88	120.60
1	B	40	ILE	N-CA-C	-5.41	100.33	108.12
1	F	73	HIS	ND1-CE1-NE2	5.41	113.81	108.40
2	1	66	LEU	CA-C-N	5.41	127.53	120.28
2	1	66	LEU	C-N-CA	5.41	127.53	120.28
3	H	371	THR	CA-C-N	5.41	127.53	120.28
3	H	371	THR	C-N-CA	5.41	127.53	120.28
3	K	102	PRO	CB-CA-C	-5.41	104.67	111.71
1	A	207	GLU	CA-CB-CG	-5.41	103.28	114.10
1	f	14	VAL	CA-C-N	5.41	128.40	120.71
1	f	14	VAL	C-N-CA	5.41	128.40	120.71
3	K	72	LEU	N-CA-C	-5.41	101.07	109.24
3	L	281	VAL	CA-C-N	5.41	131.44	121.70
3	L	281	VAL	C-N-CA	5.41	131.44	121.70
1	D	118	ASP	CB-CA-C	-5.41	101.65	110.85
3	H	205	ARG	CA-C-O	5.41	126.27	120.32
3	M	266	MET	CA-C-N	5.41	127.53	120.28
3	M	266	MET	C-N-CA	5.41	127.53	120.28
1	F	144	VAL	CA-C-O	-5.41	113.59	120.95
1	G	65	GLU	CA-C-O	5.41	130.00	120.80
2	7	49	ALA	O-C-N	-5.41	117.20	122.99
3	K	356	THR	CA-C-N	5.41	128.53	120.31
3	K	356	THR	C-N-CA	5.41	128.53	120.31
1	a	190	VAL	CA-CB-CG2	-5.41	101.21	110.40
1	E	18	ASP	CA-C-N	5.41	131.12	122.25
1	E	18	ASP	C-N-CA	5.41	131.12	122.25
1	g	134	VAL	O-C-N	-5.41	117.05	123.00
1	D	168	ARG	CB-CA-C	-5.41	101.81	110.79
2	l	190	LYS	N-CA-C	-5.41	99.48	108.34
3	I	345	GLY	N-CA-C	-5.41	107.08	115.67
1	c	83	ALA	CA-C-N	5.40	127.96	120.29
1	c	83	ALA	C-N-CA	5.40	127.96	120.29
1	D	239	ARG	CA-C-O	5.40	126.49	120.82
1	E	10	ARG	CA-C-O	-5.40	113.19	119.14
1	f	175	PHE	CA-C-O	5.40	125.61	119.18
1	G	168	ARG	CA-C-N	5.40	129.82	120.58
1	G	168	ARG	C-N-CA	5.40	129.82	120.58
2	i	55	THR	N-CA-C	-5.40	99.60	108.41
1	C	222	LYS	CB-CA-C	-5.40	100.27	110.16
3	M	59	ARG	N-CA-C	5.40	117.25	111.36
1	a	32	LYS	CG-CD-CE	5.40	123.72	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	230	LYS	O-C-N	-5.40	115.42	120.55
1	E	83	ALA	CA-C-N	5.40	127.52	120.28
1	E	83	ALA	C-N-CA	5.40	127.52	120.28
1	g	157	LEU	N-CA-C	-5.40	98.76	108.48
2	k	113	GLY	CA-C-O	-5.40	115.78	121.56
3	H	36	PHE	CA-C-N	5.40	127.86	120.46
3	H	36	PHE	C-N-CA	5.40	127.86	120.46
3	H	272	LEU	N-CA-C	-5.40	104.34	111.96
3	H	273	ASP	CB-CA-C	5.40	119.42	110.78
2	l	78	GLU	O-C-N	5.40	127.63	122.07
1	G	232	TYR	CA-CB-CG	-5.40	104.18	113.90
2	3	47	GLN	N-CA-CB	5.40	118.32	109.95
2	n	136	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	174	PHE	CA-CB-CG	5.40	119.20	113.80
2	4	62	ASP	CA-C-N	5.40	127.51	120.28
2	4	62	ASP	C-N-CA	5.40	127.51	120.28
2	6	97	LEU	CA-C-O	5.40	126.27	120.55
1	G	58	LEU	CA-C-N	5.39	128.75	120.82
1	G	58	LEU	C-N-CA	5.39	128.75	120.82
2	i	87	VAL	CA-C-N	5.39	127.51	120.28
2	i	87	VAL	C-N-CA	5.39	127.51	120.28
2	i	116	ASP	CA-C-O	5.39	127.75	121.49
2	7	157	PRO	N-CA-CB	5.39	108.33	103.20
3	L	55	VAL	CA-C-O	-5.39	115.45	121.17
1	E	115	LYS	CA-C-O	5.39	126.14	120.42
1	e	90	ASP	N-CA-CB	5.39	118.05	110.12
1	B	218	ASP	CA-C-O	-5.39	114.26	120.24
2	i	203	GLU	CA-C-N	5.39	128.07	120.42
2	i	203	GLU	C-N-CA	5.39	128.07	120.42
2	3	112	ILE	CB-CA-C	5.39	118.42	110.77
2	l	68	ARG	NE-CZ-NH2	-5.39	114.35	119.20
2	m	17	LEU	CA-C-N	5.39	129.10	121.66
2	m	17	LEU	C-N-CA	5.39	129.10	121.66
3	K	384	LYS	N-CA-CB	5.39	118.05	110.12
3	M	207	VAL	CA-C-O	-5.39	116.06	121.45
2	1	60	VAL	CA-C-O	-5.39	115.07	121.05
2	1	125	ILE	O-C-N	-5.39	117.38	123.20
3	I	214	LYS	O-C-N	-5.39	114.93	122.37
3	K	106	VAL	CA-C-O	5.39	127.53	121.28
3	J	73	GLU	N-CA-CB	5.39	116.39	110.35
1	d	136	LEU	N-CA-C	-5.39	101.17	109.52
2	6	109	GLN	N-CA-C	-5.39	99.74	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	214	LYS	CA-C-O	5.39	125.80	119.28
1	c	118	ASP	CA-CB-CG	-5.38	107.22	112.60
1	D	103	TYR	N-CA-CB	5.38	118.16	111.00
1	D	111	GLU	CA-C-N	5.38	127.50	120.28
1	D	111	GLU	C-N-CA	5.38	127.50	120.28
1	F	14	VAL	O-C-N	-5.38	117.44	123.26
1	G	20	ARG	N-CA-C	-5.38	99.96	108.14
1	g	95	GLU	CA-C-O	5.38	126.18	120.10
2	h	17	LEU	CA-C-N	5.38	129.72	122.93
2	h	17	LEU	C-N-CA	5.38	129.72	122.93
2	7	202	GLU	CA-C-N	5.38	127.50	120.28
2	7	202	GLU	C-N-CA	5.38	127.50	120.28
3	K	90	ASN	CA-C-N	5.38	131.83	121.54
3	K	90	ASN	C-N-CA	5.38	131.83	121.54
3	L	61	PRO	N-CD-CG	5.38	111.28	103.20
3	L	254	ASP	CA-CB-CG	-5.38	107.22	112.60
2	n	47	GLN	CA-C-N	5.38	129.62	121.65
2	n	47	GLN	C-N-CA	5.38	129.62	121.65
1	g	85	ALA	CA-C-N	5.38	127.49	120.28
1	g	85	ALA	C-N-CA	5.38	127.49	120.28
2	j	194	ASP	N-CA-C	-5.38	105.75	114.09
2	4	190	LYS	N-CA-C	-5.38	100.13	108.90
2	6	131	ALA	N-CA-C	-5.38	98.79	108.48
3	H	310	PRO	CA-C-N	5.38	127.88	120.67
3	H	310	PRO	C-N-CA	5.38	127.88	120.67
3	I	263	ARG	NE-CZ-NH2	-5.38	114.36	119.20
3	K	28	ARG	CG-CD-NE	-5.38	100.16	112.00
1	b	10	ARG	NE-CZ-NH1	-5.38	116.12	121.50
3	K	176	LYS	N-CA-CB	5.38	117.81	110.01
3	M	303	PHE	CA-CB-CG	-5.38	108.42	113.80
1	b	98	ILE	CB-CA-C	-5.38	104.80	112.22
1	C	142	ASP	CA-CB-CG	-5.38	107.22	112.60
2	l	171	ALA	N-CA-C	5.38	117.14	111.28
3	M	89	VAL	CA-C-O	5.38	127.52	121.28
1	C	244	LEU	N-CA-C	-5.38	106.59	112.72
2	2	77	TYR	N-CA-CB	-5.38	102.20	110.16
2	6	36	PHE	N-CA-C	-5.38	100.14	108.90
3	H	290	ILE	O-C-N	-5.38	117.25	122.09
3	M	289	ARG	CA-C-N	5.38	128.94	122.16
3	M	289	ARG	C-N-CA	5.38	128.94	122.16
1	a	100	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	H	150	ILE	O-C-N	-5.38	116.62	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	27	TYR	CB-CA-C	-5.38	99.42	110.38
1	e	89	ILE	CA-C-N	5.37	127.48	120.28
1	e	89	ILE	C-N-CA	5.37	127.48	120.28
1	a	238	GLU	N-CA-CB	5.37	118.11	110.16
1	B	157	LEU	N-CA-C	-5.37	99.56	108.75
1	d	65	GLU	CA-C-O	5.37	127.17	121.16
2	k	64	GLN	N-CA-C	-5.37	105.46	112.23
2	1	45	ILE	O-C-N	-5.37	117.46	123.26
2	7	152	GLU	CA-C-N	5.37	127.47	120.28
2	7	152	GLU	C-N-CA	5.37	127.47	120.28
3	M	137	GLU	CB-CG-CD	-5.37	103.47	112.60
1	D	163	ALA	CA-C-N	5.37	131.69	122.67
1	D	163	ALA	C-N-CA	5.37	131.69	122.67
2	2	97	LEU	CA-C-N	5.37	128.01	120.28
2	2	97	LEU	C-N-CA	5.37	128.01	120.28
2	m	33	MET	N-CA-C	-5.37	96.26	107.37
3	M	163	LYS	O-C-N	-5.37	116.56	121.34
3	J	117	ASN	O-C-N	-5.37	116.17	123.15
1	C	87	VAL	CA-C-O	-5.37	115.16	120.85
1	e	91	ARG	CA-C-N	5.37	127.47	120.28
1	e	91	ARG	C-N-CA	5.37	127.47	120.28
2	3	104	PHE	CA-CB-CG	-5.37	108.44	113.80
2	k	73	GLU	CA-C-N	5.37	127.47	120.28
2	k	73	GLU	C-N-CA	5.37	127.47	120.28
2	l	126	ASP	CA-C-N	5.37	125.06	119.64
2	l	126	ASP	C-N-CA	5.37	125.06	119.64
2	l	201	PRO	N-CA-CB	5.37	108.88	103.25
3	I	224	ARG	CA-C-O	5.37	126.11	120.42
3	I	227	PHE	N-CA-CB	5.37	118.01	110.12
1	a	81	LEU	CA-C-N	5.36	127.81	120.46
1	a	81	LEU	C-N-CA	5.36	127.81	120.46
1	B	119	PHE	O-C-N	5.36	128.26	122.15
1	e	230	LYS	CA-C-N	5.36	124.70	118.85
1	e	230	LYS	C-N-CA	5.36	124.70	118.85
3	H	248	ALA	CA-C-O	5.36	125.93	120.24
1	B	16	SER	CA-C-O	-5.36	113.58	121.46
1	e	84	ASP	CA-C-N	5.36	127.47	120.28
1	e	84	ASP	C-N-CA	5.36	127.47	120.28
1	F	132	PHE	CA-CB-CG	-5.36	108.44	113.80
2	i	199	TYR	CB-CA-C	-5.36	102.46	110.88
1	d	97	GLN	O-C-N	-5.36	115.15	122.33
1	F	165	GLY	CA-C-O	-5.36	116.94	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	h	210	LYS	N-CA-C	-5.36	106.51	113.16
1	f	41	LYS	O-C-N	-5.36	117.22	123.27
2	1	30	ARG	NE-CZ-NH1	-5.36	116.14	121.50
2	3	38	ALA	N-CA-C	-5.36	105.39	112.94
2	4	132	ILE	CA-CB-CG2	-5.36	101.39	110.50
2	k	61	GLY	CA-C-N	5.36	129.79	120.68
2	k	61	GLY	C-N-CA	5.36	129.79	120.68
3	J	254	ASP	N-CA-CB	5.36	119.55	110.49
1	D	237	ASN	N-CA-CB	5.36	118.47	110.22
1	G	169	ASN	N-CA-CB	5.36	118.18	110.20
2	2	153	ASP	CA-CB-CG	5.36	117.96	112.60
2	4	23	VAL	N-CA-CB	5.36	120.23	111.45
2	5	83	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	l	70	ILE	N-CA-CB	5.36	116.82	110.55
3	H	216	ILE	O-C-N	5.36	127.98	122.79
3	K	85	PRO	N-CA-C	5.36	119.02	110.40
1	f	60	GLU	O-C-N	5.35	129.29	123.13
2	n	103	TYR	N-CA-C	-5.35	106.79	113.38
2	n	139	ALA	CA-C-N	5.35	131.77	121.54
2	n	139	ALA	C-N-CA	5.35	131.77	121.54
1	F	212	GLY	N-CA-C	-5.35	102.98	110.96
2	3	104	PHE	N-CA-CB	5.35	117.24	110.23
2	4	161	VAL	CA-C-O	-5.35	114.47	120.25
2	m	199	TYR	O-C-N	5.35	127.87	122.09
3	I	234	ALA	O-C-N	-5.35	115.43	121.43
3	K	356	THR	O-C-N	-5.35	115.69	122.27
1	E	231	PRO	CA-C-N	5.35	127.89	120.29
1	E	231	PRO	C-N-CA	5.35	127.89	120.29
2	4	43	LYS	CB-CG-CD	5.35	123.61	111.30
1	A	10	ARG	N-CA-C	-5.35	106.34	112.92
1	A	135	SER	N-CA-CB	5.35	120.05	110.80
1	A	145	PRO	CA-C-O	-5.35	115.34	121.86
1	a	56	SER	CA-C-N	5.35	127.45	120.28
1	a	56	SER	C-N-CA	5.35	127.45	120.28
1	C	230	LYS	CA-C-N	5.35	124.53	118.97
1	C	230	LYS	C-N-CA	5.35	124.53	118.97
1	d	100	ARG	CD-NE-CZ	-5.35	116.91	124.40
2	1	178	ARG	NE-CZ-NH2	-5.35	114.39	119.20
3	I	276	ASP	N-CA-CB	5.35	117.92	110.11
3	K	192	ALA	N-CA-CB	5.35	118.08	110.16
3	M	84	GLY	CA-C-O	-5.35	113.87	121.52
3	M	117	ASN	CA-C-O	-5.35	114.12	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	189	MET	CA-C-O	-5.35	114.75	120.42
2	l	45	ILE	N-CA-C	-5.35	100.42	108.12
2	l	210	LYS	CA-C-O	5.35	125.96	119.38
1	C	138	ILE	N-CA-CB	5.34	117.46	111.21
2	k	201	PRO	N-CA-CB	5.34	109.35	103.26
2	l	14	THR	CA-CB-CG2	-5.34	101.41	110.50
2	6	170	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	J	49	ARG	CA-C-O	-5.34	114.75	120.42
3	J	313	THR	CA-C-N	5.34	127.76	120.54
3	J	313	THR	C-N-CA	5.34	127.76	120.54
2	h	48	ILE	N-CA-C	-5.34	105.64	110.82
1	E	70	ILE	CA-C-N	5.34	131.13	122.53
1	E	70	ILE	C-N-CA	5.34	131.13	122.53
3	K	195	VAL	N-CA-CB	5.34	117.80	110.54
1	e	160	LYS	N-CA-C	-5.34	106.70	114.12
2	j	161	VAL	N-CA-C	5.34	116.11	110.72
2	j	211	PHE	CA-C-N	5.34	131.74	121.54
2	j	211	PHE	C-N-CA	5.34	131.74	121.54
3	H	217	GLY	CA-C-N	5.34	128.43	120.31
3	H	217	GLY	C-N-CA	5.34	128.43	120.31
1	B	182	ASP	CA-C-O	5.34	125.67	119.32
1	C	136	LEU	N-CA-CB	5.34	119.39	110.85
2	k	196	PHE	N-CA-C	-5.34	100.47	108.96
1	B	53	ARG	CD-NE-CZ	-5.34	116.93	124.40
1	D	141	VAL	CB-CA-C	-5.34	104.05	110.99
1	d	147	LEU	N-CA-CB	5.34	119.78	110.81
3	K	241	ASP	CB-CA-C	-5.34	102.28	109.16
1	a	208	ASN	CA-C-N	5.33	131.11	122.68
1	a	208	ASN	C-N-CA	5.33	131.11	122.68
1	E	78	THR	CA-CB-CG2	5.33	119.57	110.50
2	l	63	ALA	CA-C-N	5.33	127.87	120.29
2	l	63	ALA	C-N-CA	5.33	127.87	120.29
3	I	52	ARG	N-CA-CB	5.33	118.55	110.28
3	K	49	ARG	NE-CZ-NH1	-5.33	116.17	121.50
3	M	126	MET	N-CA-CB	5.33	119.50	110.49
3	M	135	LYS	CB-CA-C	5.33	120.68	110.17
3	M	362	ALA	N-CA-CB	5.33	117.75	110.01
1	A	35	ALA	N-CA-C	5.33	122.16	110.80
1	d	124	THR	N-CA-C	-5.33	106.94	113.50
2	k	128	ILE	N-CA-CB	-5.33	103.12	112.08
2	m	185	GLY	CA-C-N	5.33	128.23	120.98
2	m	185	GLY	C-N-CA	5.33	128.23	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	104	PHE	CA-C-N	-5.33	113.18	119.84
2	7	104	PHE	C-N-CA	-5.33	113.18	119.84
2	3	155	PHE	CA-C-N	5.33	132.65	123.11
2	3	155	PHE	C-N-CA	5.33	132.65	123.11
2	l	206	GLN	N-CA-C	-5.33	106.78	113.28
1	a	44	GLU	O-C-N	-5.33	114.91	122.15
3	H	138	VAL	CA-C-N	5.33	130.84	122.21
3	H	138	VAL	C-N-CA	5.33	130.84	122.21
1	f	59	LEU	N-CA-C	-5.33	101.79	110.20
1	G	169	ASN	CA-C-O	-5.33	114.33	120.24
1	G	233	VAL	CA-C-O	-5.33	115.21	120.85
1	g	171	VAL	CA-C-N	5.33	127.42	120.28
1	g	171	VAL	C-N-CA	5.33	127.42	120.28
2	i	193	GLU	O-C-N	-5.33	115.51	122.59
1	c	106	PRO	N-CA-C	5.32	119.57	111.11
1	c	142	ASP	CA-C-N	5.32	127.85	120.29
1	c	142	ASP	C-N-CA	5.32	127.85	120.29
1	E	238	GLU	CB-CA-C	-5.32	102.52	110.88
3	M	53	SER	CA-C-O	-5.32	114.78	120.42
3	J	393	LYS	CG-CD-CE	5.32	123.55	111.30
2	n	203	GLU	CA-C-N	5.32	127.98	120.42
2	n	203	GLU	C-N-CA	5.32	127.98	120.42
3	H	310	PRO	CA-C-O	-5.32	110.91	120.60
1	B	179	TYR	CB-CG-CD1	-5.32	112.82	120.80
1	c	219	ARG	N-CA-CB	5.32	119.48	110.49
2	5	99	ASN	CA-CB-CG	-5.32	107.28	112.60
2	n	212	ARG	CD-NE-CZ	-5.32	116.95	124.40
3	L	374	ASP	CB-CA-C	-5.32	101.96	110.79
3	J	84	GLY	N-CA-C	-5.32	101.49	112.34
3	I	234	ALA	CA-C-O	-5.32	114.68	120.69
3	L	323	ILE	CA-C-N	5.32	127.84	120.29
3	L	323	ILE	C-N-CA	5.32	127.84	120.29
1	A	191	LEU	N-CA-C	5.32	117.83	111.71
1	e	240	ILE	N-CA-C	-5.32	105.20	110.62
1	f	14	VAL	CA-CB-CG2	5.32	119.44	110.40
2	3	63	ALA	N-CA-C	5.32	116.76	111.07
2	5	168	ALA	CA-C-N	5.32	127.26	120.56
2	5	168	ALA	C-N-CA	5.32	127.26	120.56
3	H	350	ASP	O-C-N	-5.32	116.09	122.15
3	K	67	VAL	O-C-N	-5.32	117.46	123.20
3	K	149	GLN	N-CA-C	5.32	122.13	110.80
3	L	77	VAL	CA-CB-CG2	5.32	119.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	37	ALA	N-CA-C	-5.32	100.02	109.06
1	d	196	MET	N-CA-C	-5.32	105.48	111.28
2	j	147	ALA	CA-C-N	5.32	127.40	120.28
2	j	147	ALA	C-N-CA	5.32	127.40	120.28
2	4	192	THR	O-C-N	5.32	128.62	122.19
2	7	168	ALA	CA-C-O	5.32	126.18	120.55
1	A	111	GLU	CA-C-N	5.31	127.83	120.29
1	A	111	GLU	C-N-CA	5.31	127.83	120.29
1	F	11	ALA	N-CA-C	-5.31	101.37	108.86
2	i	192	THR	CA-C-N	5.31	131.69	121.54
2	i	192	THR	C-N-CA	5.31	131.69	121.54
1	b	154	GLY	N-CA-C	-5.31	107.46	115.32
1	c	163	ALA	CA-C-O	-5.31	115.59	121.33
1	e	142	ASP	N-CA-C	-5.31	108.56	114.62
2	3	197	TYR	CA-CB-CG	5.31	123.46	113.90
2	7	14	THR	CA-CB-OG1	5.31	117.57	109.60
1	E	142	ASP	N-CA-C	-5.31	99.49	110.80
2	j	158	GLU	O-C-N	5.31	129.79	122.83
1	C	227	GLU	O-C-N	5.31	127.75	122.12
1	D	64	ILE	O-C-N	-5.31	115.93	122.57
1	G	77	ALA	N-CA-C	-5.31	101.23	109.14
2	2	144	SER	CA-C-N	5.31	127.83	120.29
2	2	144	SER	C-N-CA	5.31	127.83	120.29
3	L	361	PHE	CA-CB-CG	-5.31	108.49	113.80
1	b	194	VAL	CA-CB-CG1	5.31	119.42	110.40
1	C	148	TYR	CA-C-N	5.31	130.25	122.77
1	C	148	TYR	C-N-CA	5.31	130.25	122.77
2	h	200	SER	O-C-N	-5.31	115.22	121.32
1	B	111	GLU	N-CA-CB	5.31	118.47	110.30
2	n	56	THR	CA-CB-CG2	-5.31	101.48	110.50
1	b	100	ARG	NE-CZ-NH1	-5.30	116.19	121.50
1	G	67	ILE	N-CA-C	-5.30	97.17	106.61
2	i	15	VAL	N-CA-CB	5.30	121.70	111.62
2	5	156	THR	CA-C-O	-5.30	114.47	120.46
3	J	224	ARG	CA-C-O	5.30	126.17	120.55
1	B	42	CYS	CA-C-O	-5.30	115.34	121.49
1	B	219	ARG	CB-CA-C	5.30	119.61	111.39
1	d	20	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	d	170	ALA	CA-C-O	5.30	126.16	120.70
1	d	237	ASN	CA-C-N	5.30	127.39	120.28
1	d	237	ASN	C-N-CA	5.30	127.39	120.28
3	M	157	VAL	O-C-N	5.30	129.20	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	ALA	N-CA-C	5.30	116.74	111.07
1	d	110	LYS	CA-C-N	5.30	127.38	120.28
1	d	110	LYS	C-N-CA	5.30	127.38	120.28
1	E	81	LEU	N-CA-C	-5.30	101.52	109.15
2	7	55	THR	CA-CB-OG1	5.30	117.55	109.60
3	J	387	THR	N-CA-CB	5.30	119.81	110.37
1	f	97	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	g	173	GLU	CA-C-N	5.30	127.91	120.28
1	g	173	GLU	C-N-CA	5.30	127.91	120.28
3	I	104	ALA	N-CA-CB	5.30	118.50	109.87
2	i	162	ASP	N-CA-C	5.29	117.05	111.28
3	L	26	LEU	CA-C-N	5.29	127.38	120.28
3	L	26	LEU	C-N-CA	5.29	127.38	120.28
1	B	91	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	e	65	GLU	CA-C-O	-5.29	115.02	121.05
1	G	245	LYS	N-CA-C	-5.29	105.59	111.36
1	g	166	MET	CB-CA-C	-5.29	101.86	110.85
2	3	24	VAL	O-C-N	-5.29	117.47	123.03
2	k	124	SER	N-CA-C	-5.29	100.61	109.24
2	5	100	SER	CA-C-O	5.29	126.16	120.55
2	m	202	GLU	N-CA-C	5.29	117.46	111.11
2	m	205	GLU	N-CA-C	5.29	117.80	111.71
2	n	180	SER	N-CA-CB	5.29	118.23	110.35
3	M	65	VAL	CA-CB-CG1	5.29	119.39	110.40
1	e	60	GLU	CB-CG-CD	-5.29	103.61	112.60
1	E	237	ASN	N-CA-CB	5.29	117.89	110.12
2	i	147	ALA	O-C-N	5.29	127.72	122.12
3	I	152	GLU	N-CA-CB	5.29	117.68	110.01
3	L	193	LYS	O-C-N	5.29	128.77	122.27
1	c	87	VAL	CA-C-N	5.29	127.36	120.28
1	c	87	VAL	C-N-CA	5.29	127.36	120.28
1	E	185	PHE	O-C-N	-5.29	116.12	122.15
1	A	77	ALA	N-CA-CB	5.29	118.92	110.46
2	l	29	LYS	CA-C-N	5.29	131.63	121.54
2	l	29	LYS	C-N-CA	5.29	131.63	121.54
2	6	127	PRO	N-CA-C	5.29	120.88	113.53
3	M	90	ASN	N-CA-C	-5.29	100.56	108.96
1	f	97	GLN	N-CA-C	5.28	117.95	111.82
2	j	131	ALA	CA-C-N	5.28	130.06	123.14
2	j	131	ALA	C-N-CA	5.28	130.06	123.14
2	5	125	ILE	N-CA-C	-5.28	100.71	108.11
2	n	176	MET	CA-C-O	-5.28	114.13	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	178	VAL	N-CA-C	-5.28	101.38	108.35
1	f	200	ILE	CA-C-N	5.28	129.64	122.19
1	f	200	ILE	C-N-CA	5.28	129.64	122.19
2	i	61	GLY	N-CA-C	5.28	119.03	112.64
1	B	58	LEU	CA-C-O	-5.28	113.04	119.43
1	b	16	SER	N-CA-C	-5.28	98.14	109.81
1	d	107	ILE	CB-CA-C	5.28	119.93	111.32
1	G	117	CYS	CB-CA-C	-5.28	102.02	110.79
2	7	156	THR	N-CA-C	-5.28	102.02	110.10
2	n	67	ALA	CB-CA-C	-5.28	100.86	110.63
3	K	272	LEU	O-C-N	5.28	127.72	122.12
3	L	235	PRO	N-CA-CB	5.28	108.41	102.60
2	i	172	ILE	N-CA-CB	-5.28	102.66	110.58
2	4	139	ALA	O-C-N	-5.28	117.34	122.99
3	I	36	PHE	CA-CB-CG	-5.28	108.52	113.80
2	j	108	VAL	CA-CB-CG1	5.28	119.37	110.40
2	m	200	SER	N-CA-CB	5.28	119.76	110.37
3	K	296	ALA	N-CA-C	-5.28	99.56	110.80
1	A	228	GLU	CA-C-N	5.27	127.87	120.28
1	A	228	GLU	C-N-CA	5.27	127.87	120.28
1	F	143	GLU	N-CA-C	-5.27	99.57	110.80
1	F	150	THR	CA-CB-CG2	-5.27	101.54	110.50
2	1	45	ILE	N-CA-C	-5.27	100.73	108.11
2	i	85	PRO	N-CA-C	5.27	120.48	111.68
2	i	116	ASP	CB-CA-C	5.27	122.18	111.11
3	I	254	ASP	N-CA-C	-5.27	99.57	110.80
1	B	42	CYS	N-CA-CB	5.27	119.55	111.22
2	1	104	PHE	CA-C-N	5.27	125.73	120.14
2	1	104	PHE	C-N-CA	5.27	125.73	120.14
2	m	186	ILE	O-C-N	-5.27	116.93	122.67
3	H	133	GLU	O-C-N	5.27	129.23	123.22
3	M	268	LEU	O-C-N	5.27	128.16	122.15
1	b	150	THR	N-CA-CB	5.27	119.28	110.85
1	C	212	GLY	N-CA-C	-5.27	102.80	111.38
1	d	208	ASN	N-CA-C	-5.27	106.36	114.16
3	H	290	ILE	N-CA-C	-5.27	107.34	112.29
3	K	30	LEU	CA-C-N	5.27	127.34	120.28
3	K	30	LEU	C-N-CA	5.27	127.34	120.28
3	M	294	ASP	N-CA-CB	5.27	117.05	109.78
2	n	63	ALA	CA-C-O	-5.27	115.29	120.82
3	I	353	ALA	N-CA-C	5.27	117.10	111.36
3	L	325	THR	CA-CB-OG1	-5.27	101.70	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	109	VAL	N-CA-C	-5.26	105.40	110.72
1	g	94	ILE	CA-C-N	5.26	127.86	120.28
1	g	94	ILE	C-N-CA	5.26	127.86	120.28
2	m	59	SER	N-CA-CB	5.26	117.75	110.17
3	I	358	ALA	N-CA-CB	5.26	117.86	110.12
3	K	49	ARG	CG-CD-NE	-5.26	100.42	112.00
3	J	196	ALA	CA-C-O	-5.26	114.97	120.55
1	d	68	TYR	CA-CB-CG	-5.26	104.43	113.90
3	I	285	GLY	O-C-N	5.26	129.54	122.70
1	e	173	GLU	CB-CG-CD	-5.26	103.66	112.60
1	d	49	ILE	N-CA-C	-5.26	101.41	108.35
2	m	83	ARG	CA-C-N	5.26	128.14	120.51
2	m	83	ARG	C-N-CA	5.26	128.14	120.51
1	B	98	ILE	CA-C-N	5.26	127.33	120.28
1	B	98	ILE	C-N-CA	5.26	127.33	120.28
1	G	102	THR	CA-CB-OG1	5.26	117.49	109.60
1	G	193	LEU	N-CA-CB	5.26	118.03	110.20
3	I	350	ASP	CA-CB-CG	-5.26	107.34	112.60
1	E	86	ARG	CA-C-N	5.26	127.89	120.42
1	E	86	ARG	C-N-CA	5.26	127.89	120.42
1	f	216	VAL	CA-CB-CG1	5.26	119.34	110.40
3	K	319	GLN	N-CA-CB	5.26	117.85	110.12
3	M	128	TYR	CB-CG-CD1	5.26	128.69	120.80
1	C	217	ASP	O-C-N	5.25	127.77	122.09
3	I	78	VAL	N-CA-C	-5.25	100.32	107.99
1	c	129	VAL	O-C-N	-5.25	117.38	123.00
2	7	159	ILE	N-CA-CB	5.25	116.26	110.53
1	f	28	ARG	N-CA-C	5.25	116.69	111.07
2	4	140	THR	N-CA-C	-5.25	99.61	110.80
2	7	198	GLN	N-CA-CB	5.25	118.84	110.65
2	n	170	ARG	CB-CA-C	5.25	120.75	110.67
2	n	173	TYR	CA-C-N	5.25	127.32	120.28
2	n	173	TYR	C-N-CA	5.25	127.32	120.28
1	F	235	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	C	90	ASP	O-C-N	5.25	127.68	122.12
1	e	23	GLN	CA-C-N	5.25	127.28	120.56
1	e	23	GLN	C-N-CA	5.25	127.28	120.56
2	4	13	THR	CA-C-N	5.25	130.83	121.75
2	4	13	THR	C-N-CA	5.25	130.83	121.75
3	H	37	ILE	N-CA-C	5.25	115.97	110.62
3	H	381	LYS	CA-C-O	-5.25	115.49	121.00
1	d	239	ARG	N-CA-CB	5.25	118.02	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	165	VAL	CA-C-N	5.25	127.58	120.44
2	k	165	VAL	C-N-CA	5.25	127.58	120.44
3	L	32	ASP	O-C-N	5.25	127.68	122.12
2	k	20	LYS	CB-CG-CD	5.25	123.36	111.30
1	C	168	ARG	N-CA-C	5.24	117.67	111.33
1	G	34	GLY	CA-C-O	-5.24	115.28	122.31
2	1	152	GLU	CA-C-N	5.24	127.25	120.44
2	1	152	GLU	C-N-CA	5.24	127.25	120.44
3	J	143	ILE	N-CA-C	-5.24	100.01	107.77
1	A	23	GLN	CA-C-N	5.24	127.86	120.42
1	A	23	GLN	C-N-CA	5.24	127.86	120.42
1	C	52	LYS	N-CA-C	-5.24	106.66	113.16
2	i	110	LEU	CA-C-O	5.24	126.09	120.38
3	J	241	ASP	O-C-N	-5.24	117.19	123.06
2	m	79	ILE	CA-C-N	5.24	127.57	120.44
2	m	79	ILE	C-N-CA	5.24	127.57	120.44
2	m	81	ARG	NE-CZ-NH2	-5.24	114.48	119.20
2	7	69	ILE	O-C-N	5.24	127.18	121.94
3	H	137	GLU	CA-C-O	-5.24	112.94	119.28
3	I	345	GLY	O-C-N	5.24	128.29	122.47
1	C	149	GLU	N-CA-CB	5.24	118.99	110.77
2	i	18	VAL	O-C-N	-5.24	116.75	122.83
2	3	67	ALA	CA-C-N	5.24	127.30	120.28
2	3	67	ALA	C-N-CA	5.24	127.30	120.28
2	j	35	ASN	CA-CB-CG	-5.24	107.36	112.60
2	4	64	GLN	OE1-CD-NE2	5.24	127.84	122.60
3	L	360	MET	CA-C-N	5.24	127.73	120.29
3	L	360	MET	C-N-CA	5.24	127.73	120.29
2	j	202	GLU	CA-C-N	5.24	127.30	120.28
2	j	202	GLU	C-N-CA	5.24	127.30	120.28
1	a	134	VAL	CA-C-N	5.24	130.80	122.74
1	a	134	VAL	C-N-CA	5.24	130.80	122.74
1	G	18	ASP	N-CA-CB	-5.24	102.74	110.49
1	g	218	ASP	CA-C-N	5.24	129.62	122.34
1	g	218	ASP	C-N-CA	5.24	129.62	122.34
2	5	64	GLN	CA-C-O	-5.24	113.95	119.97
3	K	337	LYS	CB-CA-C	-5.24	101.95	110.85
3	J	63	LEU	N-CA-C	-5.24	98.70	108.02
1	D	101	LEU	O-C-N	5.23	128.12	122.15
2	i	143	GLY	N-CA-C	-5.23	106.51	115.61
2	j	153	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	100	ARG	CA-C-N	5.23	127.72	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	C-N-CA	5.23	127.72	120.29
1	a	155	ALA	CA-C-O	5.23	127.89	121.72
1	g	212	GLY	CA-C-O	5.23	126.18	121.47
2	k	132	ILE	N-CA-C	-5.23	100.79	108.11
2	k	212	ARG	CB-CG-CD	5.23	123.33	111.30
2	5	105	PRO	CA-C-N	5.23	130.13	122.39
2	5	105	PRO	C-N-CA	5.23	130.13	122.39
3	I	374	ASP	N-CA-C	5.23	117.06	111.36
1	C	45	GLY	CA-C-O	-5.23	117.30	120.91
3	L	94	TYR	N-CA-C	-5.23	106.29	113.30
1	d	53	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	F	191	LEU	O-C-N	-5.23	115.84	122.27
1	f	94	ILE	CA-C-O	-5.23	115.31	120.85
2	4	196	PHE	N-CA-CB	5.23	120.49	110.82
2	6	75	ASN	OD1-CG-ND2	5.23	127.83	122.60
2	m	199	TYR	CA-C-O	-5.23	115.32	120.70
3	I	221	ARG	CB-CG-CD	5.23	123.33	111.30
3	K	42	ILE	CB-CA-C	-5.23	105.01	112.22
1	A	65	GLU	CA-C-N	5.23	131.52	121.54
1	A	65	GLU	C-N-CA	5.23	131.52	121.54
2	h	104	PHE	CA-C-O	-5.23	116.16	120.71
2	4	72	ILE	CB-CA-C	5.23	118.66	111.97
2	6	71	LYS	O-C-N	5.23	127.66	122.12
3	M	265	MET	CA-C-N	5.23	128.25	120.31
3	M	265	MET	C-N-CA	5.23	128.25	120.31
1	d	168	ARG	CB-CA-C	-5.22	102.61	110.92
2	n	140	THR	N-CA-CB	5.22	119.32	110.49
3	I	283	VAL	CA-C-N	5.22	131.10	121.70
3	I	283	VAL	C-N-CA	5.22	131.10	121.70
3	K	126	MET	CB-CA-C	-5.22	101.80	110.68
1	b	32	LYS	CA-C-N	5.22	127.54	120.38
1	b	32	LYS	C-N-CA	5.22	127.54	120.38
1	C	234	GLU	N-CA-CB	5.22	117.55	109.98
1	E	144	VAL	N-CA-CB	5.22	118.52	111.21
3	H	189	THR	CA-C-O	-5.22	115.34	120.82
2	5	170	ARG	CB-CA-C	-5.22	102.12	110.79
2	j	132	ILE	N-CA-CB	5.22	118.61	111.41
2	j	150	VAL	CA-C-N	5.22	127.27	120.28
2	j	150	VAL	C-N-CA	5.22	127.27	120.28
2	6	31	ALA	N-CA-CB	5.22	119.45	110.68
3	H	155	GLU	CA-C-O	5.22	126.08	120.55
1	a	179	TYR	N-CA-CB	5.22	117.64	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	19	GLY	O-C-N	-5.22	115.76	122.39
1	F	169	ASN	O-C-N	5.22	127.65	122.12
2	k	201	PRO	CA-C-N	5.22	127.58	120.54
2	k	201	PRO	C-N-CA	5.22	127.58	120.54
1	a	168	ARG	CA-C-N	5.21	128.64	120.82
1	a	168	ARG	C-N-CA	5.21	128.64	120.82
1	E	172	THR	CA-C-N	5.21	127.69	120.29
1	E	172	THR	C-N-CA	5.21	127.69	120.29
2	h	199	TYR	N-CA-C	5.21	117.87	111.82
3	M	145	GLY	CA-C-N	5.21	131.08	121.70
3	M	145	GLY	C-N-CA	5.21	131.08	121.70
1	g	95	GLU	CB-CG-CD	5.21	121.46	112.60
2	j	125	ILE	N-CA-C	-5.21	100.97	108.53
3	J	381	LYS	CB-CA-C	-5.21	102.70	110.88
1	b	92	ALA	O-C-N	5.21	128.68	122.27
2	m	73	GLU	CA-C-N	5.21	127.69	120.29
2	m	73	GLU	C-N-CA	5.21	127.69	120.29
3	I	362	ALA	N-CA-C	5.21	116.96	111.28
3	L	191	LEU	CA-C-N	5.21	127.78	120.28
3	L	191	LEU	C-N-CA	5.21	127.78	120.28
3	M	391	ASP	N-CA-C	-5.21	99.70	110.80
1	b	74	ILE	CA-CB-CG1	5.21	119.26	110.40
2	l	117	SER	N-CA-C	-5.21	106.43	112.89
3	H	351	ILE	CA-C-O	5.21	126.37	120.95
3	I	158	GLU	CA-C-N	5.21	126.60	120.09
3	I	158	GLU	C-N-CA	5.21	126.60	120.09
3	M	47	GLU	CB-CG-CD	5.21	121.46	112.60
1	C	90	ASP	CA-C-N	5.21	127.53	120.44
1	C	90	ASP	C-N-CA	5.21	127.53	120.44
1	f	168	ARG	N-CA-C	-5.21	105.50	111.07
2	3	193	GLU	O-C-N	5.21	129.52	122.59
1	A	75	CYS	CA-C-O	-5.21	115.52	121.40
1	b	10	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	186	ASP	N-CA-CB	5.21	117.87	110.16
1	g	104	ASP	CA-CB-CG	5.21	117.81	112.60
2	h	168	ALA	CA-C-O	5.21	125.94	120.42
2	7	132	ILE	CA-C-N	5.21	131.48	121.54
2	7	132	ILE	C-N-CA	5.21	131.48	121.54
3	J	241	ASP	CA-C-N	5.21	131.07	121.70
3	J	241	ASP	C-N-CA	5.21	131.07	121.70
3	J	258	ASP	CA-C-O	-5.21	115.03	120.55
1	a	126	TYR	O-C-N	5.21	129.40	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	150	THR	N-CA-C	-5.21	101.67	109.95
1	D	153	SER	O-C-N	5.21	127.64	122.12
1	f	109	VAL	CB-CA-C	-5.21	105.11	112.14
2	2	212	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	a	98	ILE	N-CA-C	-5.20	105.46	110.72
1	F	43	LYS	N-CA-C	-5.20	106.52	112.92
2	h	201	PRO	CA-C-N	5.20	127.20	120.44
2	h	201	PRO	C-N-CA	5.20	127.20	120.44
3	H	294	ASP	CA-C-O	-5.20	114.81	120.69
1	F	119	PHE	CA-CB-CG	-5.20	108.60	113.80
3	I	19	ASP	CA-C-O	-5.20	114.91	120.42
3	L	317	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	d	112	LEU	CB-CA-C	-5.20	102.01	110.85
1	E	90	ASP	CA-C-N	5.20	127.25	120.28
1	E	90	ASP	C-N-CA	5.20	127.25	120.28
1	E	223	GLU	N-CA-CB	5.20	118.76	110.65
1	F	35	ALA	CA-C-N	5.20	128.49	121.05
1	F	35	ALA	C-N-CA	5.20	128.49	121.05
2	7	89	ALA	CA-C-N	5.20	127.80	120.42
2	7	89	ALA	C-N-CA	5.20	127.80	120.42
3	I	52	ARG	CA-C-N	5.20	127.67	120.29
3	I	52	ARG	C-N-CA	5.20	127.67	120.29
3	K	173	GLU	O-C-N	-5.20	116.57	121.35
3	L	377	LYS	N-CA-CB	5.20	117.86	110.16
3	J	356	THR	CA-C-N	5.20	128.21	120.31
3	J	356	THR	C-N-CA	5.20	128.21	120.31
2	h	212	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	J	132	VAL	O-C-N	-5.20	117.65	123.26
1	C	91	ARG	NE-CZ-NH1	-5.20	116.31	121.50
1	e	22	PHE	CA-C-N	5.20	127.76	120.28
1	e	22	PHE	C-N-CA	5.20	127.76	120.28
1	f	77	ALA	N-CA-C	-5.20	101.64	109.85
1	G	122	GLN	N-CA-CB	5.20	117.85	110.16
2	1	57	ALA	CA-C-O	-5.20	115.24	121.11
2	6	151	LEU	CA-C-O	-5.20	114.91	120.42
3	H	96	ASN	CA-CB-CG	-5.20	107.41	112.60
3	K	337	LYS	CA-C-O	5.20	125.93	120.42
2	l	23	VAL	N-CA-C	-5.19	100.76	108.45
3	H	129	GLY	N-CA-C	-5.19	108.22	114.66
1	c	213	TYR	CA-C-O	5.19	126.88	121.38
3	H	361	PHE	CA-C-N	5.19	127.23	120.28
3	H	361	PHE	C-N-CA	5.19	127.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	123	LYS	O-C-N	-5.19	115.69	122.59
3	J	371	THR	CA-CB-CG2	-5.19	101.68	110.50
1	a	18	ASP	N-CA-C	-5.19	107.12	113.50
1	C	16	SER	CA-C-O	-5.19	115.31	120.96
2	h	171	ALA	O-C-N	-5.19	116.49	122.09
2	6	56	THR	N-CA-C	-5.19	100.58	109.24
3	H	333	ASP	CA-C-N	5.19	128.85	122.37
3	H	333	ASP	C-N-CA	5.19	128.85	122.37
1	a	62	ASP	N-CA-CB	-5.19	102.02	110.42
1	a	187	ASP	CA-CB-CG	5.19	117.79	112.60
1	c	168	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	d	170	ALA	CB-CA-C	-5.19	102.71	110.90
1	f	89	ILE	CA-CB-CG2	-5.19	101.68	110.50
3	I	121	THR	N-CA-C	-5.19	100.58	109.24
1	d	105	GLU	CA-C-N	5.18	125.12	119.78
1	d	105	GLU	C-N-CA	5.18	125.12	119.78
1	d	123	TYR	N-CA-C	5.18	118.86	112.54
1	e	112	LEU	CA-C-N	5.18	127.49	120.44
1	e	112	LEU	C-N-CA	5.18	127.49	120.44
3	K	242	GLU	N-CA-C	-5.18	99.76	110.80
3	M	395	VAL	N-CA-C	-5.18	106.84	113.22
3	J	281	VAL	CB-CA-C	-5.18	105.05	111.32
1	E	174	PHE	CB-CA-C	-5.18	102.75	110.88
2	j	111	LEU	N-CA-C	-5.18	98.80	108.02
3	H	358	ALA	N-CA-C	5.18	116.93	111.28
3	I	102	PRO	CA-C-O	-5.18	115.69	121.23
3	L	263	ARG	NE-CZ-NH1	5.18	126.68	121.50
3	M	127	VAL	N-CA-C	-5.18	98.56	109.34
1	b	110	LYS	CA-C-O	-5.18	114.93	120.42
2	2	21	ASP	CA-CB-CG	5.18	117.78	112.60
3	L	101	LYS	CA-CB-CG	5.18	124.46	114.10
1	b	186	ASP	N-CA-CB	5.18	117.82	110.16
3	H	384	LYS	CA-C-N	5.18	131.75	122.38
3	H	384	LYS	C-N-CA	5.18	131.75	122.38
1	c	217	ASP	N-CA-C	-5.18	106.47	112.89
1	C	207	GLU	CA-C-N	5.17	128.14	120.17
1	C	207	GLU	C-N-CA	5.17	128.14	120.17
1	e	84	ASP	N-CA-C	-5.17	105.72	111.36
1	F	5	GLN	OE1-CD-NE2	5.17	127.77	122.60
2	1	105	PRO	CA-C-O	-5.17	115.55	121.86
2	1	116	ASP	N-CA-C	-5.17	101.60	108.74
3	K	215	TYR	CB-CG-CD2	-5.17	113.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	32	LYS	CG-CD-CE	5.17	123.20	111.30
2	l	188	VAL	CA-C-N	5.17	130.16	122.71
2	l	188	VAL	C-N-CA	5.17	130.16	122.71
1	B	168	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	C	184	SER	CA-C-N	5.17	127.21	120.28
1	C	184	SER	C-N-CA	5.17	127.21	120.28
1	c	100	ARG	CB-CA-C	5.17	120.20	110.63
2	1	165	VAL	CA-C-N	5.17	127.16	120.44
2	1	165	VAL	C-N-CA	5.17	127.16	120.44
2	2	82	GLU	CB-CA-C	5.17	118.66	111.63
2	j	139	ALA	N-CA-CB	5.17	119.23	110.49
2	4	158	GLU	CA-C-N	5.17	128.10	120.91
2	4	158	GLU	C-N-CA	5.17	128.10	120.91
3	L	139	SER	N-CA-C	-5.17	101.84	109.18
3	M	36	PHE	CA-CB-CG	-5.17	108.63	113.80
3	J	235	PRO	O-C-N	-5.17	111.28	121.10
3	J	385	LYS	CA-C-N	5.17	131.42	121.54
3	J	385	LYS	C-N-CA	5.17	131.42	121.54
2	k	136	ASP	CB-CA-C	5.17	120.71	110.42
1	b	54	VAL	CA-C-N	5.17	130.31	120.07
1	b	54	VAL	C-N-CA	5.17	130.31	120.07
2	4	204	VAL	O-C-N	5.17	127.64	121.80
2	k	109	GLN	N-CA-C	-5.17	100.48	108.90
3	L	56	GLU	CA-C-N	5.17	127.16	120.44
3	L	56	GLU	C-N-CA	5.17	127.16	120.44
1	c	11	ALA	CA-C-O	-5.17	115.56	121.40
1	e	156	LEU	CA-C-O	5.17	126.01	120.38
2	k	110	LEU	CA-C-N	5.17	130.05	122.77
2	k	110	LEU	C-N-CA	5.17	130.05	122.77
2	m	180	SER	CA-C-O	5.17	124.88	119.51
3	H	349	ALA	CA-C-O	-5.17	114.94	120.42
3	K	150	ILE	CB-CA-C	-5.17	105.17	112.14
2	3	200	SER	CA-C-O	-5.17	113.84	120.04
2	1	195	GLU	N-CA-C	-5.16	100.88	108.99
3	J	183	PRO	CA-C-O	-5.16	113.07	120.56
1	C	59	LEU	CA-C-O	-5.16	114.80	120.43
2	1	181	ALA	O-C-N	-5.16	116.00	122.35
2	l	30	ARG	CA-C-N	5.16	130.57	122.21
2	l	30	ARG	C-N-CA	5.16	130.57	122.21
1	b	189	MET	O-C-N	5.16	127.39	122.07
2	i	155	PHE	N-CA-CB	5.16	117.54	109.85
2	5	113	GLY	CA-C-O	5.16	127.75	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	77	VAL	CB-CA-C	5.16	119.64	110.71
3	J	313	THR	CA-C-O	-5.16	116.05	121.88
1	B	52	LYS	CA-C-N	5.16	128.15	120.31
1	B	52	LYS	C-N-CA	5.16	128.15	120.31
1	F	28	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	F	40	ILE	N-CA-C	-5.16	100.77	108.46
2	j	63	ALA	CB-CA-C	-5.16	102.75	110.90
1	D	160	LYS	CB-CG-CD	5.16	123.16	111.30
2	j	205	GLU	O-C-N	5.16	128.25	122.22
2	5	72	ILE	CA-C-O	-5.16	115.33	121.05
3	K	340	ALA	CA-C-N	5.16	127.19	120.28
3	K	340	ALA	C-N-CA	5.16	127.19	120.28
1	B	180	ARG	CA-C-N	5.16	131.03	122.73
1	B	180	ARG	C-N-CA	5.16	131.03	122.73
1	d	242	GLU	CA-C-N	5.16	127.19	120.28
1	d	242	GLU	C-N-CA	5.16	127.19	120.28
3	H	84	GLY	CA-C-N	5.16	125.44	119.92
3	H	84	GLY	C-N-CA	5.16	125.44	119.92
3	L	375	PHE	CA-CB-CG	-5.16	108.64	113.80
1	d	64	ILE	CA-CB-CG1	-5.15	101.64	110.40
3	J	136	PRO	CA-C-O	-5.15	115.48	122.08
1	A	27	ALA	CA-C-N	5.15	128.14	120.31
1	A	27	ALA	C-N-CA	5.15	128.14	120.31
1	E	25	GLU	CA-C-N	5.15	129.32	120.72
1	E	25	GLU	C-N-CA	5.15	129.32	120.72
2	k	84	LYS	CA-C-N	5.15	125.16	119.90
2	k	84	LYS	C-N-CA	5.15	125.16	119.90
2	5	52	MET	N-CA-CB	5.15	119.47	110.81
2	6	42	ALA	CA-C-N	5.15	128.39	120.82
2	6	42	ALA	C-N-CA	5.15	128.39	120.82
3	I	271	GLU	CA-C-N	5.15	127.61	120.29
3	I	271	GLU	C-N-CA	5.15	127.61	120.29
1	c	206	PRO	CA-C-N	5.15	130.63	122.60
1	c	206	PRO	C-N-CA	5.15	130.63	122.60
1	f	73	HIS	N-CA-C	-5.15	105.35	113.02
1	f	158	GLU	CA-C-O	-5.15	115.00	120.92
2	1	156	THR	O-C-N	-5.15	116.56	121.20
3	H	40	GLU	N-CA-CB	5.15	117.69	110.12
3	K	210	GLU	N-CA-C	-5.15	106.68	113.17
3	L	305	ARG	N-CA-C	-5.15	100.13	108.52
2	i	86	THR	CA-C-N	5.15	127.73	120.42
2	i	86	THR	C-N-CA	5.15	127.73	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	125	ILE	CA-CB-CG2	-5.15	101.75	110.50
1	b	120	LYS	CB-CA-C	-5.15	102.10	110.85
1	g	80	GLY	CA-C-O	-5.15	116.26	121.30
2	l	186	ILE	CA-CB-CG1	5.15	119.15	110.40
2	6	28	GLU	CB-CA-C	5.15	118.02	109.53
1	A	126	TYR	CB-CG-CD2	5.14	128.52	120.80
1	F	103	TYR	CA-C-N	5.14	129.43	122.07
1	F	103	TYR	C-N-CA	5.14	129.43	122.07
1	f	112	LEU	CA-C-N	5.14	127.44	120.44
1	f	112	LEU	C-N-CA	5.14	127.44	120.44
2	k	102	ARG	NE-CZ-NH1	-5.14	116.36	121.50
2	l	30	ARG	N-CA-CB	5.14	119.18	110.49
3	J	107	ALA	CA-C-O	-5.14	114.77	120.38
2	i	106	TYR	CB-CG-CD2	-5.14	113.08	120.80
2	5	212	ARG	CA-C-O	5.14	127.86	120.51
3	I	77	VAL	CB-CA-C	-5.14	102.96	110.62
3	I	200	ARG	CB-CA-C	5.14	119.62	112.11
1	A	58	LEU	N-CA-C	-5.14	105.37	111.69
1	B	81	LEU	N-CA-CB	5.14	117.63	109.71
1	D	6	MET	CG-SD-CE	-5.14	89.59	100.90
2	3	153	ASP	CB-CA-C	-5.14	102.78	110.90
2	4	189	VAL	CB-CA-C	-5.14	102.16	110.28
2	n	163	GLU	CB-CA-C	-5.14	102.11	110.85
1	E	189	MET	O-C-N	5.14	128.01	122.15
2	i	126	ASP	CA-C-N	5.14	124.80	119.56
2	i	126	ASP	C-N-CA	5.14	124.80	119.56
3	I	303	PHE	N-CA-CB	5.14	119.18	110.49
3	L	397	PHE	N-CA-C	-5.14	107.04	113.72
1	A	99	ASN	CA-C-N	5.14	128.12	120.31
1	A	99	ASN	C-N-CA	5.14	128.12	120.31
1	F	184	SER	N-CA-CB	5.14	117.47	110.38
2	k	150	VAL	CA-C-N	5.14	127.58	120.29
2	k	150	VAL	C-N-CA	5.14	127.58	120.29
3	L	81	SER	CA-CB-OG	5.14	121.38	111.10
1	b	218	ASP	N-CA-C	-5.14	104.64	112.04
2	6	143	GLY	N-CA-C	-5.14	107.09	115.46
2	1	191	ILE	CA-CB-CG1	5.13	119.13	110.40
2	7	75	ASN	OD1-CG-ND2	-5.13	117.47	122.60
3	I	15	LYS	N-CA-C	5.13	116.88	111.28
3	I	395	VAL	CA-C-O	5.13	126.26	119.53
3	K	110	GLN	O-C-N	5.13	127.56	122.12
1	A	102	THR	CA-C-O	-5.13	113.40	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	44	LYS	N-CA-C	-5.13	99.87	110.80
3	J	371	THR	CB-CA-C	-5.13	107.98	114.40
1	b	194	VAL	N-CA-CB	5.13	117.52	110.54
1	F	231	PRO	N-CA-CB	5.13	108.97	103.33
1	g	27	ALA	CA-C-N	5.13	128.11	120.31
1	g	27	ALA	C-N-CA	5.13	128.11	120.31
1	g	137	LEU	N-CA-C	-5.13	100.87	109.24
1	g	221	PHE	N-CA-CB	5.13	119.16	110.49
2	l	17	LEU	O-C-N	-5.13	117.53	123.33
1	c	77	ALA	O-C-N	-5.13	116.48	123.15
2	i	87	VAL	CB-CA-C	-5.13	105.14	112.22
3	J	267	GLN	CA-C-N	5.13	127.11	120.44
3	J	267	GLN	C-N-CA	5.13	127.11	120.44
1	B	185	PHE	O-C-N	5.13	127.35	122.07
1	b	75	CYS	N-CA-C	-5.13	101.27	109.07
1	D	144	VAL	CA-C-O	5.13	122.69	119.51
1	F	53	ARG	CD-NE-CZ	-5.13	117.22	124.40
2	j	29	LYS	CB-CA-C	5.13	118.21	109.24
2	4	66	LEU	CA-C-N	5.13	127.15	120.28
2	4	66	LEU	C-N-CA	5.13	127.15	120.28
2	n	159	ILE	CA-C-N	5.13	128.29	121.01
2	n	159	ILE	C-N-CA	5.13	128.29	121.01
3	H	220	ALA	N-CA-CB	5.13	117.50	110.07
3	L	302	ARG	CA-C-O	-5.13	113.08	118.77
3	M	211	PHE	CA-CB-CG	-5.13	108.67	113.80
3	J	368	ALA	N-CA-C	-5.13	106.99	114.12
1	D	41	LYS	CB-CA-C	5.13	118.94	109.71
2	5	212	ARG	NE-CZ-NH1	5.13	126.63	121.50
2	l	77	TYR	CA-C-N	5.13	127.11	120.44
2	l	77	TYR	C-N-CA	5.13	127.11	120.44
3	L	292	ILE	CA-C-N	5.13	132.38	122.07
3	L	292	ILE	C-N-CA	5.13	132.38	122.07
3	J	299	ARG	CA-C-N	5.13	125.12	119.89
3	J	299	ARG	C-N-CA	5.13	125.12	119.89
1	F	236	ALA	N-CA-C	5.12	116.95	111.36
2	i	28	GLU	CA-C-N	5.12	127.57	120.29
2	i	28	GLU	C-N-CA	5.12	127.57	120.29
1	e	187	ASP	CA-C-N	5.12	127.66	120.28
1	e	187	ASP	C-N-CA	5.12	127.66	120.28
2	i	144	SER	CA-C-N	5.12	127.10	120.44
2	i	144	SER	C-N-CA	5.12	127.10	120.44
2	4	112	ILE	N-CA-C	-5.12	101.10	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	l	121	SER	N-CA-CB	5.12	119.35	111.56
2	7	87	VAL	CA-C-N	5.12	127.15	120.28
2	7	87	VAL	C-N-CA	5.12	127.15	120.28
2	1	68	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	7	20	LYS	N-CA-C	-5.12	106.87	113.02
3	I	317	ARG	NH1-CZ-NH2	-5.12	112.64	119.30
3	J	255	THR	N-CA-C	-5.12	101.47	108.38
1	f	31	VAL	CA-C-O	5.12	125.78	119.58
2	5	14	THR	N-CA-C	-5.12	101.51	109.24
2	5	73	GLU	CA-C-N	5.12	127.40	120.44
2	5	73	GLU	C-N-CA	5.12	127.40	120.44
2	n	191	ILE	N-CA-CB	5.12	118.35	111.90
3	J	159	LEU	CA-C-O	-5.12	113.37	118.34
2	h	47	GLN	CA-C-N	5.12	128.06	120.74
2	h	47	GLN	C-N-CA	5.12	128.06	120.74
2	l	48	ILE	N-CA-C	-5.12	105.13	112.35
3	M	132	VAL	N-CA-CB	5.12	118.29	111.64
3	J	371	THR	O-C-N	-5.12	117.65	123.13
1	D	225	SER	N-CA-CB	5.12	116.95	110.04
2	3	31	ALA	N-CA-C	-5.12	102.49	109.71
3	M	380	GLU	CA-C-N	5.12	127.40	120.44
3	M	380	GLU	C-N-CA	5.12	127.40	120.44
1	E	158	GLU	N-CA-C	-5.12	101.37	109.76
1	G	215	LYS	O-C-N	-5.12	117.33	123.06
2	5	113	GLY	N-CA-C	-5.12	101.15	110.97
3	H	175	PRO	N-CA-CB	5.12	108.65	102.72
3	I	226	VAL	CB-CA-C	-5.12	105.16	112.22
2	7	141	GLY	N-CA-C	-5.11	103.13	110.60
3	L	205	ARG	CA-C-O	5.11	125.93	120.46
1	a	120	LYS	O-C-N	5.11	127.98	122.15
1	B	172	THR	N-CA-CB	5.11	117.42	110.01
3	I	152	GLU	CA-C-N	5.11	127.46	120.46
3	I	152	GLU	C-N-CA	5.11	127.46	120.46
1	A	208	ASN	CA-C-N	5.11	129.59	122.23
1	A	208	ASN	C-N-CA	5.11	129.59	122.23
1	E	120	LYS	CA-C-O	5.11	126.19	120.82
2	1	40	LYS	N-CA-C	-5.11	106.29	112.88
3	M	56	GLU	CB-CG-CD	-5.11	103.91	112.60
1	c	198	LEU	CA-C-N	5.11	127.13	120.28
1	c	198	LEU	C-N-CA	5.11	127.13	120.28
1	f	192	GLY	CA-C-N	5.11	127.54	120.29
1	f	192	GLY	C-N-CA	5.11	127.54	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	245	LYS	N-CA-C	-5.11	107.02	114.12
1	f	139	ALA	N-CA-C	-5.11	100.58	108.90
2	1	169	VAL	O-C-N	5.11	127.09	121.83
2	h	53	ALA	N-CA-C	-5.11	102.00	109.81
2	2	205	GLU	N-CA-C	5.11	118.98	112.34
3	M	335	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	67	ILE	CB-CA-C	5.11	119.66	111.29
1	a	122	GLN	OE1-CD-NE2	-5.11	117.50	122.60
1	c	38	ILE	N-CA-C	-5.11	100.99	108.85
1	c	87	VAL	N-CA-C	5.11	115.32	110.42
1	E	105	GLU	CA-C-N	5.11	125.11	119.90
1	E	105	GLU	C-N-CA	5.11	125.11	119.90
2	4	143	GLY	CA-C-N	5.11	127.63	120.28
2	4	143	GLY	C-N-CA	5.11	127.63	120.28
3	M	261	VAL	N-CA-CB	5.11	117.48	110.54
1	B	62	ASP	N-CA-C	-5.10	106.64	112.92
2	3	72	ILE	O-C-N	-5.10	116.57	121.83
2	j	88	ARG	NE-CZ-NH1	-5.10	116.40	121.50
3	L	17	GLU	CA-C-N	5.10	127.38	120.44
3	L	17	GLU	C-N-CA	5.10	127.38	120.44
1	e	167	GLY	CA-C-N	5.10	131.29	121.54
1	e	167	GLY	C-N-CA	5.10	131.29	121.54
2	h	126	ASP	N-CA-C	-5.10	102.75	110.50
2	4	178	ARG	NH1-CZ-NH2	5.10	125.93	119.30
2	k	86	THR	N-CA-C	-5.10	101.61	109.52
3	M	176	LYS	O-C-N	5.10	128.85	122.22
2	3	102	ARG	CA-C-N	5.10	127.53	120.29
2	3	102	ARG	C-N-CA	5.10	127.53	120.29
2	n	154	ARG	CD-NE-CZ	-5.10	117.26	124.40
3	K	324	HIS	ND1-CE1-NE2	5.10	113.50	108.40
1	c	10	ARG	CD-NE-CZ	-5.10	117.26	124.40
2	j	99	ASN	CA-CB-CG	-5.10	107.50	112.60
3	I	83	THR	CA-C-N	-5.10	113.86	121.87
3	I	83	THR	C-N-CA	-5.10	113.86	121.87
1	b	189	MET	N-CA-C	5.10	116.53	111.07
1	C	17	PRO	N-CA-CB	5.10	108.29	103.19
1	d	176	GLU	CB-CG-CD	-5.10	103.93	112.60
1	E	214	VAL	CA-C-O	5.10	125.76	120.36
1	G	99	ASN	CA-C-N	5.10	127.11	120.28
1	G	99	ASN	C-N-CA	5.10	127.11	120.28
3	H	38	GLU	CA-C-N	5.10	127.53	120.29
3	H	38	GLU	C-N-CA	5.10	127.53	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	259	ARG	NE-CZ-NH1	-5.10	116.40	121.50
3	J	235	PRO	N-CA-CB	5.10	108.21	102.60
2	i	155	PHE	CA-CB-CG	5.10	118.90	113.80
2	5	101	TYR	CB-CG-CD1	-5.10	113.16	120.80
3	L	288	ASN	CB-CA-C	-5.10	102.88	110.88
3	M	271	GLU	CA-C-O	-5.10	114.11	119.97
3	M	380	GLU	CB-CG-CD	-5.10	103.94	112.60
1	D	66	LYS	N-CA-C	-5.09	108.09	114.56
1	F	36	THR	CA-C-N	5.09	130.91	121.94
1	F	36	THR	C-N-CA	5.09	130.91	121.94
2	3	116	ASP	CB-CA-C	5.09	120.39	110.30
2	k	14	THR	CA-CB-OG1	5.09	117.24	109.60
3	J	188	LYS	N-CA-C	-5.09	105.91	111.82
1	a	187	ASP	CA-C-O	5.09	125.95	120.55
2	h	192	THR	OG1-CB-CG2	5.09	119.49	109.30
1	c	85	ALA	N-CA-C	5.09	116.52	111.07
2	3	136	ASP	O-C-N	5.09	129.36	122.59
2	5	36	PHE	CA-CB-CG	5.09	118.89	113.80
2	n	23	VAL	N-CA-C	-5.09	100.56	108.81
3	M	13	LEU	CA-C-N	5.09	127.10	120.28
3	M	13	LEU	C-N-CA	5.09	127.10	120.28
3	M	264	THR	N-CA-C	5.09	117.73	111.82
1	F	63	THR	N-CA-CB	5.09	119.09	110.69
1	G	159	TYR	CB-CG-CD1	-5.09	113.17	120.80
2	3	43	LYS	O-C-N	-5.09	117.01	123.17
2	4	37	ILE	CA-CB-CG2	-5.09	101.85	110.50
2	k	126	ASP	CA-CB-CG	-5.09	107.51	112.60
2	5	110	LEU	CA-C-O	-5.09	115.49	121.44
2	m	125	ILE	CA-C-O	5.09	125.73	120.39
3	H	19	ASP	N-CA-CB	5.09	118.17	110.28
3	H	121	THR	CA-C-O	-5.09	113.23	120.51
3	L	265	MET	CA-C-O	-5.09	114.35	120.10
3	J	358	ALA	CA-C-O	-5.09	115.02	120.42
1	D	221	PHE	CB-CG-CD1	5.09	129.35	120.70
2	h	55	THR	N-CA-C	-5.09	101.11	109.40
2	i	55	THR	CA-C-N	5.09	130.31	122.93
2	i	55	THR	C-N-CA	5.09	130.31	122.93
3	I	42	ILE	O-C-N	5.09	127.07	121.83
3	L	335	ASP	N-CA-C	-5.09	98.96	108.02
3	M	258	ASP	CA-C-N	5.09	128.04	120.31
3	M	258	ASP	C-N-CA	5.09	128.04	120.31
1	B	213	TYR	O-C-N	5.09	128.86	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	68	TYR	N-CA-C	-5.09	101.40	109.59
1	d	73	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
1	g	49	ILE	CA-CB-CG1	5.09	119.05	110.40
2	1	196	PHE	CA-CB-CG	-5.09	108.71	113.80
2	6	94	THR	CA-CB-OG1	5.09	117.23	109.60
3	L	148	VAL	CA-C-O	-5.09	115.66	120.95
3	J	170	VAL	CA-C-N	5.09	130.59	122.25
3	J	170	VAL	C-N-CA	5.09	130.59	122.25
1	D	151	ASP	N-CA-C	-5.08	101.28	109.82
1	F	32	LYS	CA-C-N	5.08	127.51	120.29
1	F	32	LYS	C-N-CA	5.08	127.51	120.29
2	m	156	THR	N-CA-C	-5.08	100.24	109.09
3	H	367	ARG	N-CA-C	-5.08	100.73	108.76
3	L	29	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	d	62	ASP	N-CA-C	-5.08	106.32	112.88
2	6	162	ASP	CA-CB-CG	-5.08	107.52	112.60
2	m	53	ALA	CA-C-O	-5.08	115.84	121.33
3	H	280	ASP	N-CA-C	-5.08	99.97	110.80
3	I	189	THR	CA-CB-CG2	5.08	119.14	110.50
3	M	390	PRO	CA-C-O	-5.08	115.66	121.86
3	J	390	PRO	CA-C-N	5.08	128.92	120.94
3	J	390	PRO	C-N-CA	5.08	128.92	120.94
1	B	31	VAL	CB-CA-C	-5.08	105.21	112.22
1	g	242	GLU	CB-CA-C	-5.08	102.35	110.79
2	3	63	ALA	N-CA-CB	5.08	117.38	110.01
2	4	162	ASP	N-CA-CB	5.08	117.59	110.12
2	n	97	LEU	N-CA-CB	5.08	117.44	110.07
2	n	107	LEU	N-CA-C	-5.08	99.98	110.80
3	K	103	GLY	CA-C-N	5.08	128.76	121.50
3	K	103	GLY	C-N-CA	5.08	128.76	121.50
1	C	92	ALA	CB-CA-C	-5.08	102.36	110.79
1	c	137	LEU	N-CA-C	-5.08	100.01	108.34
1	d	166	MET	O-C-N	5.08	127.94	122.15
1	f	193	LEU	CA-C-N	5.08	127.42	120.46
1	f	193	LEU	C-N-CA	5.08	127.42	120.46
1	C	124	THR	CA-C-O	5.08	125.17	119.18
1	d	33	ARG	N-CA-C	-5.08	106.94	113.23
2	1	31	ALA	N-CA-CB	5.08	118.55	110.84
2	h	73	GLU	CA-CB-CG	-5.08	103.95	114.10
2	j	206	GLN	N-CA-C	-5.08	105.83	111.36
2	l	53	ALA	O-C-N	5.08	129.89	122.94
2	6	99	ASN	O-C-N	5.08	127.94	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	265	MET	CA-C-O	5.08	125.93	120.70
3	K	282	LYS	O-C-N	5.08	129.05	123.16
1	a	25	GLU	CA-C-N	5.07	127.08	120.28
1	a	25	GLU	C-N-CA	5.07	127.08	120.28
1	B	147	LEU	CA-C-O	5.07	126.52	120.28
1	F	173	GLU	CB-CG-CD	5.07	121.23	112.60
2	l	80	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	e	58	LEU	CA-C-N	5.07	128.05	120.95
1	e	58	LEU	C-N-CA	5.07	128.05	120.95
2	1	88	ARG	CD-NE-CZ	-5.07	117.30	124.40
2	4	80	ARG	NE-CZ-NH1	-5.07	116.43	121.50
2	n	199	TYR	CB-CG-CD1	5.07	128.41	120.80
3	K	220	ALA	N-CA-C	5.07	117.93	111.69
3	K	305	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	D	105	GLU	CA-C-N	5.07	126.18	119.84
1	D	105	GLU	C-N-CA	5.07	126.18	119.84
1	g	72	GLU	N-CA-C	-5.07	106.94	112.72
2	3	55	THR	CA-C-N	5.07	131.09	122.37
2	3	55	THR	C-N-CA	5.07	131.09	122.37
3	M	237	ILE	N-CA-C	-5.07	100.82	108.12
2	h	64	GLN	OE1-CD-NE2	5.07	127.67	122.60
3	J	34	LYS	N-CA-C	-5.07	107.05	113.18
1	a	154	GLY	N-CA-C	-5.07	107.82	115.32
1	D	240	ILE	O-C-N	5.07	126.88	121.91
1	d	87	VAL	N-CA-C	5.07	115.84	110.72
3	I	165	GLU	O-C-N	-5.07	115.80	122.39
3	L	211	PHE	CB-CG-CD2	5.07	129.32	120.70
3	J	272	LEU	N-CA-CB	5.07	117.57	110.12
1	c	150	THR	N-CA-CB	5.07	118.52	110.57
1	D	98	ILE	O-C-N	-5.07	116.96	121.87
1	e	233	VAL	CA-CB-CG2	-5.07	101.79	110.40
2	j	15	VAL	O-C-N	5.07	128.66	123.04
2	m	58	GLY	O-C-N	-5.07	116.15	123.39
3	H	192	ALA	CA-C-O	-5.07	115.05	120.42
3	L	37	ILE	CA-C-N	5.07	127.48	120.29
3	L	37	ILE	C-N-CA	5.07	127.48	120.29
3	M	36	PHE	CA-C-N	5.07	126.94	120.56
3	M	36	PHE	C-N-CA	5.07	126.94	120.56
1	D	232	TYR	CA-CB-CG	-5.06	104.78	113.90
3	J	38	GLU	O-C-N	-5.06	116.75	122.12
3	J	294	ASP	CA-CB-CG	-5.06	107.54	112.60
1	e	105	GLU	N-CA-C	-5.06	101.58	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	235	ARG	CA-C-N	5.06	127.06	120.28
1	f	235	ARG	C-N-CA	5.06	127.06	120.28
1	g	104	ASP	N-CA-C	-5.06	106.68	112.86
3	I	377	LYS	CA-C-N	5.06	127.06	120.28
3	I	377	LYS	C-N-CA	5.06	127.06	120.28
1	A	192	GLY	CA-C-O	-5.06	115.30	120.66
1	c	191	LEU	O-C-N	5.06	127.48	122.12
1	F	224	VAL	CA-CB-CG2	-5.06	101.80	110.40
2	l	31	ALA	CA-C-O	5.06	127.12	121.40
1	e	39	GLY	CA-C-N	5.06	129.97	122.94
1	e	39	GLY	C-N-CA	5.06	129.97	122.94
2	k	139	ALA	N-CA-C	-5.06	100.02	110.80
3	K	44	TYR	CA-C-N	5.06	127.06	120.28
3	K	44	TYR	C-N-CA	5.06	127.06	120.28
3	K	352	LYS	CA-C-O	-5.06	115.19	120.55
3	L	328	MET	N-CA-C	5.06	117.21	109.07
3	J	128	TYR	N-CA-C	-5.06	102.03	110.17
1	G	8	TYR	CA-CB-CG	-5.06	104.80	113.90
2	k	69	ILE	N-CA-C	5.06	115.28	110.53
3	I	282	LYS	N-CA-CB	5.06	119.09	110.50
3	K	350	ASP	O-C-N	5.06	127.91	122.15
1	d	129	VAL	CG1-CB-CG2	5.05	121.92	110.80
2	l	57	ALA	N-CA-C	-5.05	100.80	109.24
2	7	47	GLN	N-CA-C	-5.05	99.56	108.20
3	H	221	ARG	N-CA-C	5.05	119.71	111.37
3	I	332	GLU	N-CA-C	-5.05	106.42	112.59
3	K	259	ARG	CA-C-N	5.05	127.05	120.28
3	K	259	ARG	C-N-CA	5.05	127.05	120.28
3	J	167	PHE	CB-CA-C	-5.05	100.50	110.11
1	B	163	ALA	CA-C-N	5.05	129.99	122.71
1	B	163	ALA	C-N-CA	5.05	129.99	122.71
1	E	109	VAL	CA-C-N	5.05	127.01	120.44
1	E	109	VAL	C-N-CA	5.05	127.01	120.44
1	g	134	VAL	CA-CB-CG1	5.05	118.99	110.40
3	K	28	ARG	N-CA-CB	-5.05	102.68	110.01
1	B	63	THR	CA-C-N	5.05	131.06	121.97
1	B	63	THR	C-N-CA	5.05	131.06	121.97
1	G	175	PHE	CA-CB-CG	5.05	118.85	113.80
2	h	114	GLY	N-CA-C	-5.05	103.76	110.58
2	i	192	THR	OG1-CB-CG2	5.05	119.40	109.30
2	l	136	ASP	N-CA-CB	5.05	119.02	110.49
3	I	70	ASP	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	156	THR	N-CA-C	-5.05	100.05	108.23
1	b	173	GLU	CA-C-O	5.05	125.77	120.42
1	C	224	VAL	CB-CA-C	-5.05	105.18	111.08
3	K	209	SER	N-CA-C	-5.05	106.63	112.89
3	L	156	ALA	CA-C-O	5.05	125.78	119.97
2	i	161	VAL	CA-C-O	5.04	125.92	120.47
2	j	136	ASP	CA-CB-CG	5.04	117.64	112.60
3	J	41	ARG	CB-CG-CD	5.04	122.90	111.30
1	a	198	LEU	CA-C-N	5.04	127.00	120.44
1	a	198	LEU	C-N-CA	5.04	127.00	120.44
1	b	130	ARG	CA-C-O	-5.04	115.47	120.66
1	C	121	GLN	OE1-CD-NE2	5.04	127.64	122.60
2	j	112	ILE	N-CA-C	-5.04	100.39	107.75
2	4	14	THR	O-C-N	5.04	129.00	123.25
2	n	108	VAL	CA-C-O	-5.04	116.00	121.19
3	H	151	GLU	N-CA-CB	5.04	117.53	110.12
3	H	350	ASP	CA-CB-CG	5.04	117.64	112.60
3	J	379	ILE	CA-C-N	5.04	127.00	120.44
3	J	379	ILE	C-N-CA	5.04	127.00	120.44
1	c	196	MET	CA-C-N	5.04	125.69	119.99
1	c	196	MET	C-N-CA	5.04	125.69	119.99
2	4	55	THR	N-CA-C	-5.04	101.71	109.52
2	k	109	GLN	OE1-CD-NE2	5.04	127.64	122.60
2	6	201	PRO	CA-C-N	5.04	127.35	120.54
2	6	201	PRO	C-N-CA	5.04	127.35	120.54
1	b	89	ILE	CA-CB-CG1	5.04	118.97	110.40
1	C	63	THR	CA-C-N	5.04	128.87	122.37
1	C	63	THR	C-N-CA	5.04	128.87	122.37
1	D	229	LEU	CB-CA-C	-5.04	102.94	110.90
2	l	212	ARG	CA-C-O	-5.04	115.53	120.82
3	K	182	GLY	O-C-N	-5.04	116.73	121.77
1	G	164	ILE	N-CA-C	-5.04	101.03	108.23
1	G	220	THR	N-CA-CB	5.04	119.07	110.71
2	1	86	THR	CB-CA-C	5.04	118.65	109.83
2	h	50	ASP	CB-CA-C	-5.04	105.02	111.22
3	H	171	GLY	CA-C-N	5.04	131.04	121.97
3	H	171	GLY	C-N-CA	5.04	131.04	121.97
3	M	319	GLN	CA-C-N	5.04	127.58	120.42
3	M	319	GLN	C-N-CA	5.04	127.58	120.42
1	d	24	VAL	O-C-N	5.04	127.14	121.90
1	e	113	ALA	N-CA-C	-5.04	105.70	111.14
1	F	241	ARG	NH1-CZ-NH2	5.04	125.85	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	52	MET	CG-SD-CE	-5.04	89.82	100.90
3	I	278	ARG	N-CA-CB	5.04	117.37	110.07
1	C	100	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
3	K	170	VAL	N-CA-C	-5.04	105.80	110.53
3	K	262	GLN	CA-C-N	5.04	126.99	120.44
3	K	262	GLN	C-N-CA	5.04	126.99	120.44
3	J	397	PHE	N-CA-C	-5.04	101.03	109.24
3	H	130	PHE	N-CA-CB	5.03	117.61	110.16
3	K	94	TYR	N-CA-C	-5.03	106.56	113.30
1	D	59	LEU	N-CA-C	-5.03	100.96	108.96
1	f	69	LYS	CA-C-N	5.03	129.49	121.34
1	f	69	LYS	C-N-CA	5.03	129.49	121.34
3	J	191	LEU	N-CA-C	5.03	116.76	111.28
2	6	70	ILE	CA-C-N	5.03	127.02	120.28
2	6	70	ILE	C-N-CA	5.03	127.02	120.28
1	C	183	LEU	N-CA-C	-5.03	104.04	110.53
1	D	49	ILE	CA-C-O	-5.03	114.79	120.67
1	d	239	ARG	CD-NE-CZ	-5.03	117.36	124.40
3	H	335	ASP	N-CA-C	-5.03	99.22	108.02
3	K	125	PRO	O-C-N	5.03	128.71	122.22
2	j	90	ILE	N-CA-CB	-5.03	101.45	110.95
2	5	118	GLU	CB-CA-C	-5.03	100.07	109.72
2	m	181	ALA	CA-C-O	5.03	124.58	119.05
3	L	250	ARG	CA-C-O	5.03	127.14	121.51
3	L	255	THR	CA-CB-OG1	5.03	117.14	109.60
3	J	227	PHE	CB-CG-CD1	5.03	129.24	120.70
1	E	112	LEU	CA-C-N	5.02	127.01	120.28
1	E	112	LEU	C-N-CA	5.02	127.01	120.28
1	F	68	TYR	CA-CB-CG	-5.02	104.86	113.90
2	6	94	THR	O-C-N	5.02	127.44	122.12
1	B	190	VAL	CB-CA-C	-5.02	105.29	112.22
1	b	162	THR	CA-CB-OG1	5.02	117.13	109.60
1	b	169	ASN	O-C-N	-5.02	116.80	122.12
2	n	84	LYS	CB-CA-C	-5.02	101.39	109.67
3	L	280	ASP	N-CA-C	-5.02	104.67	111.55
3	J	116	VAL	N-CA-CB	5.02	118.34	110.31
1	A	237	ASN	CA-C-O	-5.02	114.43	120.10
1	d	172	THR	CA-CB-CG2	5.02	119.03	110.50
1	F	226	PRO	CA-C-N	5.02	127.41	120.29
1	F	226	PRO	C-N-CA	5.02	127.41	120.29
1	f	120	LYS	O-C-N	-5.02	116.43	122.15
3	L	143	ILE	N-CA-C	-5.02	101.24	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	93	GLN	N-CA-CB	5.02	118.97	110.49
1	C	172	THR	CA-C-N	5.02	127.41	120.29
1	C	172	THR	C-N-CA	5.02	127.41	120.29
1	d	146	LYS	CA-C-O	5.02	126.62	120.60
2	2	103	TYR	N-CA-CB	5.02	118.19	110.61
2	n	126	ASP	O-C-N	-5.02	115.47	121.39
1	C	205	VAL	CB-CA-C	-5.01	102.23	111.36
1	D	89	ILE	CA-C-N	5.01	127.26	120.44
1	D	89	ILE	C-N-CA	5.01	127.26	120.44
3	L	341	ARG	CA-CB-CG	-5.01	104.07	114.10
1	A	193	LEU	CA-C-N	5.01	127.33	120.46
1	A	193	LEU	C-N-CA	5.01	127.33	120.46
1	F	14	VAL	CA-C-O	5.01	125.65	120.39
2	6	20	LYS	N-CA-CB	5.01	120.30	110.88
1	f	126	TYR	CB-CG-CD1	5.01	128.32	120.80
2	3	96	ASN	CA-CB-CG	5.01	117.61	112.60
2	j	155	PHE	CA-CB-CG	-5.01	108.79	113.80
2	n	208	LEU	N-CA-CB	5.01	118.11	110.44
3	M	220	ALA	N-CA-C	-5.01	105.53	111.69
3	M	370	VAL	CA-C-O	5.01	126.55	120.74
1	A	91	ARG	CA-C-O	-5.01	114.21	119.97
1	a	106	PRO	CB-CA-C	-5.01	105.20	111.71
1	g	16	SER	N-CA-C	-5.01	100.71	109.48
2	6	201	PRO	N-CA-C	5.01	122.79	112.47
2	m	92	THR	CA-CB-OG1	5.01	117.11	109.60
1	e	190	VAL	CA-C-N	5.01	126.99	120.28
1	e	190	VAL	C-N-CA	5.01	126.99	120.28
2	4	196	PHE	N-CA-C	-5.01	96.01	107.48
3	I	196	ALA	N-CA-CB	5.01	117.48	110.12
3	K	223	VAL	CA-CB-CG1	-5.01	101.89	110.40
3	K	384	LYS	CB-CA-C	-5.01	102.48	110.79
3	M	181	TYR	CB-CG-CD2	-5.01	113.29	120.80
3	J	46	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	c	118	ASP	CB-CA-C	-5.00	102.17	110.68
1	e	12	ILE	CA-C-N	5.00	129.47	121.66
1	e	12	ILE	C-N-CA	5.00	129.47	121.66
1	G	217	ASP	CA-CB-CG	-5.00	107.59	112.60
2	k	81	ARG	CA-C-N	5.00	129.95	122.74
2	k	81	ARG	C-N-CA	5.00	129.95	122.74
2	l	151	LEU	CA-C-N	5.00	127.40	120.29
2	l	151	LEU	C-N-CA	5.00	127.40	120.29
2	m	124	SER	N-CA-C	-5.00	101.08	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	SER	CA-C-N	5.00	125.07	119.87
1	B	16	SER	C-N-CA	5.00	125.07	119.87
1	e	162	THR	CA-CB-OG1	5.00	117.10	109.60
1	F	22	PHE	N-CA-C	5.00	117.62	111.82
2	l	100	SER	N-CA-CB	5.00	119.15	110.39
3	L	248	ALA	CA-C-O	-5.00	115.30	120.70
3	L	288	ASN	CA-CB-CG	5.00	117.60	112.60
1	A	23	GLN	O-C-N	5.00	127.42	122.12
1	a	86	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	C	61	ALA	N-CA-C	5.00	117.62	111.82
2	l	38	ALA	N-CA-C	-5.00	108.45	114.75
3	H	227	PHE	CA-C-O	5.00	125.72	120.42
3	K	130	PHE	CB-CG-CD2	-5.00	112.20	120.70
3	L	9	LEU	CA-C-N	5.00	127.48	120.28
3	L	9	LEU	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (321) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	101	TYR	Sidechain
2	1	103	TYR	Sidechain
2	1	106	TYR	Sidechain
2	1	123	TYR	Sidechain
2	1	170	ARG	Sidechain
2	1	199	TYR	Sidechain
2	1	46	TYR	Sidechain
2	1	81	ARG	Sidechain
2	2	106	TYR	Sidechain
2	2	123	TYR	Sidechain
2	2	139	ALA	Peptide
2	2	148	TYR	Sidechain
2	2	178	ARG	Sidechain
2	2	197	TYR	Sidechain
2	2	212	ARG	Sidechain
2	3	102	ARG	Sidechain
2	3	106	TYR	Sidechain
2	3	197	TYR	Sidechain
2	3	51	ARG	Sidechain
2	3	83	ARG	Sidechain
2	4	101	TYR	Sidechain
2	4	103	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	4	106	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	68	ARG	Sidechain
2	4	88	ARG	Sidechain
2	5	101	TYR	Sidechain
2	5	103	TYR	Sidechain
2	5	132	ILE	Peptide
2	5	170	ARG	Sidechain
2	5	173	TYR	Sidechain
2	5	51	ARG	Sidechain
2	5	77	TYR	Sidechain
2	6	102	ARG	Sidechain
2	6	154	ARG	Sidechain
2	6	199	TYR	Sidechain
2	6	77	TYR	Sidechain
2	7	106	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	68	ARG	Sidechain
2	7	77	TYR	Sidechain
2	7	88	ARG	Sidechain
1	A	105	GLU	Peptide
1	A	148	TYR	Sidechain
1	A	168	ARG	Sidechain
1	A	179	TYR	Sidechain
1	A	22	PHE	Sidechain
1	A	53	ARG	Sidechain
1	A	65	GLU	Peptide
1	A	68	TYR	Sidechain
1	A	8	TYR	Sidechain
1	A	86	ARG	Sidechain
1	B	103	TYR	Sidechain
1	B	123	TYR	Sidechain
1	B	14	VAL	Peptide
1	B	159	TYR	Sidechain
1	B	179	TYR	Sidechain
1	B	20	ARG	Sidechain
1	B	213	TYR	Sidechain
1	B	219	ARG	Sidechain
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	66	LYS	Peptide
1	C	10	ARG	Sidechain
1	C	123	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	168	ARG	Sidechain
1	C	179	TYR	Sidechain
1	C	20	ARG	Sidechain
1	C	220	THR	Peptide
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	C	8	TYR	Sidechain
1	D	126	TYR	Sidechain
1	D	180	ARG	Sidechain
1	D	185	PHE	Sidechain
1	D	220	THR	Peptide
1	D	232	TYR	Sidechain
1	D	26	TYR	Sidechain
1	D	8	TYR	Sidechain
1	E	100	ARG	Sidechain
1	E	179	TYR	Sidechain
1	E	213	TYR	Sidechain
1	E	220	THR	Peptide
1	E	26	TYR	Sidechain
1	E	86	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	10	ARG	Sidechain
1	F	130	ARG	Sidechain
1	F	179	TYR	Sidechain
1	F	219	ARG	Sidechain
1	F	220	THR	Peptide
1	F	232	TYR	Sidechain
1	F	8	TYR	Sidechain
1	F	83	ALA	Mainchain
1	F	93	ARG	Sidechain
1	G	100	ARG	Sidechain
1	G	103	TYR	Sidechain
1	G	148	TYR	Sidechain
1	G	179	TYR	Sidechain
1	G	180	ARG	Sidechain
1	G	219	ARG	Sidechain
1	G	220	THR	Peptide
1	G	232	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	G	241	ARG	Sidechain
1	G	28	ARG	Sidechain
1	G	5	GLN	Peptide
3	H	105	ARG	Sidechain
3	H	181	TYR	Sidechain
3	H	201	ALA	Peptide,Mainchain
3	H	205	ARG	Sidechain
3	H	21	TYR	Sidechain
3	H	221	ARG	Sidechain
3	H	250	ARG	Sidechain
3	H	269	LEU	Peptide
3	H	27	TYR	Sidechain
3	H	277	PRO	Peptide
3	H	317	ARG	Sidechain
3	H	367	ARG	Sidechain
3	H	386	THR	Peptide
3	H	387	THR	Peptide
3	H	41	ARG	Sidechain
3	H	44	TYR	Sidechain
3	H	94	TYR	Sidechain
3	I	121	THR	Peptide
3	I	140	TYR	Sidechain
3	I	167	PHE	Sidechain
3	I	221	ARG	Sidechain
3	I	224	ARG	Sidechain
3	I	24	ARG	Sidechain
3	I	27	TYR	Sidechain
3	I	278	ARG	Sidechain
3	I	289	ARG	Sidechain
3	I	386	THR	Peptide
3	I	387	THR	Peptide
3	I	57	ARG	Sidechain
3	J	140	TYR	Sidechain
3	J	154	ARG	Sidechain
3	J	20	TYR	Sidechain
3	J	200	ARG	Sidechain
3	J	205	ARG	Sidechain
3	J	215	TYR	Peptide
3	J	254	ASP	Peptide
3	J	29	ARG	Sidechain
3	J	305	ARG	Sidechain
3	J	314	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	J	336	PHE	Sidechain
3	J	371	THR	Peptide
3	J	385	LYS	Peptide
3	J	386	THR	Peptide
3	J	49	ARG	Sidechain
3	J	52	ARG	Sidechain
3	K	140	TYR	Sidechain
3	K	20	TYR	Sidechain
3	K	211	PHE	Sidechain
3	K	215	TYR	Peptide,Sidechain
3	K	217	GLY	Peptide
3	K	218	GLU	Peptide
3	K	236	SER	Peptide
3	K	240	ILE	Peptide
3	K	249	ARG	Sidechain
3	K	254	ASP	Peptide
3	K	276	ASP	Peptide
3	K	311	LEU	Peptide
3	K	326	ARG	Sidechain
3	K	364	ARG	Sidechain
3	K	386	THR	Peptide
3	K	44	TYR	Sidechain
3	K	76	ARG	Sidechain
3	L	121	THR	Peptide
3	L	154	ARG	Sidechain
3	L	181	TYR	Peptide
3	L	21	TYR	Sidechain
3	L	215	TYR	Sidechain
3	L	224	ARG	Sidechain
3	L	254	ASP	Peptide
3	L	269	LEU	Mainchain
3	L	278	ARG	Sidechain
3	L	29	ARG	Sidechain
3	L	303	PHE	Peptide,Sidechain
3	L	305	ARG	Sidechain
3	L	317	ARG	Sidechain
3	L	386	THR	Peptide
3	L	387	THR	Peptide
3	L	52	ARG	Sidechain
3	M	121	THR	Peptide
3	M	128	TYR	Sidechain
3	M	181	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	M	186	THR	Peptide
3	M	190	LEU	Peptide
3	M	20	TYR	Sidechain
3	M	207	VAL	Peptide
3	M	215	TYR	Sidechain
3	M	263	ARG	Sidechain
3	M	27	TYR	Sidechain
3	M	28	ARG	Sidechain
3	M	299	ARG	Sidechain
3	M	302	ARG	Sidechain
3	M	321	PHE	Sidechain
3	M	341	ARG	Sidechain
3	M	385	LYS	Peptide
3	M	386	THR	Peptide
3	M	44	TYR	Sidechain
3	M	46	ARG	Sidechain
3	M	49	ARG	Sidechain
1	a	148	TYR	Sidechain
1	a	159	TYR	Sidechain
1	a	179	TYR	Sidechain
1	a	213	TYR	Sidechain
1	a	220	THR	Peptide
1	a	221	PHE	Sidechain
1	a	232	TYR	Sidechain
1	a	235	ARG	Sidechain
1	b	10	ARG	Sidechain
1	b	123	TYR	Sidechain
1	b	179	TYR	Sidechain
1	b	185	PHE	Sidechain
1	b	220	THR	Peptide
1	b	221	PHE	Sidechain
1	b	235	ARG	Sidechain
1	b	239	ARG	Sidechain
1	b	68	TYR	Sidechain
1	b	91	ARG	Sidechain
1	c	10	ARG	Sidechain
1	c	15	PHE	Sidechain
1	c	179	TYR	Sidechain
1	c	213	TYR	Sidechain
1	c	232	TYR	Sidechain
1	c	241	ARG	Sidechain
1	c	53	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	c	68	TYR	Sidechain
1	c	86	ARG	Sidechain
1	d	126	TYR	Sidechain
1	d	213	TYR	Sidechain
1	d	22	PHE	Sidechain
1	d	220	THR	Peptide
1	d	239	ARG	Sidechain
1	d	26	TYR	Sidechain
1	d	86	ARG	Sidechain
1	d	91	ARG	Sidechain
1	e	10	ARG	Sidechain
1	e	175	PHE	Sidechain
1	e	179	TYR	Sidechain
1	e	213	TYR	Sidechain
1	e	220	THR	Peptide
1	e	53	ARG	Sidechain
1	e	86	ARG	Sidechain
1	e	93	ARG	Sidechain
1	f	119	PHE	Sidechain
1	f	132	PHE	Sidechain
1	f	148	TYR	Sidechain
1	f	159	TYR	Sidechain
1	f	20	ARG	Sidechain
1	f	219	ARG	Sidechain
1	f	220	THR	Peptide
1	f	239	ARG	Sidechain
1	f	86	ARG	Sidechain
1	f	93	ARG	Sidechain
1	g	126	TYR	Sidechain
1	g	148	TYR	Sidechain
1	g	213	TYR	Sidechain
1	g	219	ARG	Sidechain
1	g	220	THR	Peptide
1	g	241	ARG	Sidechain
2	h	103	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	170	ARG	Sidechain
2	h	178	ARG	Sidechain
2	h	197	TYR	Sidechain
2	h	199	TYR	Sidechain
2	i	103	TYR	Sidechain
2	i	113	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	i	139	ALA	Peptide
2	i	199	TYR	Sidechain
2	i	46	TYR	Sidechain
2	i	51	ARG	Sidechain
2	i	65	PHE	Sidechain
2	i	77	TYR	Sidechain
2	i	83	ARG	Sidechain
2	j	104	PHE	Sidechain
2	j	154	ARG	Sidechain
2	j	197	TYR	Sidechain
2	j	30	ARG	Sidechain
2	k	101	TYR	Sidechain
2	k	103	TYR	Sidechain
2	k	123	TYR	Sidechain
2	k	178	ARG	Sidechain
2	k	199	TYR	Sidechain
2	k	212	ARG	Sidechain
2	k	30	ARG	Sidechain
2	k	65	PHE	Sidechain
2	k	68	ARG	Sidechain
2	k	77	TYR	Sidechain
2	k	80	ARG	Sidechain
2	l	101	TYR	Sidechain
2	l	123	TYR	Sidechain
2	l	154	ARG	Sidechain
2	l	170	ARG	Sidechain
2	l	211	PHE	Sidechain
2	l	212	ARG	Sidechain
2	l	68	ARG	Sidechain
2	l	77	TYR	Sidechain
2	l	81	ARG	Sidechain
2	l	83	ARG	Sidechain
2	m	103	TYR	Sidechain
2	m	106	TYR	Sidechain
2	m	212	ARG	Sidechain
2	m	83	ARG	Sidechain
2	n	101	TYR	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	178	ARG	Sidechain
2	n	197	TYR	Sidechain
2	n	199	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	n	30	ARG	Sidechain
2	n	77	TYR	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	8	0
1	B	1907	0	1941	10	0
1	C	1907	0	1941	3	0
1	D	1907	0	1941	12	0
1	E	1907	0	1941	4	0
1	F	1907	0	1941	5	0
1	G	1907	0	1941	5	0
1	a	1866	0	1908	11	0
1	b	1866	0	1908	10	0
1	c	1866	0	1908	8	0
1	d	1866	0	1908	7	0
1	e	1866	0	1908	12	0
1	f	1866	0	1908	10	0
1	g	1866	0	1908	5	0
2	1	1553	0	1580	3	0
2	2	1553	0	1580	4	0
2	3	1553	0	1580	3	0
2	4	1553	0	1580	5	0
2	5	1553	0	1580	27	0
2	6	1553	0	1580	5	0
2	7	1553	0	1580	4	0
2	h	1553	0	1580	9	0
2	i	1553	0	1580	4	0
2	j	1553	0	1580	4	0
2	k	1553	0	1580	5	0
2	l	1553	0	1580	26	0
2	m	1553	0	1580	3	0
2	n	1553	0	1580	2	0
3	H	3100	0	3220	30	0
3	I	3100	0	3220	36	0
3	J	3100	0	3220	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	3100	0	3220	48	0
3	L	3100	0	3220	31	0
3	M	3100	0	3220	32	0
4	H	31	0	12	2	0
4	K	31	0	12	5	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	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	I	27	0	12	10	0
All	All	66909	0	68443	392	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 (392) 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)
3:I:143:ILE:HD11	6:I:401:ADP:C6	1.42	1.52
2:l:211:PHE:CZ	2:l:211:PHE:CE2	1.97	1.49
2:5:211:PHE:CZ	2:5:211:PHE:CE2	2.01	1.47
2:l:211:PHE:CE1	2:l:211:PHE:CD1	1.99	1.47
2:5:211:PHE:CE1	2:5:211:PHE:CD1	2.02	1.47
2:5:211:PHE:CE2	2:5:211:PHE:CD2	2.04	1.45
2:5:211:PHE:CD2	2:5:211:PHE:CG	2.05	1.45
2:l:211:PHE:CE2	2:l:211:PHE:CD2	2.02	1.45
2:5:211:PHE:CZ	2:5:211:PHE:CE1	2.08	1.42
2:5:211:PHE:CD1	2:5:211:PHE:CG	2.07	1.42
3:K:144:GLY:HA3	4:K:401:ATP:N1	1.20	1.42
3:I:143:ILE:CD1	6:I:401:ADP:N1	1.84	1.41
2:l:211:PHE:CZ	2:l:211:PHE:CE1	2.08	1.40
3:I:143:ILE:CD1	6:I:401:ADP:C6	2.05	1.40
2:l:211:PHE:CD1	2:l:211:PHE:CG	2.10	1.39
2:l:211:PHE:CD2	2:l:211:PHE:CG	2.12	1.37
3:K:144:GLY:CA	4:K:401:ATP:N1	2.04	1.20
3:I:143:ILE:HD12	6:I:401:ADP:N1	1.49	1.17
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.11	1.13
3:I:143:ILE:HD11	6:I:401:ADP:N6	1.64	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:170:ARG:CZ	2:l:211:PHE:CD1	2.34	1.11
2:l:170:ARG:CZ	2:l:170:ARG:NH1	2.12	1.10
2:l:170:ARG:CZ	2:l:211:PHE:CE2	2.34	1.10
2:l:170:ARG:NH1	2:l:211:PHE:CZ	2.20	1.10
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.20	1.09
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.36	1.09
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.35	1.09
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.21	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.23	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:CD1	2.23	1.06
2:l:170:ARG:NH1	2:l:211:PHE:CD1	2.23	1.06
2:l:170:ARG:NH1	2:l:211:PHE:CE1	2.24	1.06
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.38	1.05
2:l:170:ARG:CZ	2:l:211:PHE:CZ	2.38	1.05
2:l:170:ARG:CZ	2:l:211:PHE:CD2	2.39	1.05
2:l:170:ARG:NH1	2:l:211:PHE:CD2	2.23	1.05
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.39	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.25	1.05
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.39	1.05
2:l:170:ARG:NH1	2:l:211:PHE:CG	2.24	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.41	1.04
2:l:170:ARG:CZ	2:l:211:PHE:CG	2.42	1.03
2:l:170:ARG:CZ	2:l:211:PHE:CE1	2.41	1.02
2:l:170:ARG:NH1	2:l:211:PHE:CE2	2.28	1.01
3:K:172:ILE:CG2	3:J:356:THR:HG23	1.90	1.01
3:K:320:ILE:HG22	3:K:351:ILE:HG21	1.41	0.99
3:K:172:ILE:HD11	3:J:328:MET:SD	2.03	0.98
3:K:202:THR:O	3:K:237:ILE:HG21	1.71	0.90
3:L:342:ILE:HG21	3:L:379:ILE:HG21	1.55	0.89
3:I:143:ILE:CD1	6:I:401:ADP:C2	2.57	0.88
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.42	0.87
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.42	0.86
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.45	0.85
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.45	0.83
2:l:170:ARG:NE	2:l:211:PHE:CZ	2.48	0.81
2:l:170:ARG:NH2	2:l:211:PHE:CG	2.49	0.81
3:K:320:ILE:CG2	3:K:351:ILE:HG21	2.12	0.79
3:L:342:ILE:CG2	3:L:379:ILE:HG21	2.13	0.79
3:I:143:ILE:HD13	6:I:401:ADP:C2	2.18	0.78
3:I:398:VAL:HG22	3:I:398:VAL:OXT	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:143:ILE:HD13	6:I:401:ADP:N1	1.96	0.78
3:I:342:ILE:HG21	3:I:379:ILE:HG21	1.64	0.77
2:l:170:ARG:NH2	2:l:211:PHE:CD2	2.52	0.77
3:M:153:ILE:HG21	3:M:195:VAL:HG21	1.66	0.76
3:I:354:ILE:HD13	3:I:379:ILE:HG12	1.68	0.76
2:l:170:ARG:NE	2:l:211:PHE:CE1	2.55	0.74
3:K:144:GLY:HA3	4:K:401:ATP:C2	2.19	0.74
3:M:204:ILE:HB	3:M:238:ILE:HD13	1.70	0.73
3:H:172:ILE:HG12	3:M:359:GLY:HA3	1.70	0.72
3:K:172:ILE:HG23	3:J:356:THR:HG23	1.70	0.72
3:K:216:ILE:HG23	3:K:260:GLU:HG2	1.70	0.71
3:I:320:ILE:CG2	3:I:351:ILE:HG21	2.21	0.71
3:M:204:ILE:HG13	3:M:238:ILE:CD1	2.20	0.70
3:I:143:ILE:HD13	6:I:401:ADP:C6	2.23	0.70
3:I:398:VAL:OXT	3:I:398:VAL:CG2	2.38	0.70
3:K:172:ILE:HG22	3:J:356:THR:HG23	1.74	0.70
3:I:342:ILE:CG2	3:I:379:ILE:HG21	2.21	0.69
1:D:14:VAL:HG12	1:E:23:GLN:HE22	1.57	0.69
3:I:283:VAL:HA	3:I:284:ILE:HB	1.73	0.69
3:H:320:ILE:HG22	3:H:351:ILE:HG21	1.73	0.69
3:J:211:PHE:CD1	3:J:246:ILE:HD12	2.28	0.68
3:H:342:ILE:CG2	3:H:379:ILE:HG21	2.24	0.68
3:M:204:ILE:CB	3:M:238:ILE:HD13	2.24	0.68
3:M:204:ILE:CG1	3:M:238:ILE:HD13	2.25	0.67
2:k:178:ARG:HG2	2:k:178:ARG:HH11	1.60	0.66
1:f:54:VAL:HG21	1:f:59:LEU:HD23	1.77	0.66
3:J:342:ILE:CG2	3:J:379:ILE:HG21	2.24	0.66
3:K:236:SER:CA	3:K:237:ILE:HG12	2.26	0.66
3:J:342:ILE:HG21	3:J:379:ILE:HG21	1.78	0.66
3:H:342:ILE:HG21	3:H:379:ILE:HG21	1.79	0.65
1:g:214:VAL:HA	1:g:221:PHE:H	1.62	0.64
3:J:238:ILE:HG22	3:J:240:ILE:CG1	2.28	0.64
3:M:206:VAL:CG1	3:M:240:ILE:HG12	2.27	0.64
3:K:236:SER:HA	3:K:237:ILE:HG12	1.79	0.63
3:K:199:THR:HG21	3:K:237:ILE:HD11	1.81	0.63
3:J:211:PHE:CE1	3:J:246:ILE:HD12	2.34	0.63
3:I:143:ILE:HD12	6:I:401:ADP:C2	2.28	0.62
3:K:172:ILE:CG2	3:J:356:THR:CG2	2.72	0.62
3:M:153:ILE:CG2	3:M:195:VAL:HG21	2.30	0.61
3:K:287:THR:HG21	3:K:290:ILE:HG22	1.82	0.61
3:J:398:VAL:HG22	3:J:398:VAL:OXT	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:204:ILE:HG13	3:M:238:ILE:HD13	1.84	0.60
3:K:236:SER:HA	3:K:237:ILE:CG1	2.31	0.60
3:K:202:THR:O	3:K:237:ILE:CG2	2.47	0.60
3:I:320:ILE:HG22	3:I:351:ILE:CG2	2.32	0.60
2:h:137:ILE:HG23	2:h:151:LEU:HD23	1.84	0.60
3:H:342:ILE:CG2	3:H:379:ILE:CG2	2.81	0.59
3:H:398:VAL:HG22	3:H:398:VAL:OXT	2.02	0.59
3:I:132:VAL:HG12	3:I:135:LYS:H	1.66	0.59
3:K:144:GLY:N	4:K:401:ATP:N1	2.50	0.59
3:H:153:ILE:HD12	3:H:180:LEU:HD11	1.84	0.59
3:I:320:ILE:CG2	3:I:351:ILE:CG2	2.80	0.59
1:E:73:HIS:CD2	1:E:74:ILE:HG13	2.38	0.59
3:M:318:ILE:HG23	3:M:336:PHE:HB3	1.84	0.59
1:F:49:ILE:HG23	1:F:211:VAL:HG22	1.84	0.59
3:H:146:LEU:HD11	4:H:401:ATP:N6	2.17	0.58
3:K:24:ARG:HE	3:J:23:LEU:HD13	1.68	0.58
2:m:115:ILE:HD13	2:m:193:GLU:HG3	1.85	0.58
3:K:320:ILE:HG22	3:K:351:ILE:CG2	2.26	0.58
3:H:146:LEU:HD11	4:H:401:ATP:HN61	1.68	0.58
3:L:127:VAL:HG22	3:L:229:LEU:HD22	1.85	0.58
3:K:361:PHE:HA	3:K:364:ARG:HE	1.68	0.58
3:K:125:PRO:HD3	3:L:69:SER:HA	1.86	0.58
1:b:141:VAL:HG22	1:b:145:PRO:HA	1.86	0.57
1:E:125:GLN:HA	1:F:130:ARG:HE	1.69	0.57
3:L:239:PHE:CE1	3:L:284:ILE:CG2	2.87	0.57
3:J:196:ALA:HA	3:J:237:ILE:HD12	1.85	0.57
2:h:132:ILE:HG12	2:n:64:GLN:HE22	1.70	0.57
3:L:398:VAL:HG22	3:L:398:VAL:OXT	2.05	0.57
3:H:211:PHE:HD2	3:H:246:ILE:CD1	2.17	0.56
3:K:269:LEU:HD22	3:K:302:ARG:HG2	1.88	0.56
1:d:137:LEU:HD23	1:d:149:GLU:HA	1.87	0.56
1:a:164:ILE:HG22	1:a:168:ARG:HH21	1.71	0.56
1:c:21:LEU:HD12	1:c:21:LEU:H	1.71	0.56
2:7:54:MET:HE2	2:7:112:ILE:HD11	1.87	0.56
3:K:287:THR:HG21	3:K:290:ILE:CG2	2.36	0.56
3:I:239:PHE:HA	3:I:284:ILE:HG22	1.88	0.56
3:K:236:SER:C	3:K:237:ILE:HG12	2.31	0.56
3:H:342:ILE:HG21	3:H:379:ILE:CG2	2.36	0.55
3:H:95:ILE:HD11	3:H:117:ASN:HA	1.88	0.55
1:e:12:ILE:HD13	1:e:23:GLN:HG2	1.88	0.55
2:j:42:ALA:HA	2:k:132:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:339:LEU:HD22	3:H:379:ILE:HD11	1.88	0.55
3:J:238:ILE:HG22	3:J:240:ILE:HG13	1.88	0.55
3:I:230:ALA:HB2	3:I:238:ILE:HD11	1.89	0.55
1:c:197:GLY:HA3	1:c:240:ILE:HD13	1.87	0.55
3:J:392:LEU:HG	3:J:394:GLY:H	1.72	0.55
3:I:320:ILE:HG22	3:I:351:ILE:HG21	1.89	0.54
3:K:149:GLN:CD	3:K:149:GLN:H	2.14	0.54
3:H:184:PRO:HB2	3:I:299:ARG:HG2	1.89	0.54
3:I:230:ALA:CB	3:I:238:ILE:HD11	2.38	0.54
3:J:320:ILE:HG22	3:J:351:ILE:HG21	1.89	0.54
3:H:319:GLN:O	3:H:323:ILE:HG12	2.08	0.54
3:M:323:ILE:HG12	3:M:326:ARG:HH21	1.73	0.54
2:h:191:ILE:HG23	2:h:196:PHE:CZ	2.43	0.53
3:I:215:TYR:CE2	3:K:251:THR:HG23	2.43	0.53
3:L:394:GLY:HA3	3:L:396:MET:H	1.72	0.53
2:j:159:ILE:HG23	2:j:159:ILE:O	2.08	0.53
1:A:186:ASP:O	1:A:190:VAL:HG23	2.09	0.53
1:g:205:VAL:HG23	1:g:207:GLU:H	1.72	0.53
3:M:46:ARG:HA	3:M:49:ARG:HH21	1.73	0.53
3:M:204:ILE:HG21	3:M:238:ILE:HD12	1.91	0.53
3:M:230:ALA:HB2	3:M:238:ILE:HD11	1.91	0.53
3:H:398:VAL:OXT	3:H:398:VAL:CG2	2.57	0.53
1:D:73:HIS:CE1	1:D:106:PRO:HB3	2.44	0.52
3:K:216:ILE:HG22	3:K:263:ARG:HH22	1.75	0.52
3:L:239:PHE:CE1	3:L:284:ILE:HG22	2.45	0.52
2:m:27:THR:HG21	2:m:45:ILE:HB	1.91	0.52
3:I:239:PHE:CE2	3:I:241:ASP:HB2	2.45	0.52
3:J:398:VAL:OXT	3:J:398:VAL:CG2	2.57	0.52
3:M:342:ILE:CG2	3:M:379:ILE:HG21	2.40	0.52
1:f:40:ILE:HD11	1:f:192:GLY:HA3	1.92	0.52
3:K:236:SER:HA	3:K:237:ILE:HB	1.92	0.51
1:G:74:ILE:HG21	1:G:112:LEU:HD23	1.93	0.51
2:6:65:PHE:HA	2:6:68:ARG:HH21	1.76	0.51
3:K:34:LYS:HB3	3:J:34:LYS:HB3	1.93	0.51
1:D:184:SER:H	1:D:187:ASP:HB2	1.76	0.51
1:f:20:ARG:HB3	1:g:33:ARG:NH2	2.26	0.51
2:h:165:VAL:HG12	2:h:188:VAL:HG11	1.93	0.50
3:K:224:ARG:HH21	3:K:267:GLN:HG2	1.76	0.50
1:A:206:PRO:HB3	1:A:233:VAL:HG21	1.93	0.50
2:4:167:LEU:HD13	2:4:170:ARG:HH11	1.75	0.50
3:H:206:VAL:HG22	3:H:207:VAL:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:174:PRO:HG2	3:L:278:ARG:HH22	1.76	0.50
2:4:212:ARG:HE	2:4:212:ARG:HA	1.76	0.50
1:B:141:VAL:HG22	1:B:145:PRO:HA	1.94	0.50
1:d:124:THR:HG23	1:e:130:ARG:HH21	1.76	0.50
1:e:71:ASP:OD1	1:e:73:HIS:CE1	2.64	0.50
3:J:342:ILE:HG22	3:J:379:ILE:HG21	1.94	0.50
3:J:110:GLN:H	3:J:110:GLN:CD	2.20	0.50
3:K:144:GLY:CA	4:K:401:ATP:C2	2.87	0.49
1:f:61:ALA:HA	1:f:64:ILE:HG22	1.92	0.49
3:L:323:ILE:HD12	3:L:326:ARG:NH1	2.28	0.49
3:J:350:ASP:O	3:J:354:ILE:HG13	2.12	0.49
3:J:208:GLY:HA2	3:J:211:PHE:CE2	2.47	0.49
3:L:323:ILE:HD12	3:L:326:ARG:HH12	1.77	0.49
1:G:180:ARG:HH11	1:G:183:LEU:HD23	1.77	0.49
3:H:72:LEU:HD12	3:H:76:ARG:HB2	1.94	0.49
3:K:170:VAL:HG12	3:K:172:ILE:HG12	1.95	0.49
2:m:95:SER:HB3	2:m:130:GLY:H	1.78	0.49
3:L:320:ILE:HG22	3:L:351:ILE:HG21	1.93	0.49
3:M:212:VAL:H	3:M:219:GLY:CA	2.26	0.49
2:1:19:CYS:HB2	2:1:22:GLY:H	1.78	0.49
2:h:68:ARG:HH12	2:i:131:ALA:HB3	1.77	0.49
2:4:86:THR:HG23	2:4:89:ALA:H	1.77	0.49
3:K:236:SER:HA	3:K:237:ILE:CB	2.43	0.49
3:K:398:VAL:OXT	3:K:398:VAL:HG22	2.13	0.48
1:F:9:ASP:HA	1:F:22:PHE:HB2	1.95	0.48
1:g:58:LEU:H	1:g:58:LEU:HD22	1.78	0.48
1:e:40:ILE:N	1:e:40:ILE:HD13	2.28	0.48
3:H:342:ILE:HG22	3:H:379:ILE:CG2	2.43	0.48
2:5:68:ARG:HH22	2:6:95:SER:HB2	1.78	0.48
3:K:389:ILE:HB	3:K:390:PRO:CD	2.43	0.48
3:M:204:ILE:HG13	3:M:238:ILE:HD11	1.95	0.48
1:C:88:LEU:HD11	1:C:116:ILE:HG23	1.96	0.48
1:B:141:VAL:HG11	1:B:216:VAL:HG22	1.96	0.48
3:M:234:ALA:HA	3:M:235:PRO:C	2.39	0.48
3:H:339:LEU:HD22	3:H:379:ILE:CD1	2.43	0.48
1:c:230:LYS:HB3	1:c:231:PRO:HD3	1.95	0.47
2:j:167:LEU:HA	2:j:170:ARG:HH11	1.78	0.47
3:K:389:ILE:HB	3:K:390:PRO:HD2	1.95	0.47
1:D:186:ASP:HB2	1:D:235:ARG:HH22	1.79	0.47
3:K:215:TYR:H	3:L:215:TYR:HB3	1.79	0.47
3:L:359:GLY:HA3	3:M:172:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ILE:HG21	1:D:112:LEU:HD21	1.97	0.47
1:a:17:PRO:HA	1:b:26:TYR:CD2	2.50	0.47
3:M:204:ILE:CB	3:M:238:ILE:CD1	2.91	0.47
3:M:206:VAL:HG13	3:M:240:ILE:HG12	1.95	0.47
1:D:11:ALA:HB3	1:D:14:VAL:HG22	1.97	0.47
1:f:190:VAL:HG12	1:f:239:ARG:HH11	1.80	0.47
2:h:54:MET:HE1	2:h:67:ALA:HA	1.97	0.47
1:e:54:VAL:HG22	1:e:55:GLY:H	1.80	0.46
2:k:22:GLY:HA2	2:k:115:ILE:HD11	1.97	0.46
3:J:234:ALA:HB2	3:J:280:ASP:H	1.81	0.46
2:n:151:LEU:HA	2:n:167:LEU:HD11	1.98	0.46
3:K:318:ILE:HG12	3:K:337:LYS:HA	1.98	0.46
1:C:48:LEU:HD21	1:C:77:ALA:HB2	1.97	0.46
3:L:281:VAL:HA	3:L:282:LYS:HB2	1.98	0.46
2:i:115:ILE:HD12	2:i:191:ILE:HG22	1.96	0.46
2:5:159:ILE:HG23	2:5:159:ILE:O	2.15	0.46
1:a:96:ALA:HB1	1:a:107:ILE:HG21	1.97	0.46
1:D:196:MET:HE3	1:D:209:ILE:HG22	1.98	0.46
3:I:371:THR:HG22	3:I:374:ASP:OD2	2.15	0.46
3:M:204:ILE:CG1	3:M:238:ILE:CD1	2.88	0.46
1:A:163:ALA:HB2	1:A:171:VAL:HG11	1.97	0.46
1:a:129:VAL:HG12	1:a:130:ARG:H	1.80	0.46
2:h:13:THR:HB	2:h:143:GLY:H	1.81	0.46
3:L:287:THR:HG21	3:L:293:LEU:HD11	1.97	0.46
3:M:212:VAL:H	3:M:219:GLY:HA3	1.81	0.46
1:G:49:ILE:HG23	1:G:211:VAL:HG22	1.97	0.45
3:I:132:VAL:C	3:I:134:GLU:H	2.24	0.45
3:I:342:ILE:HG21	3:I:379:ILE:CG2	2.39	0.45
1:a:17:PRO:HA	1:b:26:TYR:CG	2.51	0.45
2:h:200:SER:O	2:h:204:VAL:HG23	2.16	0.45
3:L:349:ALA:HB1	3:M:301:GLY:HA3	1.99	0.45
1:b:231:PRO:HB2	1:b:235:ARG:HH11	1.81	0.45
3:H:246:ILE:HG12	3:H:246:ILE:O	2.16	0.45
3:I:212:VAL:HG11	3:I:261:VAL:HG22	1.97	0.45
3:I:320:ILE:HG22	3:I:351:ILE:HG22	1.98	0.45
3:K:216:ILE:HG22	3:K:263:ARG:NH2	2.31	0.45
3:L:342:ILE:HG22	3:L:379:ILE:HG21	1.97	0.45
3:J:179:LEU:HD13	3:J:243:LEU:HD12	1.96	0.45
3:K:234:ALA:HA	3:K:235:PRO:C	2.42	0.45
3:L:230:ALA:CB	3:L:238:ILE:HD11	2.46	0.45
1:A:65:GLU:H	1:A:66:LYS:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:238:ILE:HG22	3:M:240:ILE:HG13	1.99	0.45
1:a:100:ARG:O	1:a:104:ASP:HA	2.16	0.45
1:d:15:PHE:HB3	1:e:26:TYR:HB3	1.99	0.45
3:L:143:ILE:HD12	3:L:190:LEU:HD23	1.99	0.45
1:a:14:VAL:HG13	1:b:12:ILE:HD11	1.98	0.45
1:b:53:ARG:HH11	1:b:200:ILE:HD12	1.82	0.45
3:K:359:GLY:HA3	3:L:172:ILE:HG21	1.99	0.45
1:B:70:ILE:HG21	1:B:112:LEU:HD21	1.98	0.44
1:c:134:VAL:HG22	1:c:135:SER:N	2.32	0.44
2:4:140:THR:H	2:4:144:SER:CB	2.31	0.44
1:f:189:MET:HE3	1:f:211:VAL:HG11	1.99	0.44
2:3:16:GLY:HA3	2:3:122:ILE:HD13	1.99	0.44
1:D:189:MET:HE3	1:D:211:VAL:HG11	2.00	0.44
2:3:24:VAL:HG12	2:3:25:MET:N	2.33	0.44
2:6:45:ILE:HD12	2:6:189:VAL:HG11	2.00	0.44
3:H:320:ILE:CG2	3:H:351:ILE:HG21	2.43	0.44
1:c:38:ILE:HD12	1:c:196:MET:HE2	1.98	0.44
3:I:269:LEU:CD1	3:I:297:ILE:HD13	2.48	0.44
3:I:331:ALA:HA	3:I:371:THR:HA	1.98	0.44
1:a:184:SER:H	1:a:187:ASP:HB2	1.83	0.44
3:L:204:ILE:N	3:L:204:ILE:HD12	2.33	0.44
3:L:394:GLY:HA3	3:L:397:PHE:H	1.83	0.44
3:K:199:THR:HG21	3:K:237:ILE:CD1	2.48	0.43
3:M:342:ILE:CG2	3:M:379:ILE:CG2	2.96	0.43
1:B:56:SER:H	1:B:59:LEU:HD13	1.83	0.43
1:e:172:THR:HG23	1:f:58:LEU:HD12	2.00	0.43
1:F:100:ARG:O	1:F:104:ASP:HA	2.18	0.43
2:l:25:MET:HE2	2:l:53:ALA:HB3	2.00	0.43
1:D:88:LEU:HD12	1:D:116:ILE:HD11	2.01	0.43
2:1:131:ALA:H	2:7:64:GLN:HE21	1.66	0.43
2:6:137:ILE:HD12	2:6:151:LEU:HB3	2.00	0.43
3:J:320:ILE:CG2	3:J:351:ILE:HG21	2.48	0.43
1:A:100:ARG:O	1:A:104:ASP:HA	2.18	0.43
1:f:237:ASN:HD22	1:f:237:ASN:HA	1.51	0.43
3:M:339:LEU:O	3:M:343:THR:HG23	2.17	0.43
1:a:241:ARG:O	1:a:245:LYS:HG3	2.19	0.43
2:7:45:ILE:HD13	2:7:55:THR:CG2	2.49	0.43
3:H:137:GLU:H	3:H:137:GLU:CD	2.26	0.43
1:A:230:LYS:HB2	1:A:231:PRO:HD3	2.01	0.43
1:a:19:GLY:HA3	1:b:30:ALA:HB2	2.01	0.43
1:B:16:SER:HB2	1:B:17:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:200:SER:O	2:l:204:VAL:HG23	2.19	0.43
3:L:298:LEU:O	3:L:306:ILE:CD1	2.67	0.43
1:e:73:HIS:CD2	1:e:74:ILE:HG13	2.54	0.43
3:H:324:HIS:CD2	3:H:351:ILE:HG22	2.54	0.43
3:K:375:PHE:O	3:K:379:ILE:HG13	2.17	0.43
3:J:208:GLY:HA2	3:J:211:PHE:CD2	2.54	0.43
3:J:389:ILE:HG13	3:J:389:ILE:O	2.18	0.43
1:D:159:TYR:HB3	1:D:161:ALA:H	1.83	0.43
3:H:230:ALA:HB2	3:H:238:ILE:HD11	2.01	0.43
1:A:151:ASP:HB2	1:A:155:ALA:HB3	2.01	0.42
2:k:18:VAL:HG21	2:k:135:LYS:HA	2.01	0.42
2:k:86:THR:HG23	2:k:89:ALA:H	1.83	0.42
3:M:242:GLU:H	3:M:286:ALA:HB3	1.83	0.42
2:2:52:MET:SD	2:2:87:VAL:HG22	2.59	0.42
3:H:138:VAL:HG12	3:H:139:SER:N	2.35	0.42
2:1:169:VAL:HA	2:1:186:ILE:HD11	2.00	0.42
2:h:26:ALA:HB2	2:h:188:VAL:HG13	2.01	0.42
3:K:186:THR:HB	3:K:309:VAL:HG12	2.02	0.42
1:B:108:THR:HB	1:B:111:GLU:H	1.85	0.42
1:f:206:PRO:HB3	1:f:233:VAL:HG21	2.01	0.42
3:L:320:ILE:HG22	3:L:324:HIS:CE1	2.55	0.42
1:D:64:ILE:HD12	1:D:86:ARG:HH22	1.85	0.42
1:f:54:VAL:HG21	1:f:59:LEU:CD2	2.46	0.42
2:4:15:VAL:HG22	2:4:26:ALA:HB3	2.01	0.42
3:M:204:ILE:HB	3:M:238:ILE:CD1	2.45	0.42
1:b:94:ILE:HG22	1:b:98:ILE:HD11	2.02	0.42
1:G:140:GLY:HA2	1:G:214:VAL:HG21	2.01	0.42
2:5:66:LEU:HD11	2:5:98:LEU:HD21	2.02	0.42
3:K:203:PHE:HA	3:K:237:ILE:HG22	2.00	0.42
3:J:312:PRO:HD2	3:J:347:SER:HA	2.02	0.42
1:a:130:ARG:HB2	1:g:11:ALA:HB2	2.01	0.42
3:H:320:ILE:O	3:H:323:ILE:HB	2.20	0.42
3:J:119:LEU:HD23	3:J:119:LEU:HA	1.88	0.42
1:d:200:ILE:HD11	1:d:204:LEU:CD2	2.49	0.41
2:2:156:THR:HB	2:2:158:GLU:H	1.84	0.41
3:J:361:PHE:CE2	3:J:377:LYS:HB3	2.55	0.41
1:F:198:LEU:HD13	1:F:243:LEU:HD22	2.02	0.41
1:d:132:PHE:HB3	1:d:134:VAL:HG22	2.03	0.41
3:L:239:PHE:CE1	3:L:284:ILE:HG21	2.53	0.41
1:D:70:ILE:HD11	1:D:76:ALA:HB2	2.02	0.41
3:J:250:ARG:HD3	3:J:250:ARG:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:109:VAL:HG23	1:d:142:ASP:OD1	2.21	0.41
2:3:142:SER:C	2:3:144:SER:H	2.27	0.41
3:H:238:ILE:HG22	3:H:240:ILE:HG13	2.02	0.41
3:J:172:ILE:HG23	3:J:172:ILE:O	2.21	0.41
1:b:159:TYR:CD2	1:b:162:THR:HB	2.56	0.41
2:7:186:ILE:HG21	2:7:208:LEU:CD2	2.50	0.41
2:i:26:ALA:HB2	2:i:188:VAL:HG13	2.01	0.41
2:i:197:TYR:CE1	2:i:199:TYR:HA	2.55	0.41
3:M:342:ILE:HG21	3:M:379:ILE:HG21	2.03	0.41
3:J:230:ALA:HB2	3:J:238:ILE:HD11	2.03	0.41
1:B:14:VAL:HG13	1:C:23:GLN:HE22	1.85	0.41
2:2:25:MET:CE	2:2:53:ALA:HB3	2.51	0.41
2:2:90:ILE:HD13	2:2:90:ILE:HA	1.86	0.41
3:J:195:VAL:HG12	3:J:237:ILE:HD13	2.02	0.41
3:J:376:THR:O	3:J:379:ILE:HB	2.21	0.41
1:d:11:ALA:HB3	1:e:13:THR:HG23	2.03	0.41
1:e:174:PHE:CE1	1:e:178:GLU:HG3	2.56	0.41
3:K:272:LEU:HA	3:K:275:PHE:CE1	2.56	0.41
3:L:398:VAL:OXT	3:L:398:VAL:CG2	2.64	0.41
1:B:141:VAL:HG13	1:B:144:VAL:C	2.46	0.41
1:E:74:ILE:HD13	1:E:74:ILE:HG21	1.90	0.41
3:I:243:LEU:HA	3:I:246:ILE:HG22	2.03	0.41
3:L:324:HIS:CE1	3:L:351:ILE:HG22	2.56	0.41
1:B:28:ARG:O	1:B:32:LYS:HG2	2.21	0.40
1:e:88:LEU:HD21	1:e:120:LYS:HE2	2.04	0.40
3:M:342:ILE:HG21	3:M:379:ILE:CG2	2.51	0.40
2:6:56:THR:HG21	2:6:63:ALA:HB1	2.03	0.40
1:B:148:TYR:CD1	1:B:156:LEU:HD11	2.56	0.40
1:b:121:GLN:HG3	1:c:83:ALA:O	2.21	0.40
2:l:57:ALA:O	2:l:108:VAL:HG23	2.22	0.40
3:H:153:ILE:HG23	3:H:154:ARG:N	2.37	0.40
3:I:391:ASP:CG	3:I:392:LEU:H	2.29	0.40
3:L:193:LYS:HD2	3:M:275:PHE:CD1	2.56	0.40
2:j:14:THR:HB	2:j:111:LEU:HD12	2.02	0.40
3:H:247:ALA:HA	3:H:265:MET:HG3	2.04	0.40
3:L:239:PHE:HE1	3:L:284:ILE:HG21	1.87	0.40
3:J:167:PHE:HA	3:J:172:ILE:HG22	2.03	0.40
3:J:178:VAL:HG21	3:J:307:ILE:HD12	2.04	0.40
1:A:70:ILE:HD11	1:A:76:ALA:HB3	2.03	0.40
1:c:197:GLY:HA3	1:c:240:ILE:CD1	2.50	0.40
1:c:216:VAL:HG13	1:c:219:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:75:CYS:HB3	1:e:221:PHE:CE1	2.56	0.40
1:G:80:GLY:O	3:L:398:VAL:O	2.39	0.40
2:5:24:VAL:HG21	2:5:164:ALA:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	4	26
1	B	240/242 (99%)	229 (95%)	7 (3%)	4 (2%)	7	36
1	C	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	5	30
1	D	240/242 (99%)	223 (93%)	12 (5%)	5 (2%)	5	30
1	E	240/242 (99%)	226 (94%)	10 (4%)	4 (2%)	7	36
1	F	240/242 (99%)	229 (95%)	8 (3%)	3 (1%)	9	42
1	G	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	5	30
1	a	235/242 (97%)	223 (95%)	8 (3%)	4 (2%)	7	36
1	b	235/242 (97%)	219 (93%)	16 (7%)	0	100	100
1	c	235/242 (97%)	223 (95%)	9 (4%)	3 (1%)	9	42
1	d	235/242 (97%)	221 (94%)	10 (4%)	4 (2%)	7	36
1	e	235/242 (97%)	217 (92%)	15 (6%)	3 (1%)	9	42
1	f	235/242 (97%)	221 (94%)	11 (5%)	3 (1%)	9	42
1	g	235/242 (97%)	223 (95%)	9 (4%)	3 (1%)	9	42
2	1	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	24	63
2	2	200/202 (99%)	176 (88%)	19 (10%)	5 (2%)	4	26
2	3	200/202 (99%)	185 (92%)	10 (5%)	5 (2%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	6	31
2	5	200/202 (99%)	182 (91%)	12 (6%)	6 (3%)	3	23
2	6	200/202 (99%)	181 (90%)	14 (7%)	5 (2%)	4	26
2	7	200/202 (99%)	186 (93%)	9 (4%)	5 (2%)	4	26
2	h	200/202 (99%)	180 (90%)	9 (4%)	11 (6%)	1	14
2	i	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	8	40
2	j	200/202 (99%)	186 (93%)	10 (5%)	4 (2%)	6	31
2	k	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	6	31
2	l	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	6	31
2	m	200/202 (99%)	191 (96%)	6 (3%)	3 (2%)	8	40
2	n	200/202 (99%)	181 (90%)	10 (5%)	9 (4%)	2	17
3	H	388/390 (100%)	344 (89%)	31 (8%)	13 (3%)	3	21
3	I	388/390 (100%)	354 (91%)	21 (5%)	13 (3%)	3	21
3	J	388/390 (100%)	353 (91%)	29 (8%)	6 (2%)	8	40
3	K	388/390 (100%)	344 (89%)	25 (6%)	19 (5%)	1	16
3	L	388/390 (100%)	348 (90%)	24 (6%)	16 (4%)	2	18
3	M	388/390 (100%)	336 (87%)	36 (9%)	16 (4%)	2	18
All	All	8453/8556 (99%)	7788 (92%)	461 (6%)	204 (2%)	7	27

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	a	54	VAL
1	B	64	ILE
1	C	20	ARG
1	C	66	LYS
1	C	67	ILE
1	c	219	ARG
1	D	56	SER
1	D	65	GLU
1	F	64	ILE
1	G	56	SER
1	g	143	GLU
2	h	128	ILE
2	h	140	THR

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Mol	Chain	Res	Type
2	2	140	THR
2	2	182	SER
2	3	212	ARG
2	4	140	THR
2	m	200	SER
2	n	131	ALA
2	n	139	ALA
3	H	120	PRO
3	H	270	ALA
3	H	278	ARG
3	H	280	ASP
3	I	124	ASP
3	I	282	LYS
3	K	163	LYS
3	K	215	TYR
3	K	237	ILE
3	K	313	THR
3	K	387	THR
3	L	125	PRO
3	L	255	THR
3	L	270	ALA
3	L	292	ILE
3	M	131	GLU
3	M	190	LEU
3	M	191	LEU
3	J	212	VAL
3	J	386	THR
1	A	106	PRO
1	A	143	GLU
1	a	34	GLY
1	B	65	GLU
1	B	143	GLU
1	c	73	HIS
1	D	161	ALA
1	d	12	ILE
1	d	161	ALA
1	d	221	PHE
1	E	221	PHE
1	F	221	PHE
1	f	143	GLU
1	f	179	TYR
1	G	221	PHE

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Mol	Chain	Res	Type
2	h	21	ASP
2	2	139	ALA
2	i	44	LYS
2	i	193	GLU
2	3	139	ALA
2	3	193	GLU
2	j	212	ARG
2	k	30	ARG
2	k	193	GLU
2	5	136	ASP
2	6	19	CYS
2	6	41	ALA
2	6	139	ALA
2	7	133	GLU
2	n	132	ILE
3	H	212	VAL
3	H	269	LEU
3	I	74	ASP
3	I	242	GLU
3	I	273	ASP
3	I	387	THR
3	K	255	THR
3	K	280	ASP
3	K	296	ALA
3	K	333	ASP
3	K	391	ASP
3	L	61	PRO
3	L	247	ALA
3	L	269	LEU
3	L	282	LYS
3	L	330	LEU
3	M	93	GLN
3	M	134	GLU
3	M	282	LYS
3	M	304	ASP
3	M	313	THR
3	M	333	ASP
3	M	386	THR
1	A	9	ASP
1	A	35	ALA
1	A	57	LYS
1	a	161	ALA

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Mol	Chain	Res	Type
1	B	221	PHE
1	C	221	PHE
1	c	62	ASP
1	e	161	ALA
1	F	9	ASP
1	G	6	MET
1	g	221	PHE
2	1	136	ASP
2	h	51	ARG
2	h	183	GLY
2	h	191	ILE
2	h	193	GLU
2	3	181	ALA
2	j	136	ASP
2	4	33	MET
2	4	44	LYS
2	5	193	GLU
2	l	40	LYS
2	6	136	ASP
2	7	83	ARG
3	H	126	MET
3	H	302	ARG
3	H	387	THR
3	I	131	GLU
3	I	212	VAL
3	K	149	GLN
3	K	201	ALA
3	K	392	LEU
3	L	146	LEU
3	L	212	VAL
3	L	221	ARG
3	L	331	ALA
3	M	122	SER
3	M	183	PRO
3	J	92	SER
1	D	55	GLY
1	d	143	GLU
1	E	6	MET
1	E	9	ASP
1	E	73	HIS
1	g	218	ASP
2	h	106	TYR

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Mol	Chain	Res	Type
2	h	137	ILE
2	2	106	TYR
2	2	212	ARG
2	k	140	THR
2	k	194	ASP
2	5	181	ALA
2	l	194	ASP
2	6	140	THR
2	m	106	TYR
2	m	193	GLU
2	n	137	ILE
2	n	140	THR
2	n	181	ALA
2	n	200	SER
3	H	209	SER
3	K	242	GLU
3	K	247	ALA
3	M	214	LYS
3	M	258	ASP
3	J	74	ASP
3	J	254	ASP
1	a	221	PHE
1	C	9	ASP
1	e	14	VAL
1	f	62	ASP
1	G	9	ASP
1	G	143	GLU
2	h	127	PRO
2	h	200	SER
2	i	200	SER
2	3	41	ALA
2	j	185	GLY
2	4	130	GLY
2	5	105	PRO
2	n	107	LEU
3	H	134	GLU
3	H	254	ASP
3	I	122	SER
3	I	135	LYS
3	I	310	PRO
3	K	91	THR
3	K	187	GLY

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Mol	Chain	Res	Type
3	L	135	LYS
3	L	396	MET
3	J	126	MET
2	5	133	GLU
2	l	136	ASP
2	7	34	GLY
3	I	284	ILE
3	I	388	PRO
3	K	135	LYS
1	D	64	ILE
2	5	191	ILE
2	7	105	PRO
3	L	310	PRO
2	7	85	PRO
3	M	124	ASP
2	j	200	SER
3	H	132	VAL
2	n	129	GLY
3	K	277	PRO
3	M	212	VAL
1	e	17	PRO
2	l	137	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	199 (98%)	4 (2%)	48	66
1	B	203/203 (100%)	199 (98%)	4 (2%)	48	66
1	C	203/203 (100%)	195 (96%)	8 (4%)	28	49
1	D	203/203 (100%)	196 (97%)	7 (3%)	32	54
1	E	203/203 (100%)	194 (96%)	9 (4%)	25	47
1	F	203/203 (100%)	196 (97%)	7 (3%)	32	54
1	G	203/203 (100%)	197 (97%)	6 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	199/203 (98%)	187 (94%)	12 (6%)	17	39
1	b	199/203 (98%)	192 (96%)	7 (4%)	32	53
1	c	199/203 (98%)	193 (97%)	6 (3%)	36	57
1	d	199/203 (98%)	192 (96%)	7 (4%)	32	53
1	e	199/203 (98%)	189 (95%)	10 (5%)	22	43
1	f	199/203 (98%)	190 (96%)	9 (4%)	24	46
1	g	199/203 (98%)	196 (98%)	3 (2%)	57	72
2	1	164/164 (100%)	158 (96%)	6 (4%)	30	51
2	2	164/164 (100%)	152 (93%)	12 (7%)	13	34
2	3	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	4	164/164 (100%)	153 (93%)	11 (7%)	15	36
2	5	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	6	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	7	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	h	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	i	164/164 (100%)	152 (93%)	12 (7%)	13	34
2	j	164/164 (100%)	155 (94%)	9 (6%)	19	41
2	k	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	l	164/164 (100%)	156 (95%)	8 (5%)	22	43
2	m	164/164 (100%)	160 (98%)	4 (2%)	43	64
2	n	164/164 (100%)	158 (96%)	6 (4%)	30	51
3	H	338/338 (100%)	324 (96%)	14 (4%)	27	49
3	I	338/338 (100%)	330 (98%)	8 (2%)	43	64
3	J	338/338 (100%)	328 (97%)	10 (3%)	36	57
3	K	338/338 (100%)	331 (98%)	7 (2%)	47	65
3	L	338/338 (100%)	325 (96%)	13 (4%)	29	50
3	M	338/338 (100%)	323 (96%)	15 (4%)	25	47
All	All	7138/7166 (100%)	6868 (96%)	270 (4%)	30	50

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG

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Mol	Chain	Res	Type
1	A	162	THR
1	A	202	SER
1	A	224	VAL
1	a	13	THR
1	a	21	LEU
1	a	33	ARG
1	a	58	LEU
1	a	120	LYS
1	a	121	GLN
1	a	129	VAL
1	a	134	VAL
1	a	142	ASP
1	a	166	MET
1	a	213	TYR
1	a	217	ASP
1	B	98	ILE
1	B	130	ARG
1	B	166	MET
1	B	205	VAL
1	b	15	PHE
1	b	28	ARG
1	b	31	VAL
1	b	182	ASP
1	b	198	LEU
1	b	209	ILE
1	b	224	VAL
1	C	57	LYS
1	C	63	THR
1	C	144	VAL
1	C	151	ASP
1	C	156	LEU
1	C	204	LEU
1	C	208	ASN
1	C	227	GLU
1	c	21	LEU
1	c	144	VAL
1	c	166	MET
1	c	182	ASP
1	c	213	TYR
1	c	224	VAL
1	D	38	ILE
1	D	41	LYS

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Mol	Chain	Res	Type
1	D	102	THR
1	D	121	GLN
1	D	213	TYR
1	D	215	LYS
1	D	231	PRO
1	d	21	LEU
1	d	40	ILE
1	d	109	VAL
1	d	142	ASP
1	d	144	VAL
1	d	145	PRO
1	d	160	LYS
1	E	6	MET
1	E	33	ARG
1	E	46	VAL
1	E	75	CYS
1	E	109	VAL
1	E	145	PRO
1	E	166	MET
1	E	191	LEU
1	E	224	VAL
1	e	21	LEU
1	e	40	ILE
1	e	46	VAL
1	e	59	LEU
1	e	63	THR
1	e	102	THR
1	e	118	ASP
1	e	129	VAL
1	e	189	MET
1	e	205	VAL
1	F	13	THR
1	F	89	ILE
1	F	97	GLN
1	F	102	THR
1	F	121	GLN
1	F	229	LEU
1	F	230	LYS
1	f	21	LEU
1	f	40	ILE
1	f	102	THR
1	f	105	GLU

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Mol	Chain	Res	Type
1	f	129	VAL
1	f	144	VAL
1	f	145	PRO
1	f	229	LEU
1	f	241	ARG
1	G	5	GLN
1	G	21	LEU
1	G	57	LYS
1	G	97	GLN
1	G	214	VAL
1	G	216	VAL
1	g	58	LEU
1	g	109	VAL
1	g	184	SER
2	1	14	THR
2	1	27	THR
2	1	45	ILE
2	1	121	SER
2	1	126	ASP
2	1	146	THR
2	h	17	LEU
2	h	52	MET
2	h	116	ASP
2	h	205	GLU
2	2	14	THR
2	2	17	LEU
2	2	45	ILE
2	2	69	ILE
2	2	71	LYS
2	2	90	ILE
2	2	106	TYR
2	2	110	LEU
2	2	121	SER
2	2	125	ILE
2	2	148	TYR
2	2	156	THR
2	i	17	LEU
2	i	45	ILE
2	i	60	VAL
2	i	72	ILE
2	i	104	PHE
2	i	107	LEU

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Mol	Chain	Res	Type
2	i	110	LEU
2	i	122	ILE
2	i	137	ILE
2	i	140	THR
2	i	169	VAL
2	i	203	GLU
2	3	12	THR
2	3	17	LEU
2	3	37	ILE
2	3	72	ILE
2	3	107	LEU
2	3	128	ILE
2	3	165	VAL
2	3	207	ILE
2	j	13	THR
2	j	14	THR
2	j	39	SER
2	j	116	ASP
2	j	121	SER
2	j	148	TYR
2	j	184	ASP
2	j	204	VAL
2	j	205	GLU
2	4	27	THR
2	4	32	THR
2	4	45	ILE
2	4	56	THR
2	4	72	ILE
2	4	108	VAL
2	4	110	LEU
2	4	123	TYR
2	4	140	THR
2	4	188	VAL
2	4	208	LEU
2	k	13	THR
2	k	108	VAL
2	k	120	LYS
2	k	148	TYR
2	5	15	VAL
2	5	27	THR
2	5	39	SER
2	5	45	ILE

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Mol	Chain	Res	Type
2	5	72	ILE
2	5	108	VAL
2	5	198	GLN
2	5	208	LEU
2	l	24	VAL
2	l	27	THR
2	l	45	ILE
2	l	104	PHE
2	l	116	ASP
2	l	128	ILE
2	l	146	THR
2	l	186	ILE
2	6	45	ILE
2	6	126	ASP
2	6	201	PRO
2	6	202	GLU
2	m	14	THR
2	m	45	ILE
2	m	172	ILE
2	m	212	ARG
2	7	28	GLU
2	7	64	GLN
2	7	72	ILE
2	7	103	TYR
2	7	108	VAL
2	7	132	ILE
2	7	163	GLU
2	7	205	GLU
2	n	60	VAL
2	n	87	VAL
2	n	115	ILE
2	n	117	SER
2	n	179	ASP
2	n	194	ASP
3	H	14	LYS
3	H	54	GLU
3	H	116	VAL
3	H	120	PRO
3	H	127	VAL
3	H	137	GLU
3	H	206	VAL
3	H	213	GLN

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Mol	Chain	Res	Type
3	H	226	VAL
3	H	268	LEU
3	H	278	ARG
3	H	298	LEU
3	H	329	LYS
3	H	360	MET
3	I	88	VAL
3	I	95	ILE
3	I	174	PRO
3	I	214	LYS
3	I	243	LEU
3	I	277	PRO
3	I	283	VAL
3	I	398	VAL
3	K	121	THR
3	K	189	THR
3	K	241	ASP
3	K	260	GLU
3	K	304	ASP
3	K	311	LEU
3	K	319	GLN
3	L	67	VAL
3	L	101	LYS
3	L	122	SER
3	L	175	PRO
3	L	179	LEU
3	L	183	PRO
3	L	212	VAL
3	L	250	ARG
3	L	304	ASP
3	L	332	GLU
3	L	339	LEU
3	L	344	GLU
3	L	370	VAL
3	M	48	VAL
3	M	67	VAL
3	M	79	VAL
3	M	91	THR
3	M	127	VAL
3	M	136	PRO
3	M	159	LEU
3	M	165	GLU

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Mol	Chain	Res	Type
3	M	176	LYS
3	M	190	LEU
3	M	249	ARG
3	M	272	LEU
3	M	347	SER
3	M	380	GLU
3	M	386	THR
3	J	85	PRO
3	J	89	VAL
3	J	101	LYS
3	J	116	VAL
3	J	122	SER
3	J	148	VAL
3	J	227	PHE
3	J	256	SER
3	J	300	PRO
3	J	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	E	23	GLN
1	E	73	HIS
1	E	97	GLN
1	E	122	GLN
1	E	237	ASN
1	e	73	HIS
1	e	97	GLN
1	e	121	GLN
1	F	125	GLN
1	f	121	GLN
1	f	122	GLN
1	f	208	ASN
1	f	237	ASN
1	G	73	HIS
1	G	97	GLN
1	G	99	ASN
1	G	125	GLN
1	g	23	GLN
1	g	208	ASN
1	g	237	ASN
2	1	64	GLN
2	1	96	ASN
2	h	35	ASN
2	h	109	GLN
2	2	96	ASN
2	2	109	GLN
2	i	96	ASN
2	i	109	GLN
2	i	198	GLN
2	3	35	ASN
2	3	75	ASN
2	3	99	ASN
2	j	47	GLN
2	j	75	ASN
2	j	99	ASN
2	j	206	GLN
2	4	64	GLN
2	4	96	ASN
2	4	99	ASN
2	k	75	ASN
2	l	47	GLN
2	6	35	ASN

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Mol	Chain	Res	Type
2	6	75	ASN
2	6	96	ASN
2	m	206	GLN
2	7	47	GLN
2	7	64	GLN
2	7	99	ASN
2	n	64	GLN
2	n	75	ASN
2	n	96	ASN
2	n	109	GLN
3	H	111	GLN
3	H	117	ASN
3	H	149	GLN
3	H	213	GLN
3	H	288	ASN
3	I	90	ASN
3	I	96	ASN
3	I	109	ASN
3	I	117	ASN
3	I	228	GLN
3	I	267	GLN
3	I	288	ASN
3	I	324	HIS
3	K	93	GLN
3	K	96	ASN
3	K	109	ASN
3	K	197	ASN
3	K	213	GLN
3	L	93	GLN
3	L	117	ASN
3	L	149	GLN
3	L	197	ASN
3	L	198	GLN
3	L	324	HIS
3	M	90	ASN
3	M	110	GLN
3	M	117	ASN
3	M	149	GLN
3	M	262	GLN
3	M	319	GLN
3	J	109	ASN
3	J	117	ASN

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Mol	Chain	Res	Type
3	J	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	4.78	6 (18%)	48,52,52	1.48	10 (20%)
4	ATP	H	401	5	32,33,33	5.20	7 (21%)	48,52,52	1.17	6 (12%)
6	ADP	I	401	5	28,29,29	2.18	4 (14%)	43,45,45	1.57	10 (23%)
4	ATP	K	401	5	32,33,33	4.07	6 (18%)	48,52,52	1.67	7 (14%)
4	ATP	M	401	5	32,33,33	4.17	3 (9%)	48,52,52	1.31	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	-	6/22/38/38	0/3/3/3
4	ATP	H	401	5	-	4/22/38/38	0/3/3/3
6	ADP	I	401	5	-	1/16/32/32	0/3/3/3
4	ATP	K	401	5	-	7/22/38/38	0/3/3/3
4	ATP	M	401	5	-	4/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	ATP	PB-O3B	21.37	1.82	1.59
4	L	401	ATP	PB-O3B	19.89	1.81	1.59
4	M	401	ATP	PB-O3B	17.69	1.78	1.59
4	L	401	ATP	PB-O3A	16.40	1.77	1.59
4	H	401	ATP	PB-O3A	15.04	1.75	1.59
4	K	401	ATP	PA-O3A	14.33	1.75	1.59
4	K	401	ATP	PB-O3B	13.59	1.74	1.59
4	M	401	ATP	PB-O3A	12.29	1.72	1.59
4	H	401	ATP	PA-O3A	11.34	1.71	1.59
4	K	401	ATP	PB-O3A	10.44	1.70	1.59
6	I	401	ADP	PA-O3A	8.94	1.69	1.59
4	M	401	ATP	PA-O3A	7.60	1.67	1.59
4	L	401	ATP	PA-O3A	4.84	1.64	1.59
4	L	401	ATP	C1'-N9	3.48	1.55	1.46
4	H	401	ATP	C5-N7	-3.38	1.32	1.39
6	I	401	ADP	C5-N7	-3.24	1.33	1.39
4	H	401	ATP	O4'-C4'	-2.63	1.39	1.45
4	K	401	ATP	C1'-N9	2.51	1.53	1.46
6	I	401	ADP	C1'-N9	2.49	1.53	1.46
4	H	401	ATP	C5'-C4'	2.44	1.58	1.51
6	I	401	ADP	PB-O1B	2.42	1.58	1.50
4	L	401	ATP	C5'-C4'	2.35	1.58	1.51
4	K	401	ATP	C2-N1	2.18	1.37	1.33
4	L	401	ATP	C5-N7	-2.11	1.35	1.39
4	K	401	ATP	PA-O2A	-2.07	1.45	1.55
4	H	401	ATP	C2-N3	2.00	1.37	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	401	ATP	C5-C4-N3	-4.78	120.14	126.72
4	K	401	ATP	C6-C5-C4	4.45	123.26	117.18
4	K	401	ATP	N3-C4-N9	3.99	133.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	401	ATP	C6-C5-C4	3.92	122.52	117.18
4	K	401	ATP	C5'-C4'-C3'	-3.73	101.79	115.21
6	I	401	ADP	N6-C6-N1	3.59	126.37	118.38
4	M	401	ATP	C5-C4-N9	3.32	109.43	105.81
6	I	401	ADP	C4-N9-C8	-3.16	102.42	105.74
4	K	401	ATP	C6-C5-N7	-3.14	126.03	132.09
6	I	401	ADP	O4'-C1'-N9	3.09	114.02	108.09
4	M	401	ATP	C4-C5-N7	-3.07	107.07	110.58
4	M	401	ATP	C5-C4-N3	-3.04	122.53	126.72
4	M	401	ATP	N6-C6-N1	2.95	124.95	118.38
4	L	401	ATP	N6-C6-N1	2.88	124.80	118.38
4	L	401	ATP	C4-N9-C8	-2.75	102.85	105.74
4	H	401	ATP	O5'-C5'-C4'	2.72	118.27	108.99
4	L	401	ATP	C6-C5-N7	-2.70	126.88	132.09
6	I	401	ADP	C2'-C1'-N9	-2.70	106.60	113.30
4	L	401	ATP	C5-C6-N1	-2.67	110.72	117.51
4	K	401	ATP	O3G-PG-O2G	2.64	117.72	107.80
4	K	401	ATP	O2B-PB-O3A	2.53	114.12	107.27
4	H	401	ATP	C6-C5-C4	2.42	120.48	117.18
4	H	401	ATP	C5'-C4'-C3'	2.40	123.87	115.21
6	I	401	ADP	C6-C5-C4	2.39	120.44	117.18
4	H	401	ATP	N6-C6-N1	2.38	123.68	118.38
6	I	401	ADP	C6-C5-N7	-2.32	127.63	132.09
4	H	401	ATP	C2'-C1'-N9	-2.28	107.65	113.30
4	M	401	ATP	C6-C5-C4	2.25	120.25	117.18
4	L	401	ATP	C2-N1-C6	2.23	122.39	118.73
6	I	401	ADP	O2B-PB-O1B	2.22	119.50	110.83
4	M	401	ATP	O4'-C4'-C3'	2.16	109.45	105.15
6	I	401	ADP	N3-C2-N1	2.15	131.83	128.58
4	L	401	ATP	O2A-PA-O3A	2.12	113.01	107.27
6	I	401	ADP	O2'-C2'-C1'	2.10	117.32	110.10
4	H	401	ATP	O4'-C1'-N9	2.08	112.09	108.09
4	L	401	ATP	O3A-PA-O1A	-2.04	104.56	110.70
4	L	401	ATP	O3B-PB-O1B	2.02	116.78	110.70
6	I	401	ADP	C1'-N9-C8	2.01	131.56	127.09
4	L	401	ATP	O3'-C3'-C4'	-2.01	105.32	111.08

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	401	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	K	401	ATP	PB-O3B-PG-O2G
4	K	401	ATP	PB-O3B-PG-O3G
4	K	401	ATP	C5'-O5'-PA-O1A
4	L	401	ATP	PB-O3B-PG-O2G
4	L	401	ATP	C5'-O5'-PA-O1A
4	L	401	ATP	C5'-O5'-PA-O2A
4	L	401	ATP	C5'-O5'-PA-O3A
4	M	401	ATP	C5'-O5'-PA-O2A
4	M	401	ATP	C5'-O5'-PA-O3A
4	K	401	ATP	C4'-C5'-O5'-PA
4	K	401	ATP	PB-O3A-PA-O5'
4	K	401	ATP	PG-O3B-PB-O2B
4	H	401	ATP	C4'-C5'-O5'-PA
4	H	401	ATP	C5'-O5'-PA-O1A
4	M	401	ATP	PB-O3B-PG-O1G
4	M	401	ATP	PA-O3A-PB-O1B
4	K	401	ATP	PB-O3B-PG-O1G
4	L	401	ATP	PB-O3B-PG-O1G
6	I	401	ADP	PA-O3A-PB-O1B
4	H	401	ATP	PA-O3A-PB-O1B
4	L	401	ATP	PG-O3B-PB-O2B

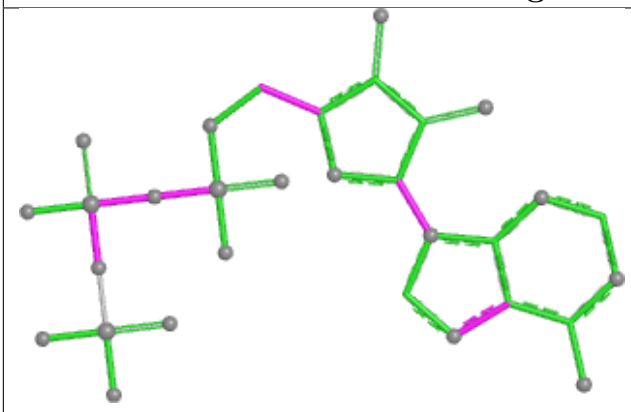
There are no ring outliers.

3 monomers are involved in 17 short contacts:

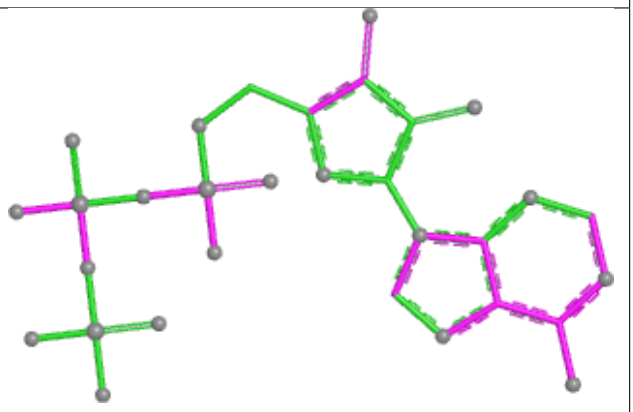
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	401	ATP	2	0
6	I	401	ADP	10	0
4	K	401	ATP	5	0

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

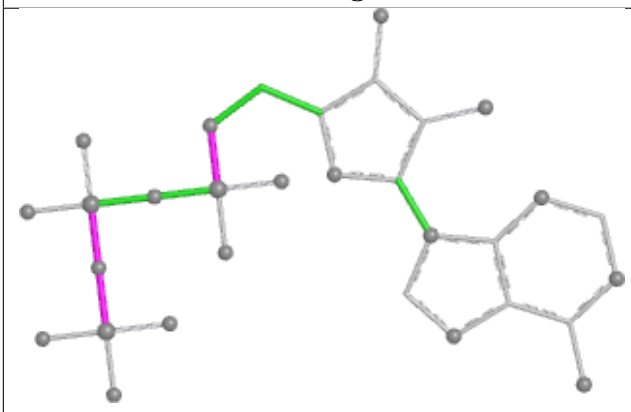
Ligand ATP L 401



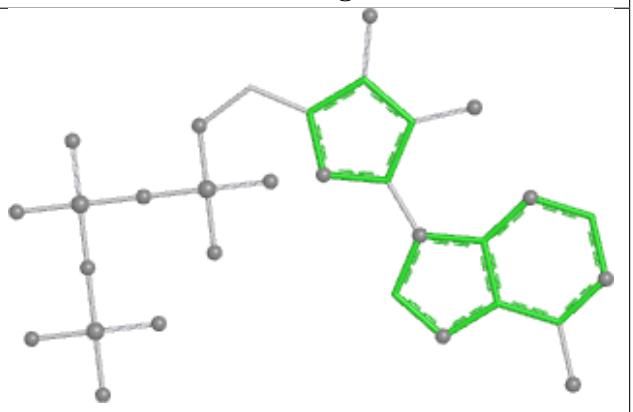
Bond lengths



Bond angles

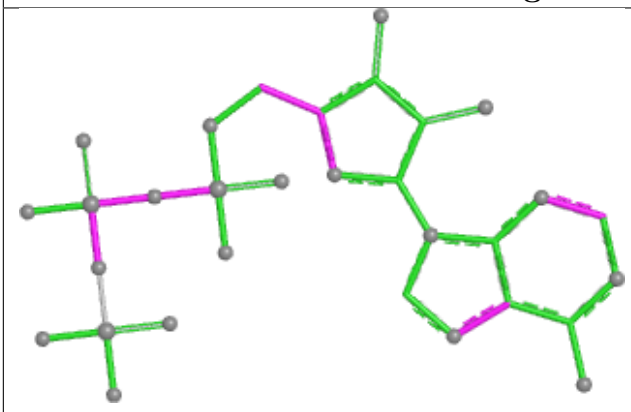


Torsions

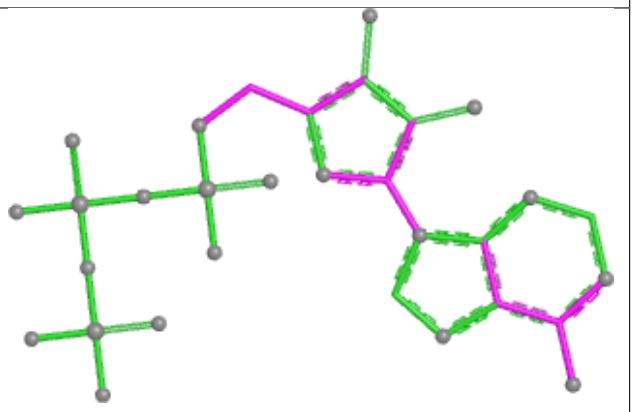


Rings

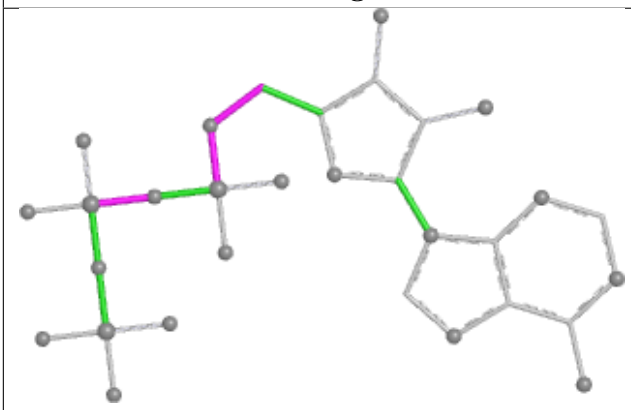
Ligand ATP H 401



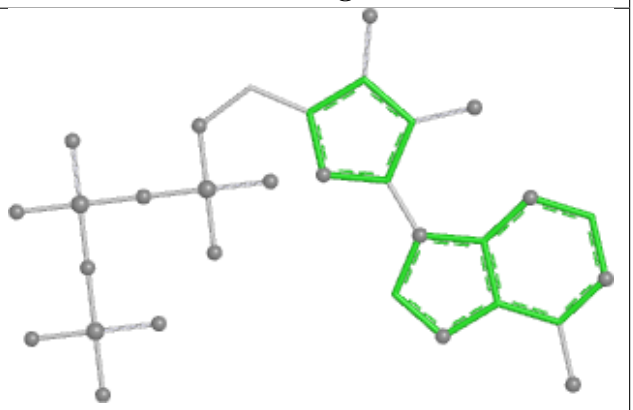
Bond lengths



Bond angles

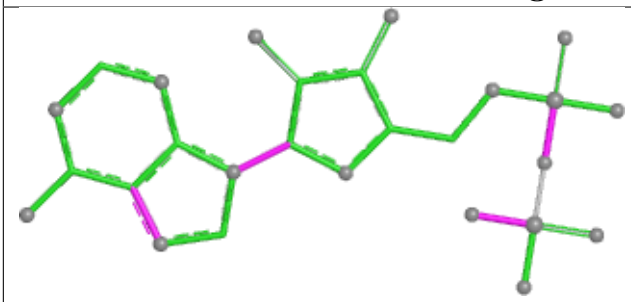


Torsions

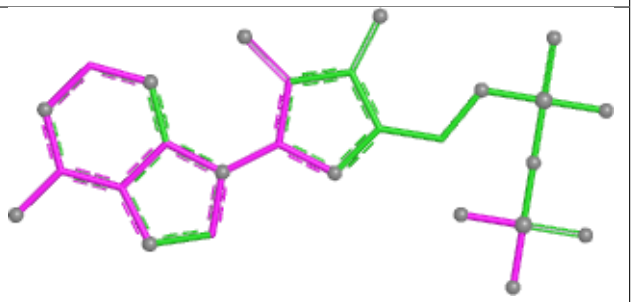


Rings

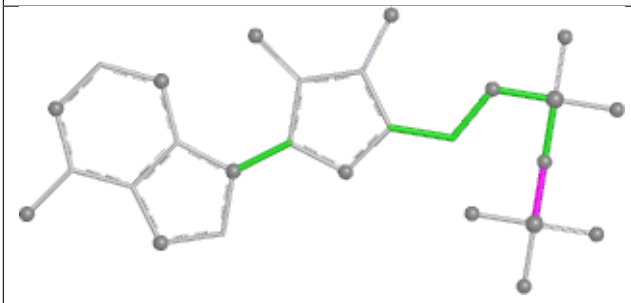
Ligand ADP I 401



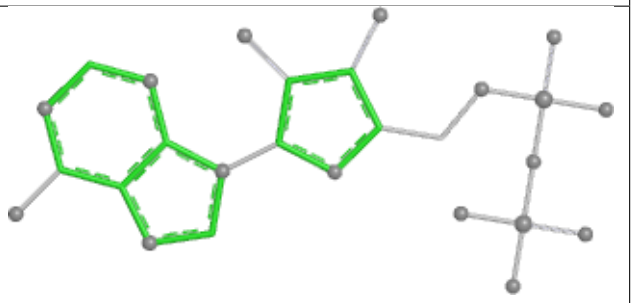
Bond lengths



Bond angles

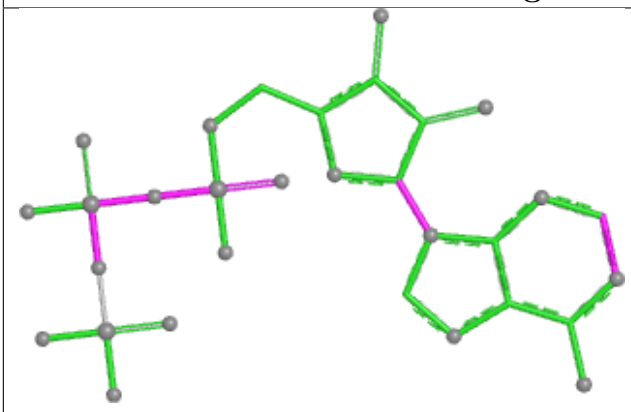


Torsions

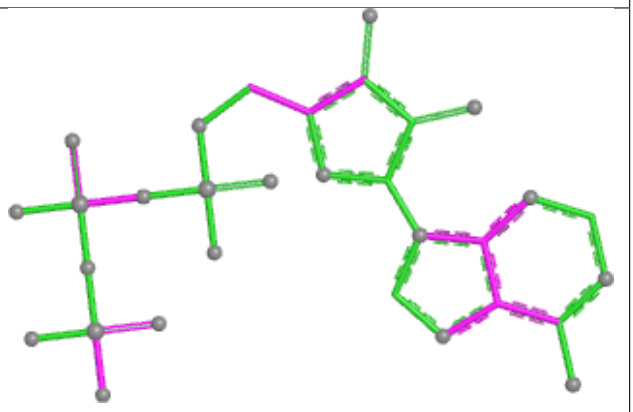


Rings

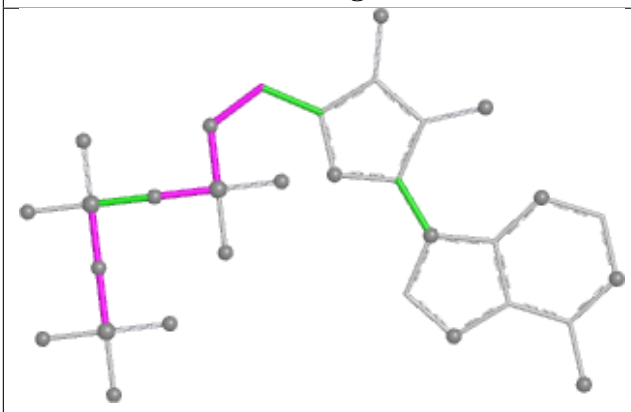
Ligand ATP K 401



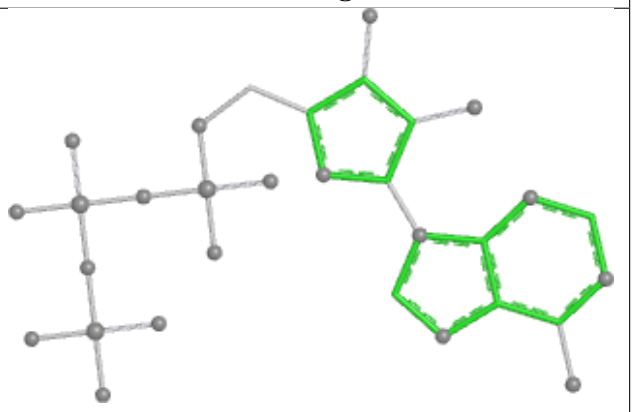
Bond lengths



Bond angles

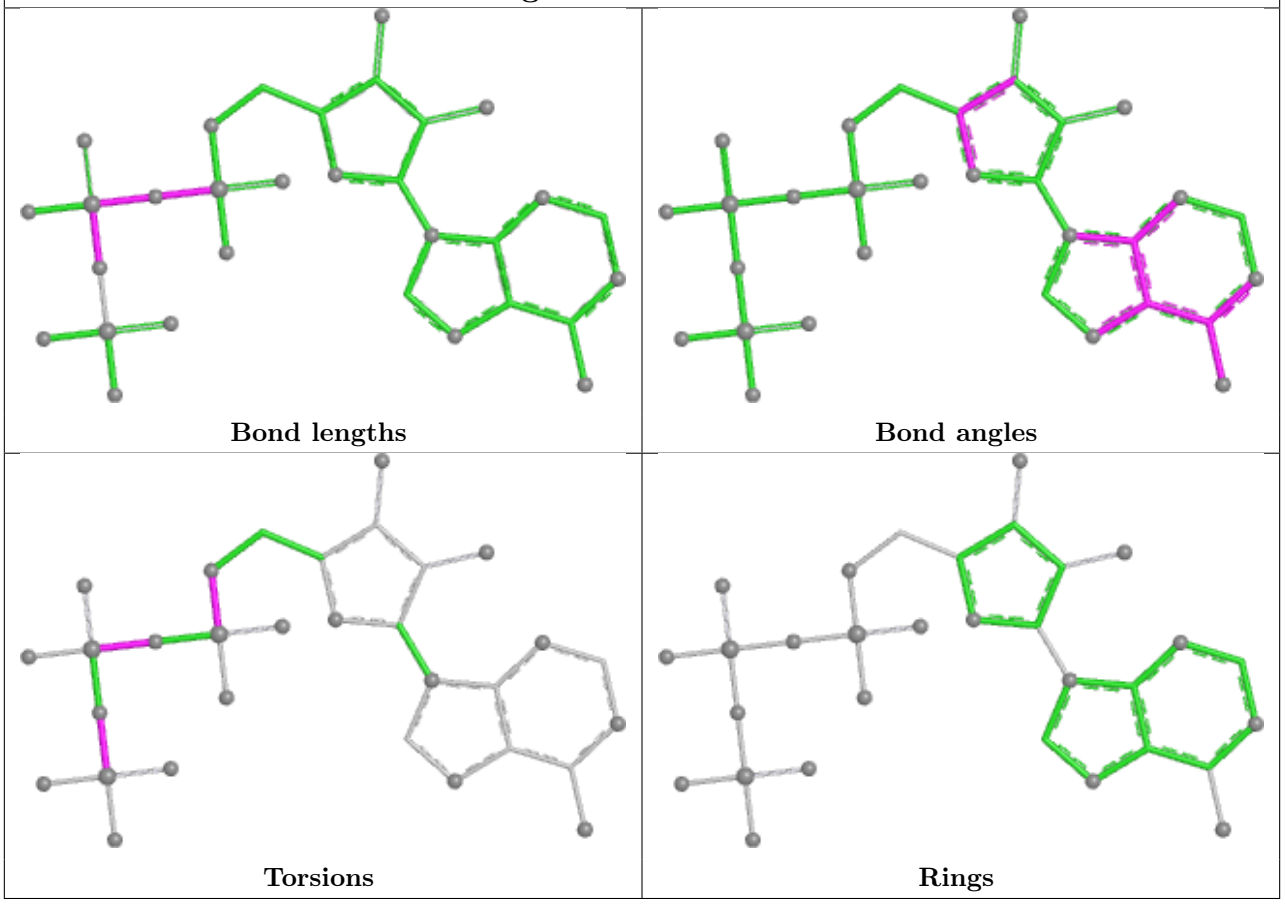


Torsions



Rings

Ligand ATP M 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

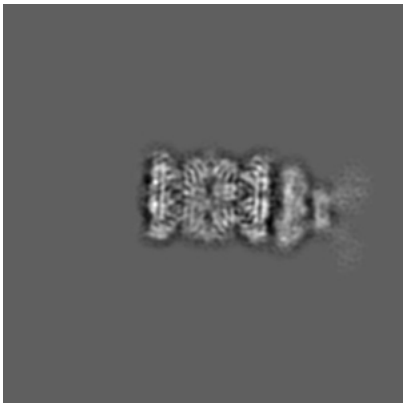
This section contains visualisations of the EMDB entry EMD-0216. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

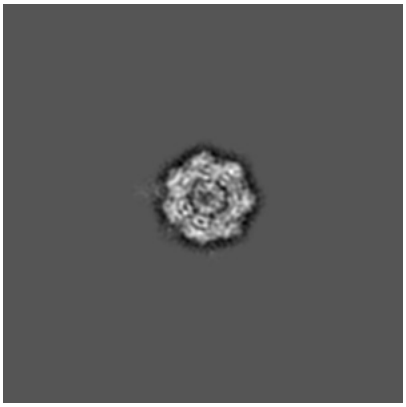
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

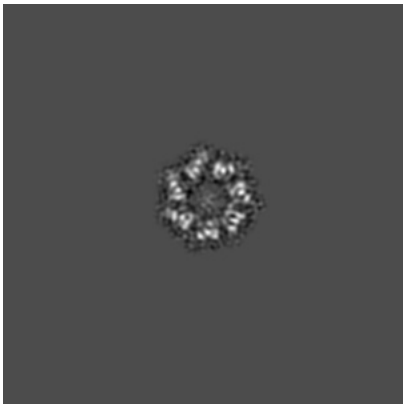
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192



Z Index: 192

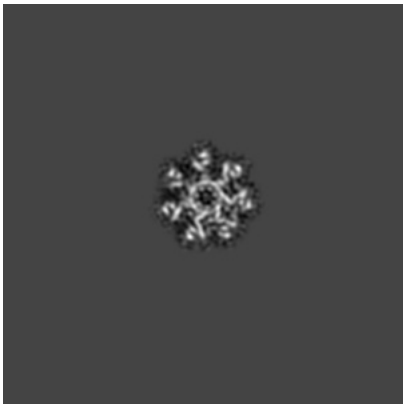
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 179

Y Index: 211

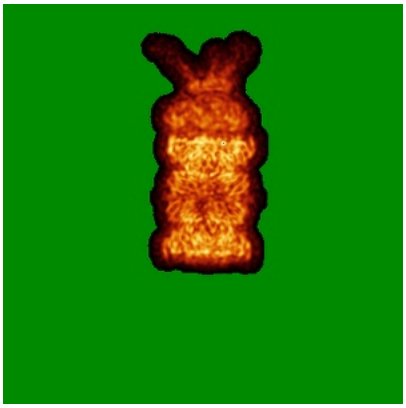


Z Index: 251

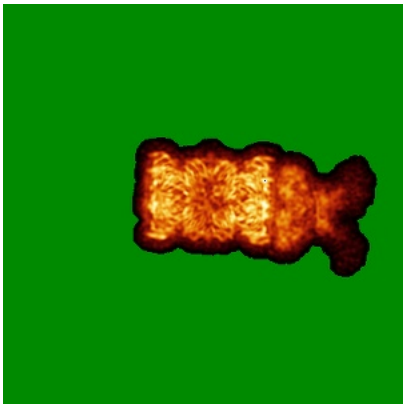
The images above show the largest variance slices of the map in three orthogonal directions.

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

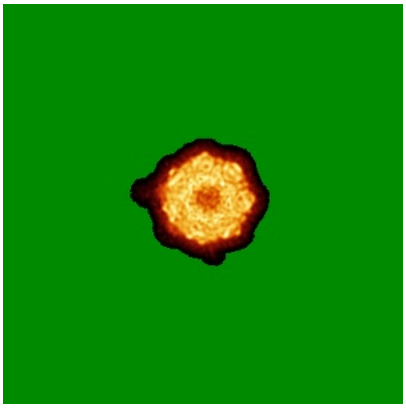
6.4.1 Primary map



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)

This section was not generated.

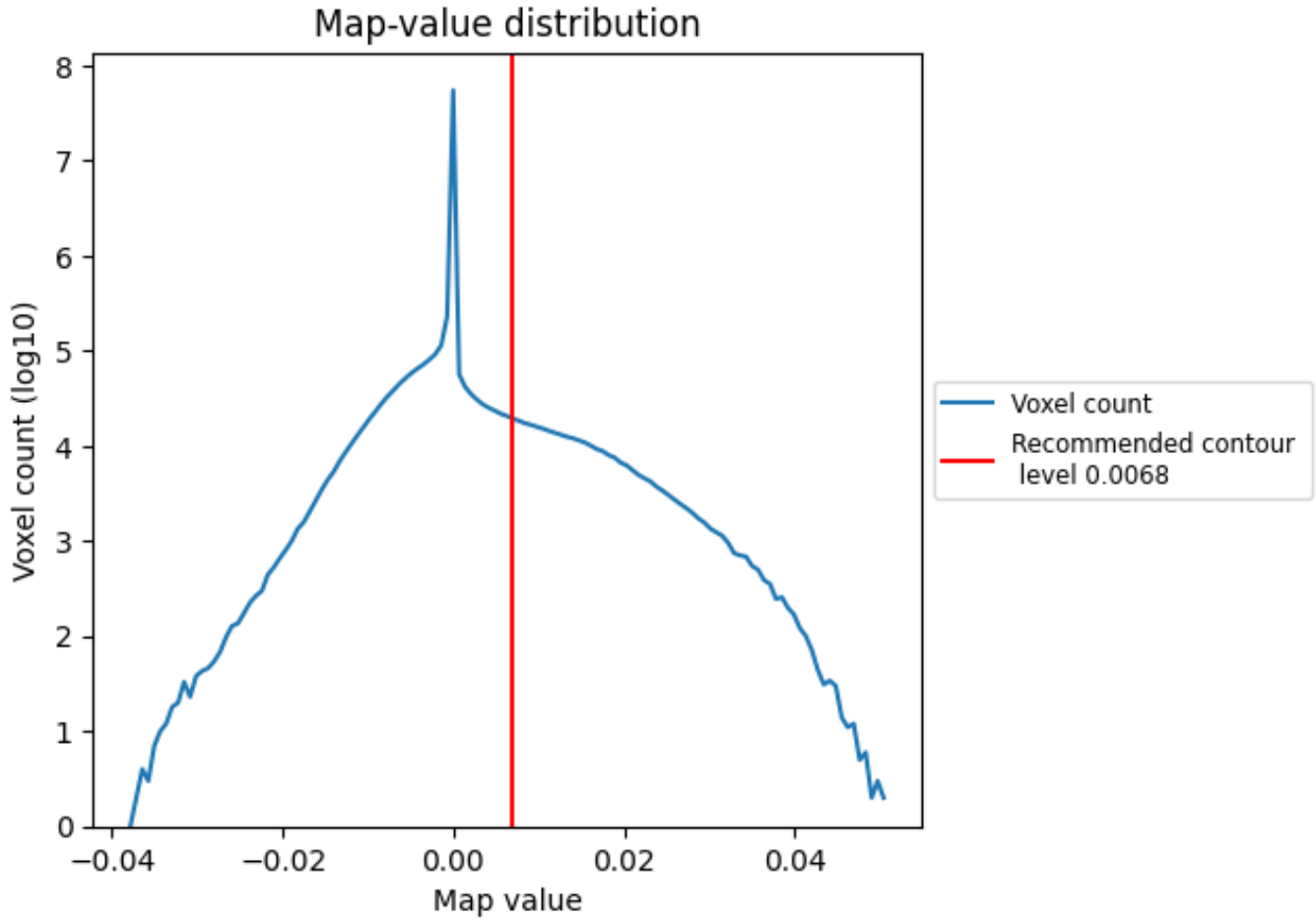
6.6 Mask visualisation (i)

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

7 Map analysis

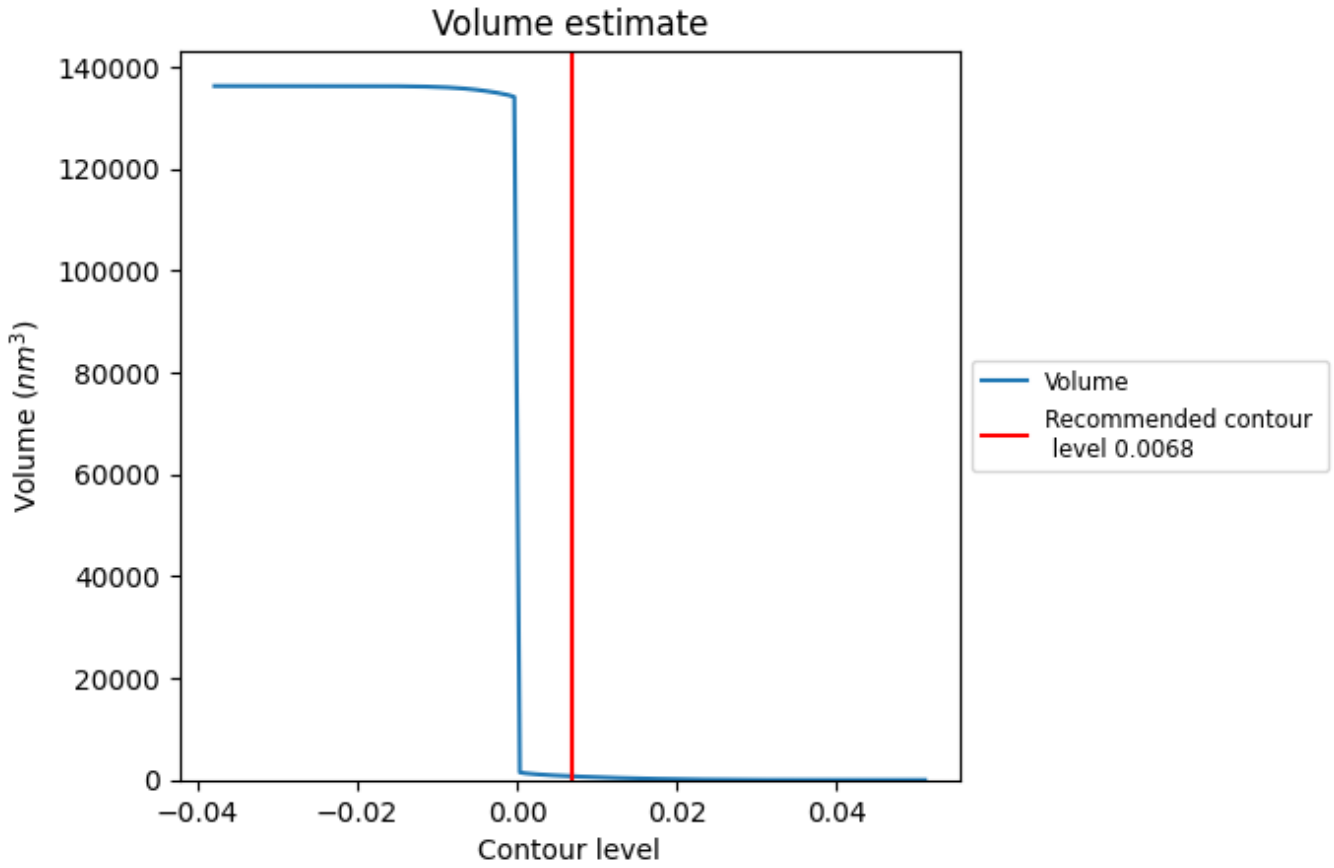
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

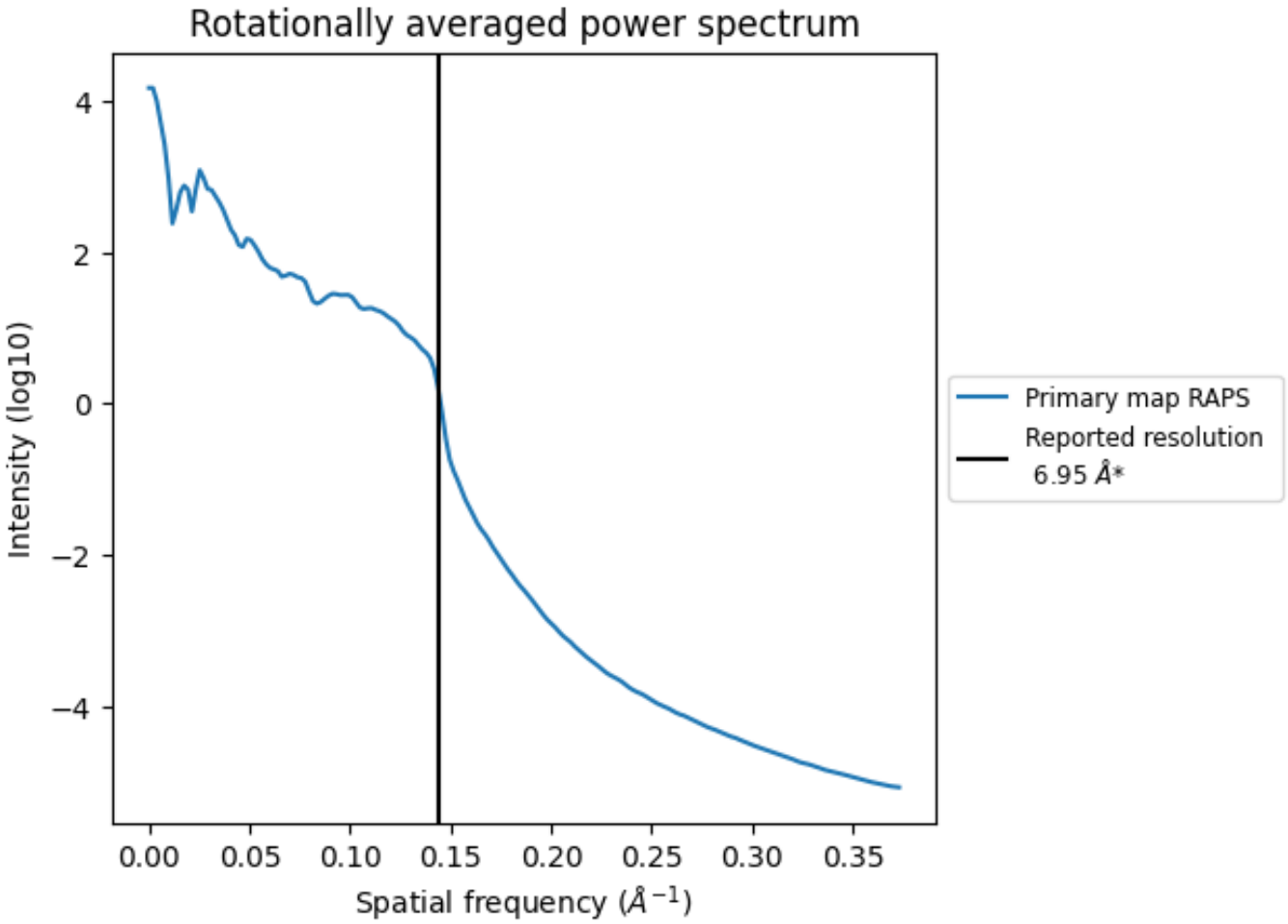
7.2 Volume estimate



The volume at the recommended contour level is 735 nm^3; this corresponds to an approximate mass of 664 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.144 Å^{-1}

8 Fourier-Shell correlation

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

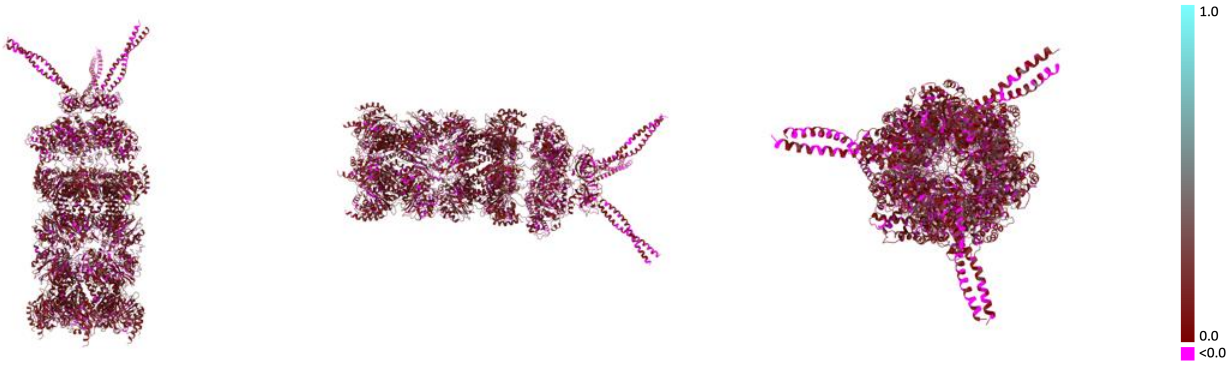
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0216 and PDB model 6HED. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay

This section was not generated.

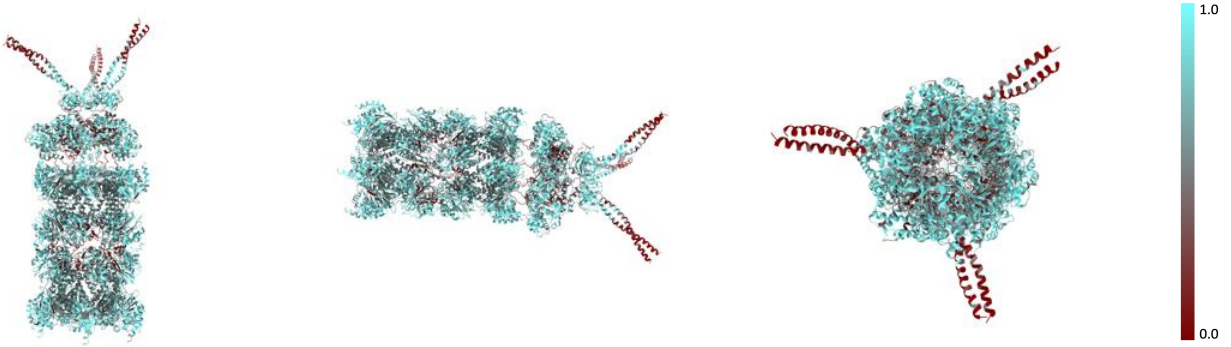
9.2 Q-score mapped to coordinate model



X Y Z

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

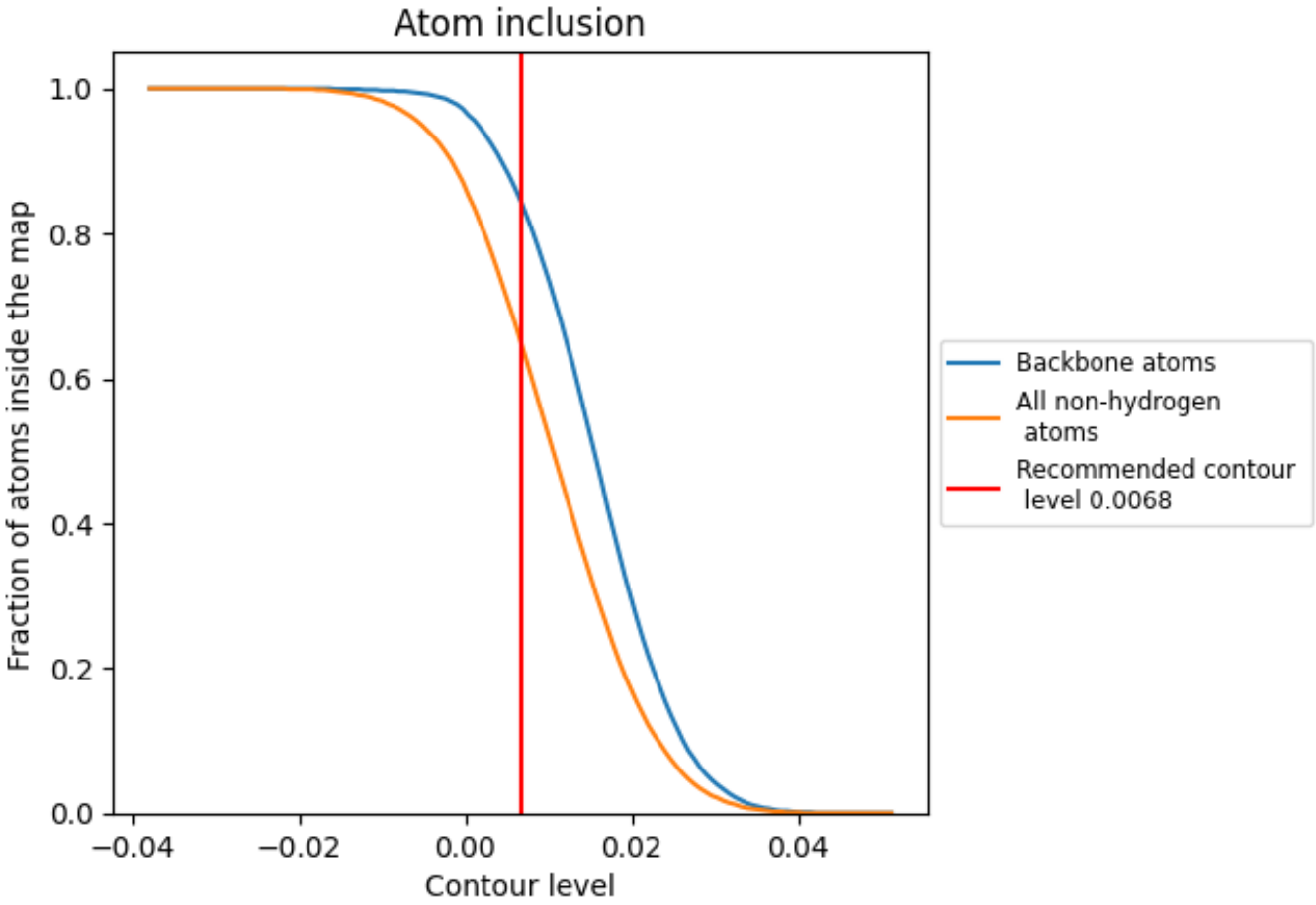
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0068).

9.4 Atom inclusion (i)



At the recommended contour level, 84% 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 (0.0068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.1140
1	0.6200	0.1150
2	0.6370	0.1220
3	0.6500	0.1250
4	0.6300	0.1240
5	0.6390	0.1210
6	0.6310	0.1130
7	0.6250	0.1180
A	0.7020	0.1320
B	0.7080	0.1380
C	0.6960	0.1320
D	0.6820	0.1340
E	0.6990	0.1300
F	0.7050	0.1370
G	0.7010	0.1310
H	0.6150	0.0960
I	0.6150	0.0860
J	0.5680	0.0880
K	0.6050	0.0950
L	0.5940	0.0860
M	0.6120	0.1000
a	0.6920	0.1210
b	0.6880	0.1220
c	0.6830	0.1180
d	0.6730	0.1160
e	0.6940	0.1220
f	0.6680	0.1160
g	0.6890	0.1270
h	0.6400	0.1210
i	0.6200	0.1210
j	0.6100	0.1160
k	0.6130	0.1210
l	0.6230	0.1210
m	0.6020	0.1080
n	0.6270	0.1080