wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	3J34
EMDB ID:	:	EMD-5582
Title	:	Structure of HIV-1 Capsid Protein by Cryo-EM
Authors	:	Zhao, G.; Perilla, J.R.; Yufenyuy, E.; Meng, X.; Chen, B.; Ning, J.; Ahn, J.; Gronenborn, A.M.; Schulten, K.; Aiken, C.; Zhang, P.
Deposited on	:	2013-02-23
Resolution	:	8.60 Å(reported)
Based on PDB ID	:	2KOD, 3H47

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

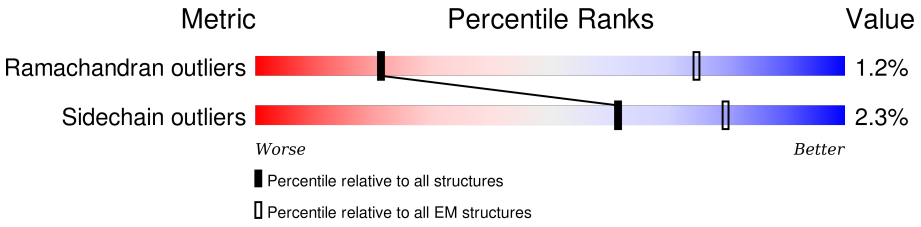
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.60 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)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	5	231	75% 23% •
1	6	231	77% 20% •
1	7	231	76% 22% •
1	A	231	77% 22% •
1	B	231	76% 23% •
1	C	231	80% 18% •
1	D	231	76% 23% •
1	E	231	77% 22% •
1	F	231	78% 21% •
1	G	231	80% 18% •
1	H	231	82% 17% •

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Mol	Chain	Length	Quality of chain
1	I	231	76% 23%
1	J	231	78% 18%
1	K	231	78% 18%
1	L	231	78% 19%
1	M	231	77% 21%
1	N	231	74% 24%
1	O	231	81% 18%
1	P	231	76% 22%
1	Q	231	80% 18%
1	R	231	82% 17%
1	S	231	82% 16%
1	T	231	82% 16%
1	U	231	77% 19%
1	V	231	77% 20%
1	W	231	73% 26%
1	X	231	79% 21%
1	Y	231	75% 22%
1	Z	231	81% 15%
1	a	231	78% 20%
1	b	231	76% 21%
1	c	231	80% 17%
1	d	231	76% 22%
1	e	231	76% 20%
1	f	231	81% 17%
1	g	231	81% 17%

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Mol	Chain	Length	Quality of chain
1	h	231	75% 22%
1	i	231	81% 17%
1	j	231	76% 22%
1	k	231	76% 21%
1	l	231	78% 20%
1	m	231	81% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 75600 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 capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
B	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
C	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
D	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
E	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
F	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
G	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
H	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
I	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
J	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
K	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
L	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
M	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
N	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
O	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
P	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
Q	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
R	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
S	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
T	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
U	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
V	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
W	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
X	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
Y	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
Z	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
5	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
a	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
b	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
c	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
6	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791

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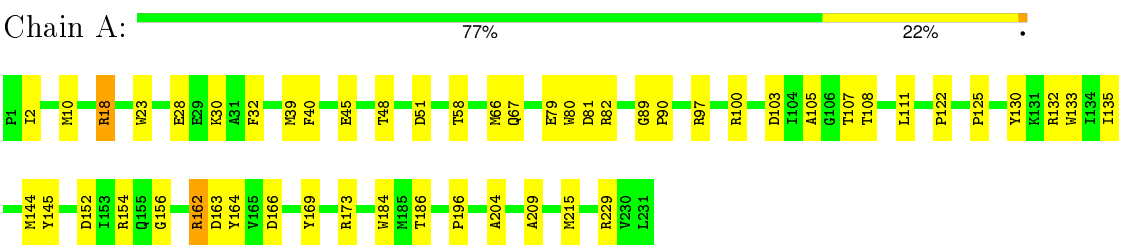
Chain	Residue	Modelled	Actual	Comment	Reference
i	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
j	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
k	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
l	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
m	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
7	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
d	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
e	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
f	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
g	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791
h	92	GLU	ALA	ENGINEERED MUTATION	UNP Q79791

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

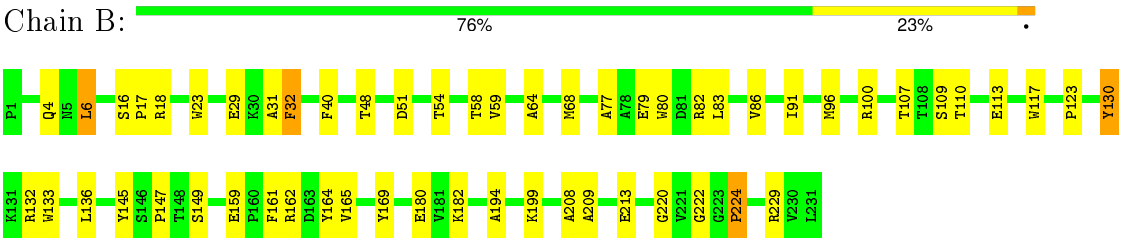
- Molecule 1: capsid protein

Chain A:



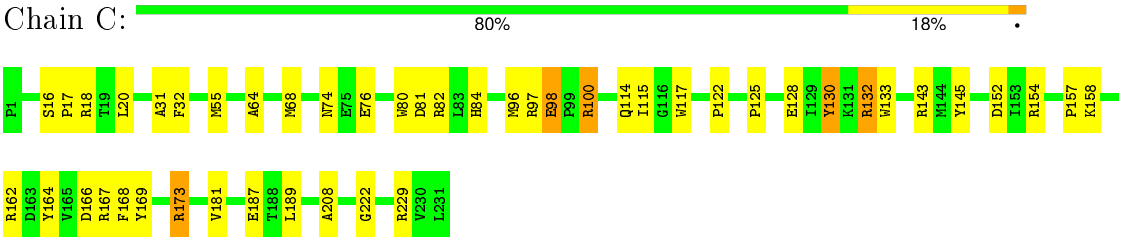
- Molecule 1: capsid protein

Chain B:



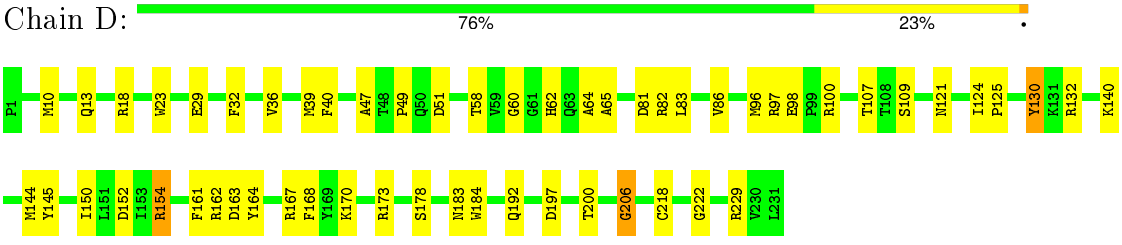
- Molecule 1: capsid protein

Chain C:



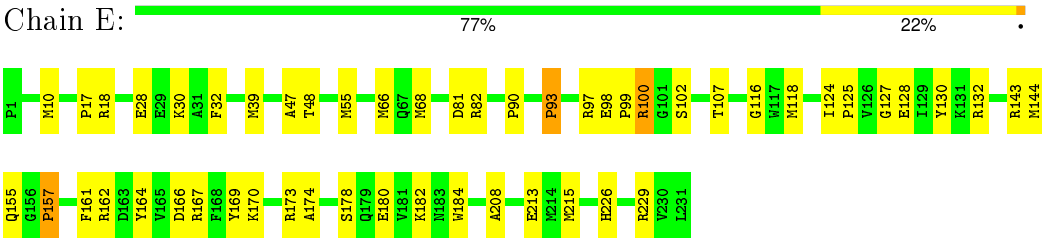
- Molecule 1: capsid protein

Chain D:



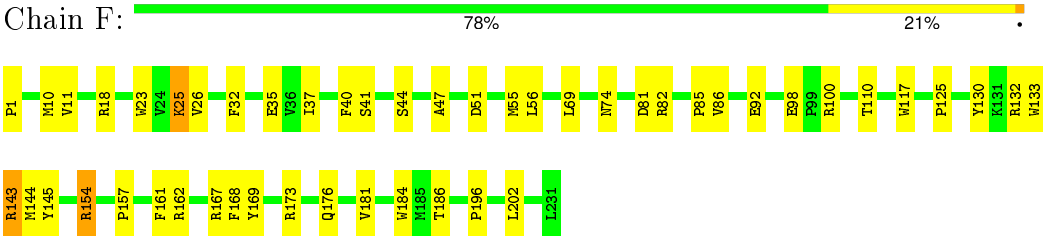
- Molecule 1: capsid protein

Chain E:



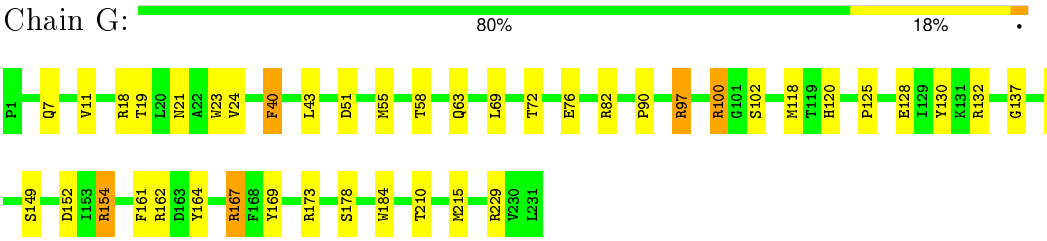
• Molecule 1: capsid protein

Chain F:



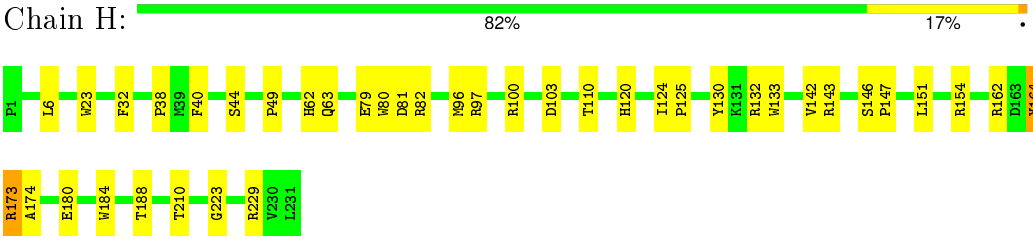
• Molecule 1: capsid protein

Chain G:



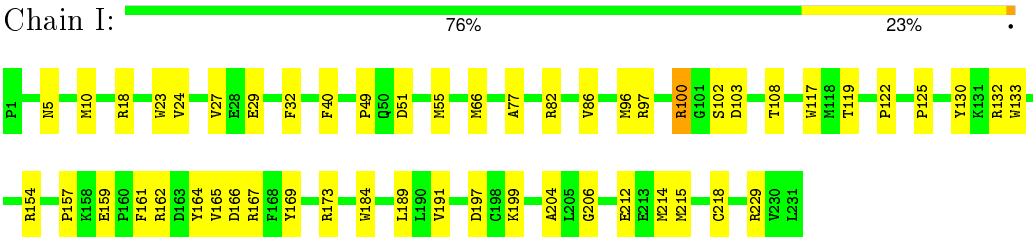
• Molecule 1: capsid protein

Chain H:



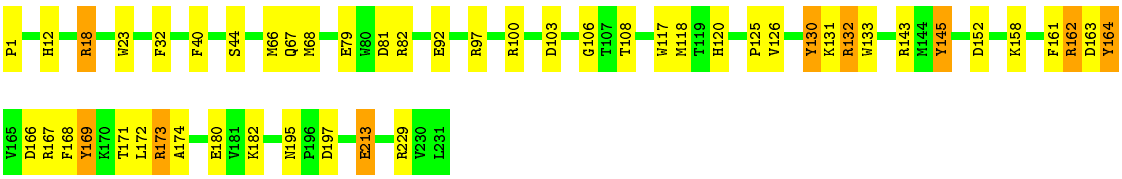
• Molecule 1: capsid protein

Chain I:



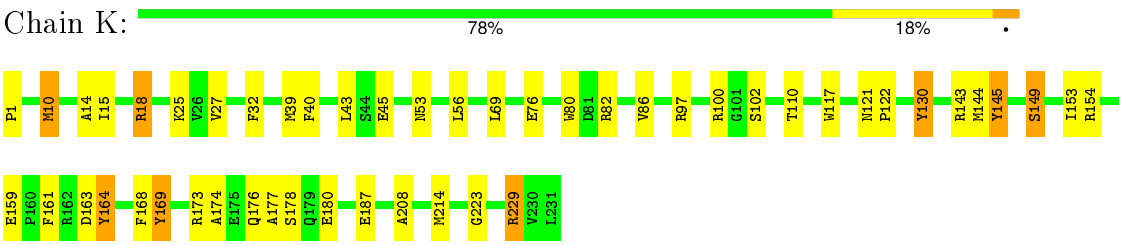
• Molecule 1: capsid protein

Chain J:



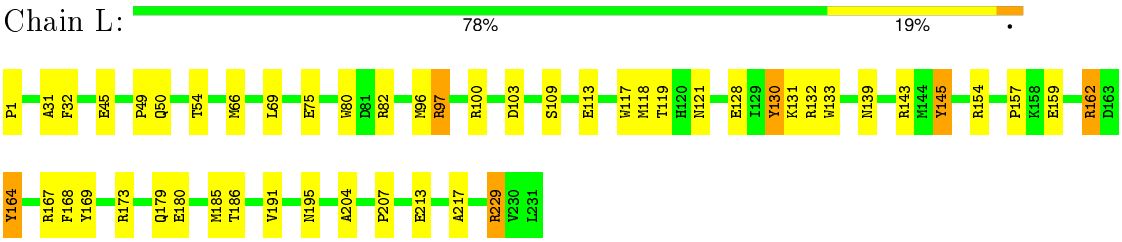
• Molecule 1: capsid protein

Chain K:



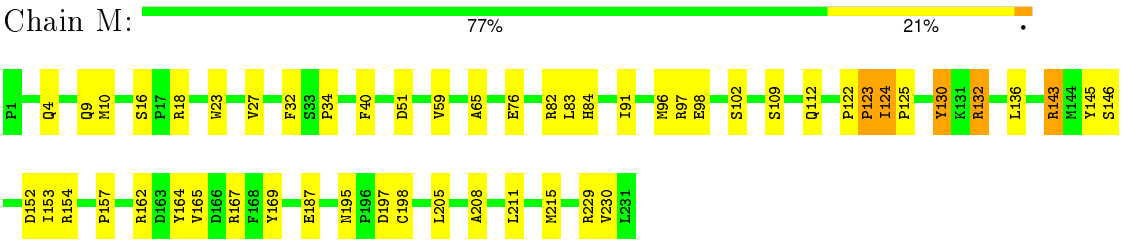
• Molecule 1: capsid protein

Chain L:



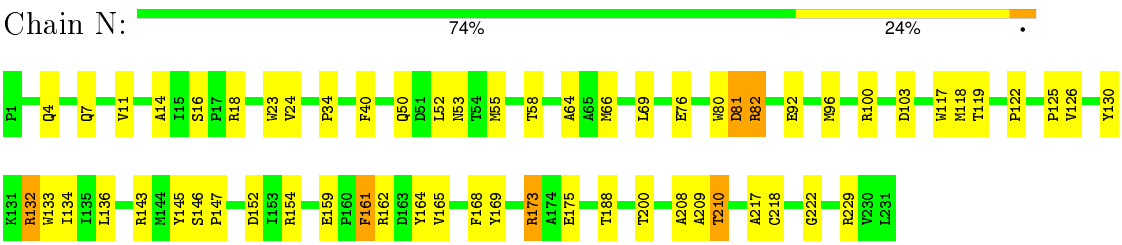
• Molecule 1: capsid protein

Chain M:



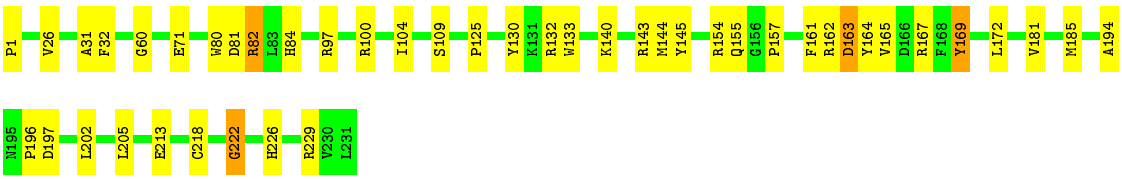
• Molecule 1: capsid protein

Chain N:



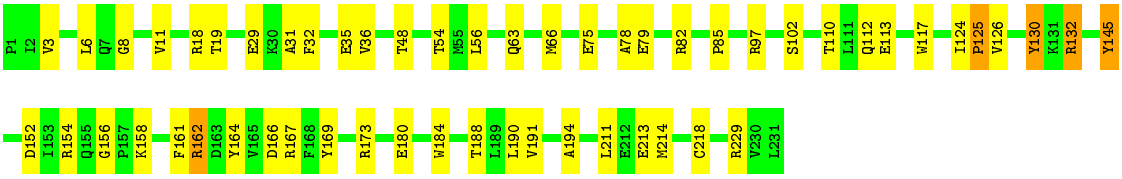
• Molecule 1: capsid protein

Chain O:



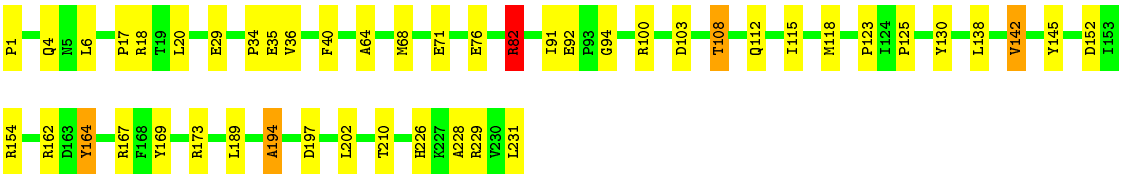
• Molecule 1: capsid protein

Chain P:



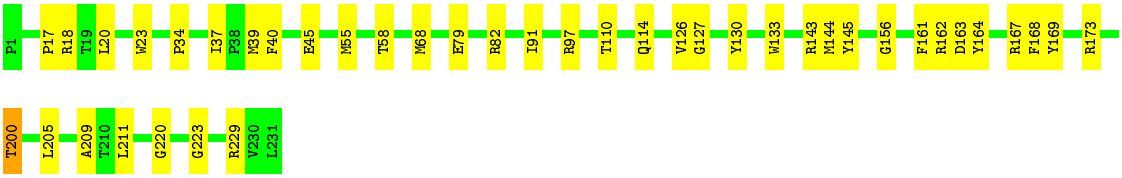
• Molecule 1: capsid protein

Chain Q:



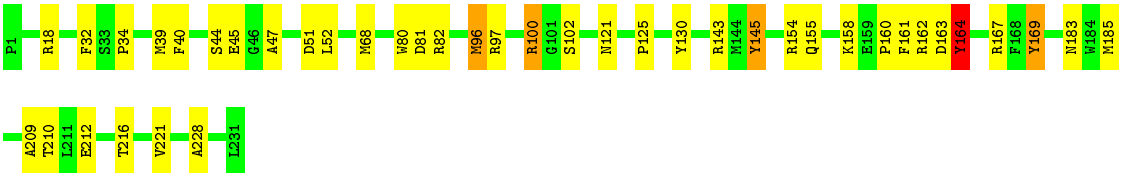
• Molecule 1: capsid protein

Chain R:



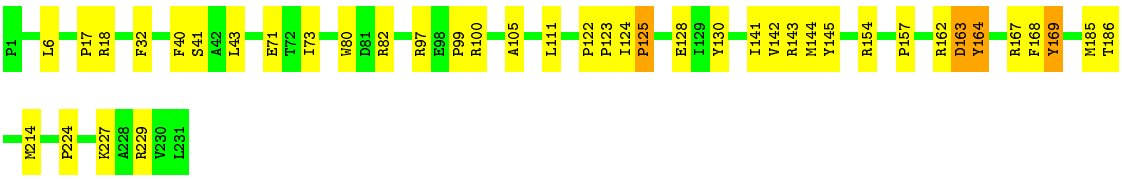
• Molecule 1: capsid protein

Chain S:



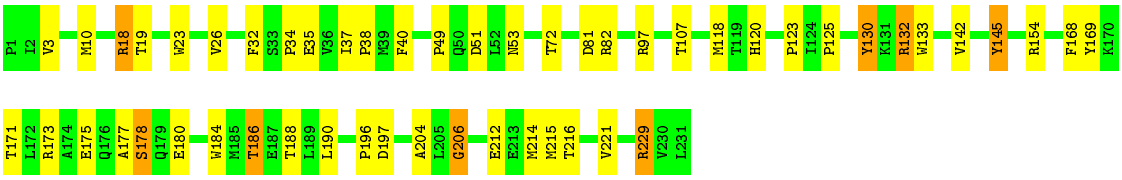
• Molecule 1: capsid protein

Chain T:



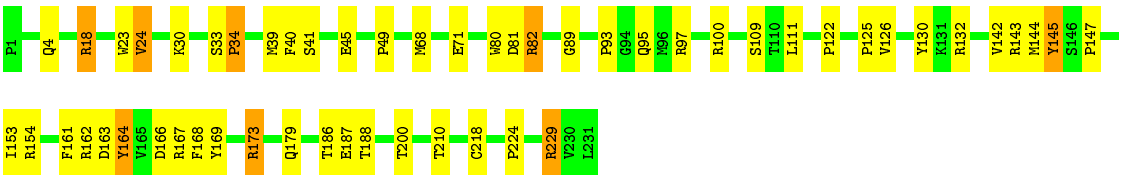
- Molecule 1: capsid protein

Chain U:



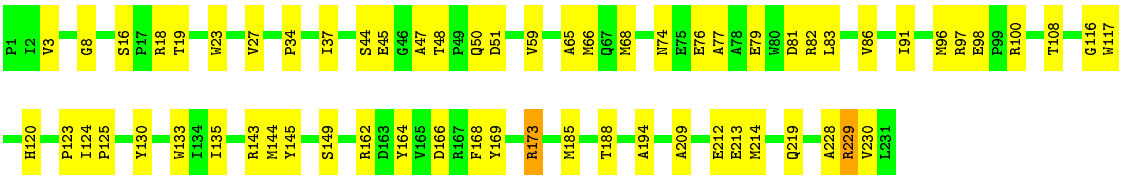
- Molecule 1: capsid protein

Chain V:



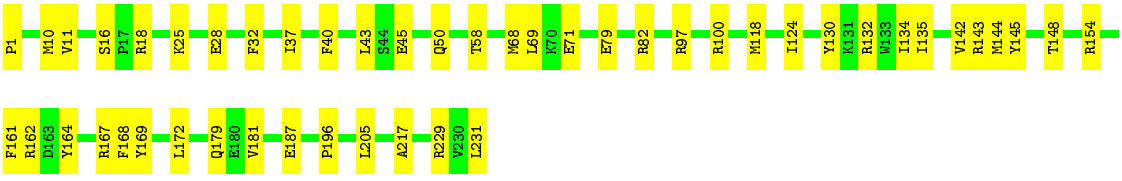
- Molecule 1: capsid protein

Chain W:



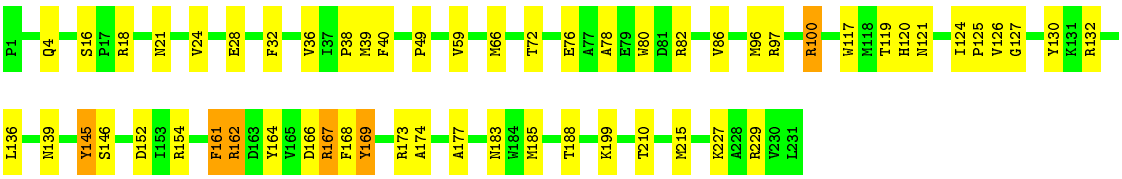
- Molecule 1: capsid protein

Chain X:



- Molecule 1: capsid protein

Chain Y:

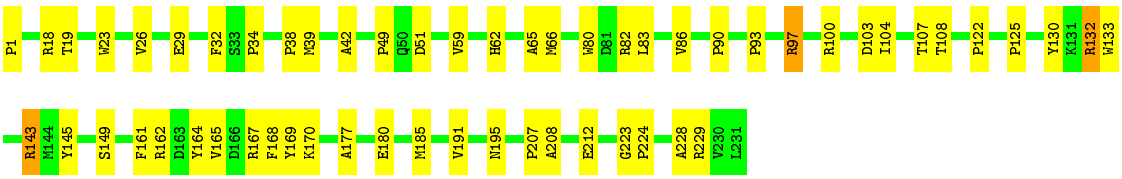


- Molecule 1: capsid protein

Chain Z:

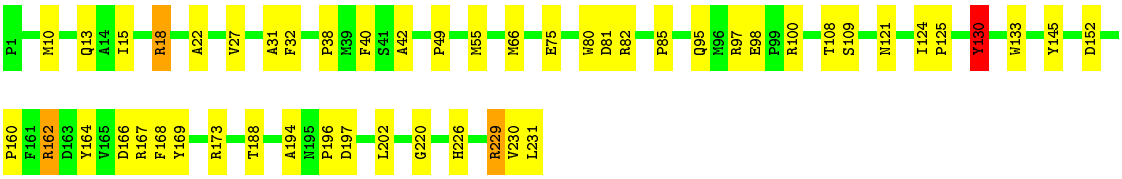
- Molecule 1: capsid protein

Chain 5:



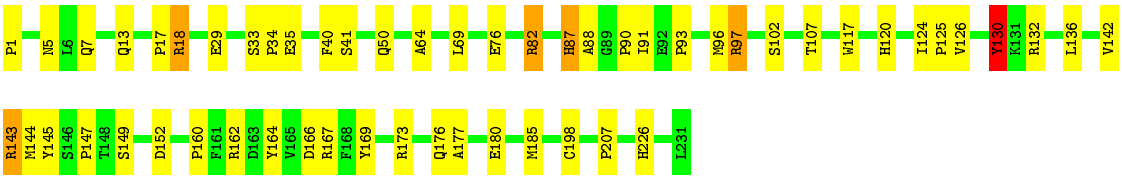
- Molecule 1: capsid protein

Chain a:



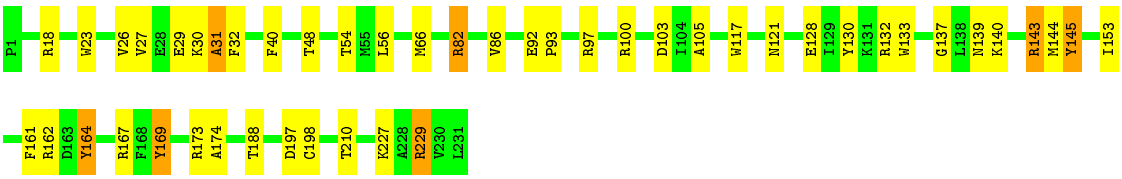
- Molecule 1: capsid protein

Chain b:



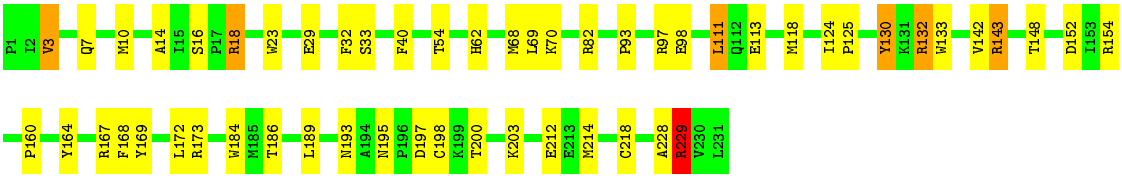
- Molecule 1: capsid protein

Chain c:



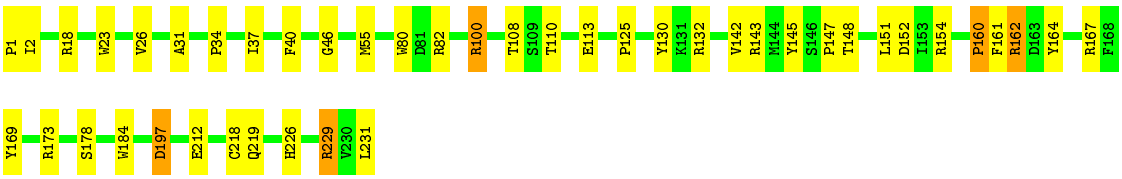
• Molecule 1: capsid protein

Chain 6:



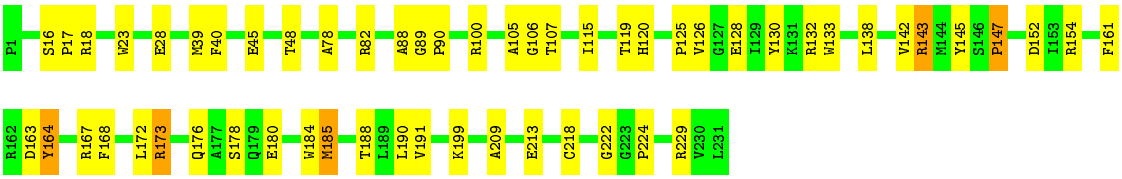
• Molecule 1: capsid protein

Chain i:



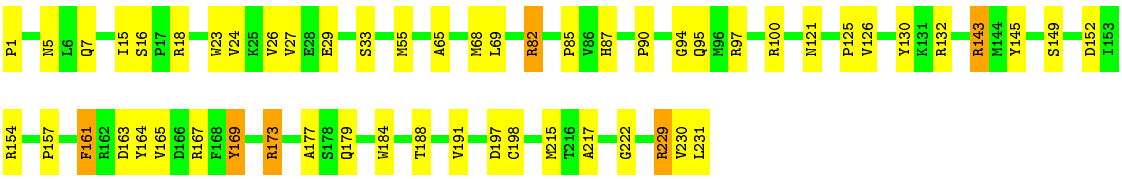
• Molecule 1: capsid protein

Chain j:



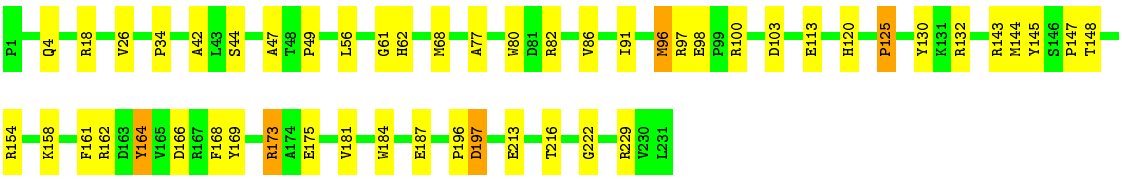
• Molecule 1: capsid protein

Chain k:



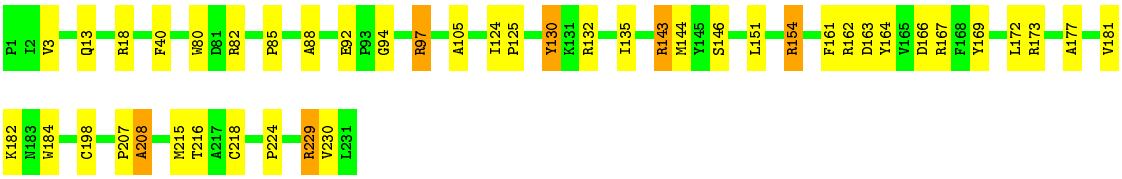
• Molecule 1: capsid protein

Chain l:



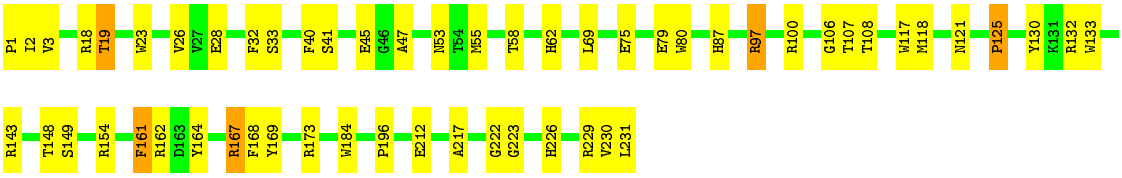
• Molecule 1: capsid protein

Chain m:



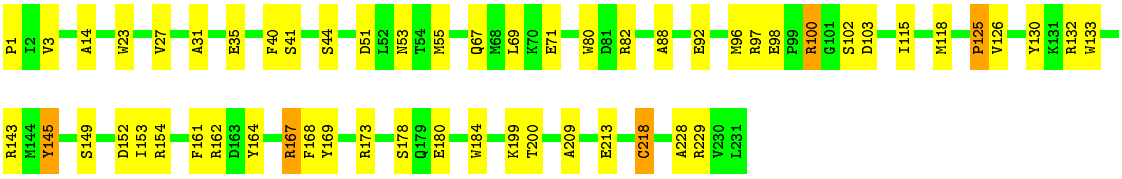
• Molecule 1: capsid protein

Chain 7:



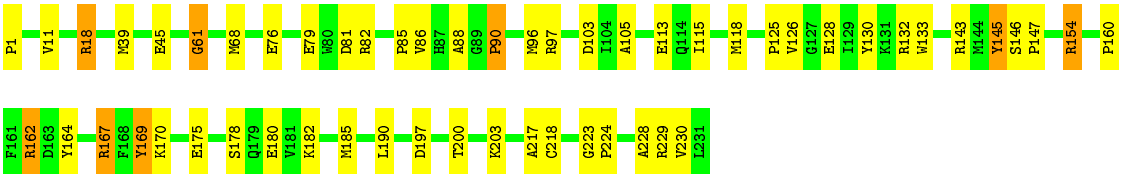
• Molecule 1: capsid protein

Chain d:



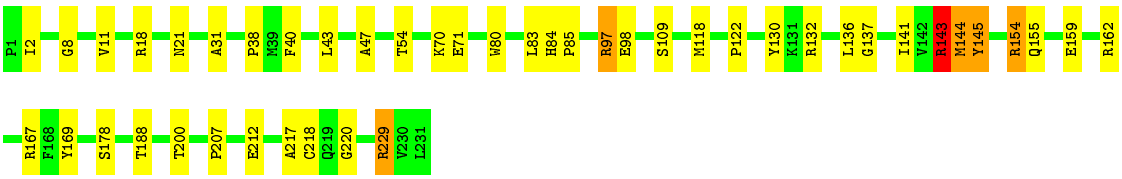
• Molecule 1: capsid protein

Chain e:



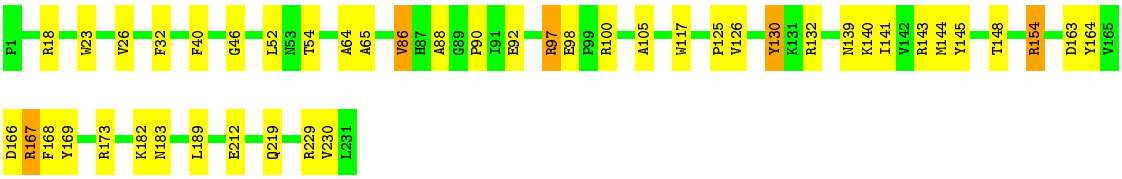
• Molecule 1: capsid protein

Chain f:



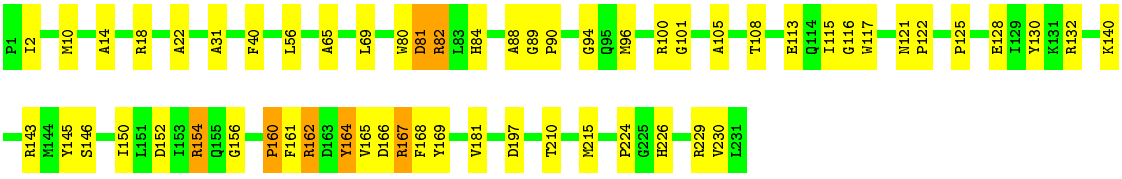
- Molecule 1: capsid protein

Chain g:



- Molecule 1: capsid protein

Chain h:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	3210	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each filament	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	Kodak SO163	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	5	1.71	15/1841 (0.8%)	1.94	46/2500 (1.8%)
1	6	1.68	9/1841 (0.5%)	2.15	60/2500 (2.4%)
1	7	1.61	13/1841 (0.7%)	2.00	51/2500 (2.0%)
1	A	1.66	14/1841 (0.8%)	2.03	47/2500 (1.9%)
1	B	1.64	8/1841 (0.4%)	2.02	50/2500 (2.0%)
1	C	1.62	5/1841 (0.3%)	1.92	41/2500 (1.6%)
1	D	1.63	9/1841 (0.5%)	1.96	51/2500 (2.0%)
1	E	1.68	12/1841 (0.7%)	1.98	40/2500 (1.6%)
1	F	1.68	10/1841 (0.5%)	1.99	52/2500 (2.1%)
1	G	1.65	6/1841 (0.3%)	2.00	50/2500 (2.0%)
1	H	1.65	10/1841 (0.5%)	1.95	41/2500 (1.6%)
1	I	1.64	10/1841 (0.5%)	1.94	48/2500 (1.9%)
1	J	1.74	18/1841 (1.0%)	2.01	52/2500 (2.1%)
1	K	1.72	14/1841 (0.8%)	1.95	42/2500 (1.7%)
1	L	1.68	12/1841 (0.7%)	2.05	59/2500 (2.4%)
1	M	1.66	12/1841 (0.7%)	2.09	56/2500 (2.2%)
1	N	1.68	11/1841 (0.6%)	2.05	62/2500 (2.5%)
1	O	1.69	12/1841 (0.7%)	2.01	42/2500 (1.7%)
1	P	1.63	16/1841 (0.9%)	2.05	54/2500 (2.2%)
1	Q	1.66	13/1841 (0.7%)	1.93	36/2500 (1.4%)
1	R	1.62	12/1841 (0.7%)	1.87	34/2500 (1.4%)
1	S	1.68	9/1841 (0.5%)	1.89	38/2500 (1.5%)
1	T	1.68	10/1841 (0.5%)	2.05	41/2500 (1.6%)
1	U	1.73	13/1841 (0.7%)	1.89	46/2500 (1.8%)
1	V	1.71	19/1841 (1.0%)	1.97	40/2500 (1.6%)
1	W	1.70	15/1841 (0.8%)	2.06	56/2500 (2.2%)
1	X	1.68	17/1841 (0.9%)	2.07	41/2500 (1.6%)
1	Y	1.68	9/1841 (0.5%)	2.00	43/2500 (1.7%)
1	Z	1.65	9/1841 (0.5%)	1.96	38/2500 (1.5%)
1	a	1.68	7/1841 (0.4%)	1.96	50/2500 (2.0%)
1	b	1.67	9/1841 (0.5%)	1.92	42/2500 (1.7%)
1	c	1.67	12/1841 (0.7%)	1.95	44/2500 (1.8%)
1	d	1.68	13/1841 (0.7%)	1.95	51/2500 (2.0%)
1	e	1.70	14/1841 (0.8%)	1.95	42/2500 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
1	f	1.70	11/1841 (0.6%)	1.89	32/2500 (1.3%)
1	g	1.64	12/1841 (0.7%)	1.94	42/2500 (1.7%)
1	h	1.69	17/1841 (0.9%)	2.07	48/2500 (1.9%)
1	i	1.63	13/1841 (0.7%)	2.01	41/2500 (1.6%)
1	j	1.66	12/1841 (0.7%)	2.02	46/2500 (1.8%)
1	k	1.70	19/1841 (1.0%)	2.03	43/2500 (1.7%)
1	l	1.66	13/1841 (0.7%)	1.95	45/2500 (1.8%)
1	m	1.64	6/1841 (0.3%)	1.97	38/2500 (1.5%)
All	All	1.67	500/77322 (0.6%)	1.99	1921/105000 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	0	4
1	6	0	5
1	7	0	4
1	A	0	4
1	B	0	5
1	C	0	6
1	D	0	8
1	E	0	4
1	F	0	3
1	G	0	7
1	H	0	5
1	I	0	3
1	J	0	10
1	K	0	11
1	L	0	6
1	M	0	4
1	N	0	6
1	O	0	4
1	P	0	5
1	Q	0	3
1	R	0	3
1	S	0	6
1	T	0	3
1	U	0	7
1	V	0	9
1	W	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	3
1	Y	0	9
1	Z	0	10
1	a	0	5
1	b	0	9
1	c	0	10
1	d	0	6
1	e	0	6
1	f	0	8
1	g	0	4
1	h	0	7
1	i	0	6
1	j	0	9
1	k	0	7
1	l	0	6
1	m	0	6
All	All	0	251

All (500) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	145	TYR	CG-CD1	9.17	1.51	1.39
1	U	23	TRP	NE1-CE2	8.38	1.48	1.37
1	Q	94	GLY	N-CA	8.12	1.58	1.46
1	A	156	GLY	CA-C	-8.04	1.39	1.51
1	F	169	TYR	CE2-CZ	7.99	1.49	1.38
1	k	1	PRO	N-CD	7.95	1.58	1.47
1	K	159	GLU	CD-OE2	7.94	1.34	1.25
1	M	229	ARG	CD-NE	7.90	1.59	1.46
1	J	97	ARG	CD-NE	7.81	1.59	1.46
1	H	130	TYR	CE2-CZ	7.80	1.48	1.38
1	6	154	ARG	CD-NE	7.76	1.59	1.46
1	Z	92	GLU	CD-OE1	7.74	1.34	1.25
1	e	45	GLU	CD-OE1	7.71	1.34	1.25
1	f	212	GLU	CB-CG	7.70	1.66	1.52
1	S	34	PRO	N-CD	-7.69	1.37	1.47
1	Z	109	SER	CA-CB	7.67	1.64	1.52
1	c	229	ARG	CD-NE	7.62	1.59	1.46
1	A	89	GLY	CA-C	7.62	1.64	1.51
1	W	98	GLU	CD-OE2	7.61	1.34	1.25
1	W	16	SER	CB-OG	7.58	1.52	1.42
1	c	130	TYR	CE1-CZ	7.58	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	161	PHE	CG-CD2	7.57	1.50	1.38
1	f	8	GLY	CA-C	-7.48	1.39	1.51
1	h	94	GLY	CA-C	-7.39	1.40	1.51
1	I	132	ARG	CD-NE	7.38	1.58	1.46
1	M	102	SER	CA-CB	7.37	1.64	1.52
1	5	32	PHE	CB-CG	7.37	1.63	1.51
1	h	117	TRP	NE1-CE2	7.33	1.47	1.37
1	U	173	ARG	CD-NE	7.32	1.58	1.46
1	L	162	ARG	CD-NE	7.32	1.58	1.46
1	h	169	TYR	CG-CD1	7.30	1.48	1.39
1	K	145	TYR	CE2-CZ	7.28	1.48	1.38
1	R	164	TYR	CG-CD2	7.22	1.48	1.39
1	J	169	TYR	CG-CD2	7.20	1.48	1.39
1	i	169	TYR	CG-CD1	7.20	1.48	1.39
1	M	98	GLU	CB-CG	7.19	1.65	1.52
1	Q	92	GLU	CD-OE2	7.17	1.33	1.25
1	J	32	PHE	CG-CD2	7.12	1.49	1.38
1	N	16	SER	CA-CB	7.12	1.63	1.52
1	L	80	TRP	NE1-CE2	-7.02	1.28	1.37
1	Y	167	ARG	CD-NE	7.00	1.58	1.46
1	7	164	TYR	CD1-CE1	6.98	1.49	1.39
1	6	62	HIS	CB-CG	6.96	1.62	1.50
1	S	164	TYR	CD1-CE1	6.95	1.49	1.39
1	O	222	GLY	C-N	6.94	1.45	1.33
1	V	49	PRO	N-CD	-6.93	1.38	1.47
1	A	169	TYR	CE1-CZ	6.93	1.47	1.38
1	P	169	TYR	CZ-OH	6.92	1.49	1.37
1	M	205	LEU	CA-CB	6.91	1.69	1.53
1	V	109	SER	CB-OG	6.88	1.51	1.42
1	j	17	PRO	N-CD	-6.88	1.38	1.47
1	X	16	SER	CA-CB	6.87	1.63	1.52
1	S	145	TYR	CZ-OH	6.87	1.49	1.37
1	Y	164	TYR	CE1-CZ	6.85	1.47	1.38
1	V	122	PRO	N-CD	-6.83	1.38	1.47
1	O	32	PHE	CG-CD1	6.83	1.49	1.38
1	R	161	PHE	CG-CD2	6.82	1.49	1.38
1	V	224	PRO	N-CD	-6.82	1.38	1.47
1	Y	38	PRO	N-CD	-6.80	1.38	1.47
1	5	130	TYR	CG-CD1	6.79	1.48	1.39
1	b	33	SER	CA-CB	6.78	1.63	1.52
1	f	109	SER	CA-CB	6.77	1.63	1.52
1	5	132	ARG	NE-CZ	6.76	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	133	TRP	CZ2-CH2	6.75	1.50	1.37
1	W	123	PRO	N-CD	-6.75	1.38	1.47
1	j	16	SER	CA-CB	6.74	1.63	1.52
1	I	146	SER	CA-CB	6.73	1.63	1.52
1	G	90	PRO	N-CD	-6.71	1.38	1.47
1	W	97	ARG	NE-CZ	6.69	1.41	1.33
1	V	145	TYR	CZ-OH	6.69	1.49	1.37
1	L	75	GLU	CB-CG	6.68	1.64	1.52
1	e	88	ALA	C-N	6.68	1.45	1.33
1	V	162	ARG	CD-NE	6.67	1.57	1.46
1	Y	16	SER	CB-OG	6.67	1.50	1.42
1	l	222	GLY	N-CA	6.67	1.56	1.46
1	W	44	SER	CA-CB	6.66	1.62	1.52
1	g	132	ARG	NE-CZ	6.66	1.41	1.33
1	k	191	VAL	CA-CB	6.65	1.68	1.54
1	i	173	ARG	CD-NE	6.62	1.57	1.46
1	Y	76	GLU	CG-CD	6.62	1.61	1.51
1	6	33	SER	CB-OG	6.62	1.50	1.42
1	b	29	GLU	CD-OE2	6.61	1.32	1.25
1	J	164	TYR	CB-CG	-6.61	1.41	1.51
1	F	132	ARG	CD-NE	6.60	1.57	1.46
1	K	102	SER	CA-CB	6.59	1.62	1.52
1	g	117	TRP	CB-CG	6.59	1.62	1.50
1	F	82	ARG	CZ-NH2	-6.59	1.24	1.33
1	5	180	GLU	CB-CG	6.59	1.64	1.52
1	M	98	GLU	CD-OE1	6.58	1.32	1.25
1	7	169	TYR	CD2-CE2	6.57	1.49	1.39
1	k	29	GLU	CD-OE1	6.56	1.32	1.25
1	X	154	ARG	CD-NE	6.56	1.57	1.46
1	Q	162	ARG	CD-NE	6.55	1.57	1.46
1	X	169	TYR	CZ-OH	6.53	1.49	1.37
1	Q	82	ARG	NE-CZ	6.51	1.41	1.33
1	P	145	TYR	CG-CD2	6.49	1.47	1.39
1	k	130	TYR	CZ-OH	6.47	1.48	1.37
1	O	1	PRO	N-CD	6.47	1.56	1.47
1	X	18	ARG	CD-NE	6.47	1.57	1.46
1	h	169	TYR	CD2-CE2	6.44	1.49	1.39
1	T	157	PRO	N-CD	-6.43	1.38	1.47
1	i	147	PRO	N-CD	-6.43	1.38	1.47
1	f	21	ASN	CB-CG	6.42	1.65	1.51
1	K	45	GLU	CD-OE2	-6.42	1.18	1.25
1	L	75	GLU	CD-OE2	6.41	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	56	LEU	CA-CB	6.39	1.68	1.53
1	J	23	TRP	NE1-CE2	6.38	1.45	1.37
1	5	143	ARG	CD-NE	6.38	1.57	1.46
1	7	212	GLU	CD-OE2	6.38	1.32	1.25
1	U	133	TRP	NE1-CE2	6.38	1.45	1.37
1	7	130	TYR	CZ-OH	6.37	1.48	1.37
1	c	169	TYR	CG-CD2	6.37	1.47	1.39
1	B	164	TYR	CG-CD1	6.36	1.47	1.39
1	T	122	PRO	N-CA	-6.35	1.36	1.47
1	G	145	TYR	CZ-OH	6.35	1.48	1.37
1	d	80	TRP	CD1-NE1	6.34	1.48	1.38
1	Q	29	GLU	CD-OE2	-6.34	1.18	1.25
1	7	106	GLY	CA-C	6.33	1.61	1.51
1	A	130	TYR	CE2-CZ	6.33	1.46	1.38
1	U	204	ALA	CA-CB	6.33	1.65	1.52
1	i	80	TRP	CD2-CE3	-6.32	1.30	1.40
1	l	145	TYR	CZ-OH	6.31	1.48	1.37
1	g	145	TYR	CZ-OH	6.31	1.48	1.37
1	J	180	GLU	N-CA	-6.30	1.33	1.46
1	K	76	GLU	CB-CG	6.27	1.64	1.52
1	k	94	GLY	CA-C	-6.27	1.41	1.51
1	H	180	GLU	CG-CD	6.27	1.61	1.51
1	l	4	GLN	CA-CB	6.24	1.67	1.53
1	T	169	TYR	CE2-CZ	6.22	1.46	1.38
1	F	41	SER	CA-CB	6.20	1.62	1.52
1	a	109	SER	CA-CB	6.20	1.62	1.52
1	I	49	PRO	N-CD	-6.19	1.39	1.47
1	k	149	SER	CA-CB	6.19	1.62	1.52
1	K	45	GLU	CD-OE1	6.19	1.32	1.25
1	c	93	PRO	C-N	6.19	1.44	1.33
1	V	33	SER	CA-CB	6.18	1.62	1.52
1	H	133	TRP	CZ2-CH2	6.17	1.49	1.37
1	X	82	ARG	CD-NE	6.17	1.56	1.46
1	P	169	TYR	CE1-CZ	6.17	1.46	1.38
1	c	137	GLY	CA-C	-6.17	1.42	1.51
1	A	90	PRO	N-CD	-6.16	1.39	1.47
1	Z	18	ARG	NE-CZ	6.16	1.41	1.33
1	b	7	GLN	C-N	6.14	1.44	1.33
1	S	160	PRO	N-CA	6.14	1.57	1.47
1	e	223	GLY	CA-C	6.14	1.61	1.51
1	l	162	ARG	CD-NE	6.14	1.56	1.46
1	F	162	ARG	NE-CZ	-6.12	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	34	PRO	N-CD	-6.11	1.39	1.47
1	l	44	SER	CA-CB	6.11	1.62	1.52
1	W	116	GLY	N-CA	-6.10	1.36	1.46
1	7	169	TYR	CG-CD1	6.08	1.47	1.39
1	O	80	TRP	CG-CD2	6.07	1.53	1.43
1	i	178	SER	CA-CB	6.07	1.62	1.52
1	5	228	ALA	N-CA	-6.06	1.34	1.46
1	f	229	ARG	CD-NE	6.06	1.56	1.46
1	E	116	GLY	CA-C	-6.05	1.42	1.51
1	k	23	TRP	CA-CB	6.05	1.67	1.53
1	j	168	PHE	CG-CD1	6.04	1.47	1.38
1	5	122	PRO	C-N	-6.04	1.22	1.34
1	6	164	TYR	CB-CG	-6.04	1.42	1.51
1	R	130	TYR	CE2-CZ	6.03	1.46	1.38
1	N	218	CYS	CA-CB	6.02	1.67	1.53
1	R	79	GLU	CD-OE1	6.01	1.32	1.25
1	H	80	TRP	NE1-CE2	6.01	1.45	1.37
1	j	184	TRP	CB-CG	6.00	1.61	1.50
1	L	128	GLU	CD-OE1	6.00	1.32	1.25
1	R	40	PHE	CG-CD1	5.99	1.47	1.38
1	E	157	PRO	N-CD	5.98	1.56	1.47
1	a	145	TYR	CZ-OH	5.98	1.48	1.37
1	k	33	SER	CA-CB	5.97	1.61	1.52
1	d	173	ARG	CD-NE	5.97	1.56	1.46
1	f	136	LEU	C-N	5.97	1.43	1.33
1	l	113	GLU	CB-CG	5.96	1.63	1.52
1	T	130	TYR	CG-CD1	5.96	1.46	1.39
1	I	149	SER	CA-CB	5.96	1.61	1.52
1	j	222	GLY	N-CA	5.94	1.54	1.46
1	W	133	TRP	CA-CB	5.94	1.67	1.53
1	5	18	ARG	CD-NE	5.94	1.56	1.46
1	K	180	GLU	CB-CG	5.94	1.63	1.52
1	g	168	PHE	CE1-CZ	5.93	1.48	1.37
1	R	223	GLY	N-CA	5.93	1.54	1.46
1	A	2	ILE	C-O	5.91	1.34	1.23
1	h	117	TRP	CD2-CE3	5.91	1.49	1.40
1	J	117	TRP	CB-CG	5.90	1.60	1.50
1	A	45	GLU	CB-CG	5.90	1.63	1.52
1	M	122	PRO	N-CD	-5.90	1.39	1.47
1	H	32	PHE	CD1-CE1	5.89	1.51	1.39
1	c	128	GLU	CD-OE2	5.89	1.32	1.25
1	J	162	ARG	CD-NE	5.89	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	k	167	ARG	CD-NE	5.89	1.56	1.46
1	L	109	SER	CA-CB	5.88	1.61	1.52
1	d	218	CYS	CB-SG	5.88	1.92	1.82
1	T	17	PRO	CA-C	-5.88	1.41	1.52
1	Z	132	ARG	CD-NE	5.88	1.56	1.46
1	b	93	PRO	N-CA	5.87	1.57	1.47
1	L	45	GLU	C-N	5.87	1.43	1.33
1	e	97	ARG	CD-NE	5.86	1.56	1.46
1	g	46	GLY	N-CA	-5.86	1.37	1.46
1	h	224	PRO	N-CA	-5.86	1.37	1.47
1	P	32	PHE	CG-CD1	5.84	1.47	1.38
1	M	136	LEU	CA-CB	5.84	1.67	1.53
1	N	34	PRO	CA-C	5.83	1.64	1.52
1	G	149	SER	CA-CB	5.83	1.61	1.52
1	K	117	TRP	CD1-NE1	5.82	1.47	1.38
1	O	60	GLY	N-CA	5.81	1.54	1.46
1	Y	161	PHE	CG-CD2	5.80	1.47	1.38
1	g	18	ARG	CA-CB	5.79	1.66	1.53
1	V	164	TYR	CD1-CE1	-5.79	1.30	1.39
1	a	133	TRP	CG-CD2	5.79	1.53	1.43
1	U	177	ALA	N-CA	-5.79	1.34	1.46
1	b	41	SER	CA-CB	5.79	1.61	1.52
1	m	82	ARG	CD-NE	5.78	1.56	1.46
1	D	164	TYR	CE2-CZ	5.78	1.46	1.38
1	E	98	GLU	CD-OE1	-5.78	1.19	1.25
1	d	92	GLU	C-N	-5.77	1.23	1.34
1	l	144	MET	CG-SD	-5.77	1.66	1.81
1	Y	169	TYR	CD2-CE2	5.76	1.48	1.39
1	e	145	TYR	CE1-CZ	5.76	1.46	1.38
1	h	65	ALA	CA-CB	5.76	1.64	1.52
1	f	220	GLY	N-CA	5.76	1.54	1.46
1	E	130	TYR	CA-CB	5.76	1.66	1.53
1	d	145	TYR	CD2-CE2	5.76	1.48	1.39
1	h	143	ARG	CD-NE	5.75	1.56	1.46
1	h	122	PRO	N-CD	5.74	1.55	1.47
1	b	160	PRO	N-CD	-5.74	1.39	1.47
1	R	45	GLU	CD-OE1	-5.73	1.19	1.25
1	a	173	ARG	NE-CZ	5.72	1.40	1.33
1	c	174	ALA	N-CA	-5.72	1.34	1.46
1	H	63	GLN	CB-CG	5.71	1.68	1.52
1	J	44	SER	CA-CB	5.71	1.61	1.52
1	K	154	ARG	NE-CZ	5.71	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	44	SER	CA-CB	5.70	1.61	1.52
1	B	29	GLU	CG-CD	5.69	1.60	1.51
1	U	184	TRP	CE3-CZ3	5.69	1.48	1.38
1	B	79	GLU	N-CA	-5.68	1.34	1.46
1	m	173	ARG	CD-NE	5.68	1.56	1.46
1	6	18	ARG	CD-NE	5.67	1.56	1.46
1	M	154	ARG	CD-NE	5.67	1.56	1.46
1	k	26	VAL	CA-CB	5.67	1.66	1.54
1	B	229	ARG	CD-NE	5.66	1.56	1.46
1	I	23	TRP	CD2-CE3	-5.66	1.31	1.40
1	W	145	TYR	CG-CD1	5.66	1.46	1.39
1	Q	164	TYR	CG-CD1	5.66	1.46	1.39
1	K	187	GLU	CD-OE1	-5.66	1.19	1.25
1	i	80	TRP	NE1-CE2	5.66	1.45	1.37
1	Q	71	GLU	CD-OE1	5.65	1.31	1.25
1	T	99	PRO	N-CD	-5.65	1.40	1.47
1	J	106	GLY	CA-C	-5.64	1.42	1.51
1	J	92	GLU	CG-CD	5.64	1.60	1.51
1	X	169	TYR	CG-CD1	5.64	1.46	1.39
1	F	157	PRO	N-CD	-5.64	1.40	1.47
1	D	184	TRP	CD2-CE3	-5.63	1.31	1.40
1	E	180	GLU	CD-OE1	5.63	1.31	1.25
1	I	117	TRP	CD2-CE3	-5.62	1.31	1.40
1	h	146	SER	CA-CB	5.62	1.61	1.52
1	P	154	ARG	NE-CZ	5.62	1.40	1.33
1	W	149	SER	CA-CB	5.62	1.61	1.52
1	m	184	TRP	CA-CB	5.62	1.66	1.53
1	T	80	TRP	NE1-CE2	5.61	1.44	1.37
1	j	147	PRO	N-CD	-5.59	1.40	1.47
1	U	221	VAL	C-N	5.59	1.43	1.33
1	b	102	SER	CA-CB	5.59	1.61	1.52
1	c	40	PHE	CG-CD1	5.58	1.47	1.38
1	h	113	GLU	N-CA	-5.58	1.35	1.46
1	I	167	ARG	CZ-NH2	-5.58	1.25	1.33
1	P	102	SER	CA-CB	5.58	1.61	1.52
1	f	47	ALA	CA-C	-5.58	1.38	1.52
1	C	98	GLU	CG-CD	-5.57	1.43	1.51
1	Q	130	TYR	CZ-OH	5.57	1.47	1.37
1	U	123	PRO	N-CD	-5.57	1.40	1.47
1	J	1	PRO	N-CD	5.56	1.55	1.47
1	U	130	TYR	CZ-OH	5.55	1.47	1.37
1	5	224	PRO	CA-C	5.55	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	161	PHE	CB-CG	5.55	1.60	1.51
1	c	198	CYS	CB-SG	5.55	1.91	1.82
1	N	145	TYR	CZ-OH	5.55	1.47	1.37
1	S	96	MET	CG-SD	5.55	1.95	1.81
1	d	98	GLU	CD-OE1	5.54	1.31	1.25
1	6	113	GLU	CG-CD	5.54	1.60	1.51
1	V	132	ARG	CD-NE	5.54	1.55	1.46
1	R	156	GLY	N-CA	5.53	1.54	1.46
1	A	184	TRP	CA-CB	5.52	1.66	1.53
1	B	16	SER	CA-CB	5.52	1.61	1.52
1	g	100	ARG	CD-NE	5.52	1.55	1.46
1	c	140	LYS	CA-CB	5.52	1.66	1.53
1	K	187	GLU	CD-OE2	5.51	1.31	1.25
1	E	128	GLU	CG-CD	5.51	1.60	1.51
1	W	45	GLU	CB-CG	5.51	1.62	1.52
1	N	23	TRP	CB-CG	-5.51	1.40	1.50
1	X	45	GLU	CG-CD	5.50	1.60	1.51
1	l	80	TRP	NE1-CE2	-5.50	1.30	1.37
1	B	80	TRP	NE1-CE2	-5.50	1.30	1.37
1	I	77	ALA	CA-CB	5.50	1.64	1.52
1	d	14	ALA	CA-CB	5.49	1.64	1.52
1	l	187	GLU	CD-OE2	5.49	1.31	1.25
1	P	36	VAL	CA-CB	5.49	1.66	1.54
1	h	167	ARG	CZ-NH2	5.49	1.40	1.33
1	d	1	PRO	N-CA	5.48	1.56	1.47
1	h	81	ASP	CA-CB	5.48	1.66	1.53
1	Y	127	GLY	N-CA	-5.47	1.37	1.46
1	O	213	GLU	CB-CG	5.47	1.62	1.52
1	X	43	LEU	N-CA	5.47	1.57	1.46
1	j	128	GLU	CD-OE1	-5.47	1.19	1.25
1	P	173	ARG	NE-CZ	5.47	1.40	1.33
1	i	212	GLU	CB-CG	5.47	1.62	1.52
1	5	23	TRP	NE1-CE2	5.46	1.44	1.37
1	E	178	SER	CA-CB	5.46	1.61	1.52
1	V	143	ARG	CD-NE	5.45	1.55	1.46
1	N	82	ARG	C-N	5.45	1.46	1.34
1	F	32	PHE	CG-CD2	5.44	1.47	1.38
1	A	229	ARG	CD-NE	5.44	1.55	1.46
1	X	71	GLU	CG-CD	-5.44	1.43	1.51
1	V	126	VAL	C-N	5.44	1.42	1.33
1	C	100	ARG	CD-NE	5.43	1.55	1.46
1	M	130	TYR	CG-CD1	5.43	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	126	VAL	C-N	5.43	1.42	1.33
1	7	168	PHE	CG-CD2	5.43	1.46	1.38
1	h	160	PRO	C-N	5.43	1.46	1.34
1	B	161	PHE	CG-CD2	5.43	1.46	1.38
1	Q	189	LEU	CA-CB	5.43	1.66	1.53
1	k	90	PRO	CA-C	5.42	1.63	1.52
1	k	164	TYR	CZ-OH	5.42	1.47	1.37
1	R	130	TYR	CA-CB	5.42	1.65	1.53
1	e	1	PRO	N-CD	5.41	1.55	1.47
1	Q	1	PRO	N-CA	5.41	1.56	1.47
1	V	89	GLY	N-CA	-5.40	1.38	1.46
1	6	173	ARG	CD-NE	5.40	1.55	1.46
1	O	109	SER	CA-CB	5.40	1.61	1.52
1	V	71	GLU	CD-OE2	-5.39	1.19	1.25
1	e	113	GLU	CD-OE1	5.39	1.31	1.25
1	A	23	TRP	CD2-CE2	-5.38	1.34	1.41
1	P	8	GLY	N-CA	5.38	1.54	1.46
1	d	149	SER	CB-OG	5.38	1.49	1.42
1	F	98	GLU	CD-OE1	5.38	1.31	1.25
1	d	102	SER	CA-CB	5.38	1.61	1.52
1	g	169	TYR	CG-CD1	5.38	1.46	1.39
1	L	191	VAL	CB-CG2	5.37	1.64	1.52
1	C	20	LEU	CA-CB	5.37	1.66	1.53
1	e	164	TYR	CZ-OH	5.37	1.47	1.37
1	V	45	GLU	CD-OE1	5.37	1.31	1.25
1	C	16	SER	CA-CB	5.37	1.61	1.52
1	L	31	ALA	CA-CB	5.37	1.63	1.52
1	d	180	GLU	CA-CB	5.37	1.65	1.53
1	T	123	PRO	CA-CB	-5.36	1.42	1.53
1	l	100	ARG	CD-NE	5.36	1.55	1.46
1	A	133	TRP	CE3-CZ3	5.36	1.47	1.38
1	P	169	TYR	CB-CG	5.36	1.59	1.51
1	E	102	SER	CB-OG	5.35	1.49	1.42
1	H	79	GLU	CB-CG	5.35	1.62	1.52
1	j	89	GLY	CA-C	5.34	1.60	1.51
1	N	76	GLU	CD-OE2	5.34	1.31	1.25
1	Z	229	ARG	NE-CZ	5.34	1.40	1.33
1	U	38	PRO	N-CD	-5.34	1.40	1.47
1	W	169	TYR	CG-CD1	5.33	1.46	1.39
1	D	36	VAL	CB-CG1	5.32	1.64	1.52
1	X	32	PHE	CG-CD1	5.32	1.46	1.38
1	J	213	GLU	CG-CD	5.31	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	100	ARG	CD-NE	5.30	1.55	1.46
1	D	109	SER	CB-OG	5.30	1.49	1.42
1	7	231	LEU	C-O	5.30	1.33	1.23
1	L	157	PRO	N-CD	5.30	1.55	1.47
1	m	80	TRP	CZ2-CH2	5.29	1.47	1.37
1	k	161	PHE	CE2-CZ	5.29	1.47	1.37
1	P	113	GLU	CA-CB	5.28	1.65	1.53
1	k	229	ARG	CB-CG	5.27	1.66	1.52
1	E	28	GLU	CB-CG	5.27	1.62	1.52
1	g	92	GLU	CB-CG	5.27	1.62	1.52
1	O	154	ARG	NE-CZ	5.26	1.39	1.33
1	S	45	GLU	CB-CG	5.26	1.62	1.52
1	X	231	LEU	C-O	5.26	1.33	1.23
1	I	159	GLU	CD-OE2	-5.26	1.19	1.25
1	P	164	TYR	CE1-CZ	5.26	1.45	1.38
1	L	49	PRO	CA-CB	-5.26	1.43	1.53
1	A	133	TRP	CG-CD1	5.26	1.44	1.36
1	G	161	PHE	CE2-CZ	5.26	1.47	1.37
1	M	16	SER	CA-CB	5.26	1.60	1.52
1	U	145	TYR	CG-CD2	5.26	1.46	1.39
1	J	229	ARG	NE-CZ	5.25	1.39	1.33
1	K	32	PHE	CA-CB	5.25	1.65	1.53
1	j	45	GLU	CB-CG	5.25	1.62	1.52
1	U	118	MET	CA-C	5.25	1.66	1.52
1	W	213	GLU	CD-OE2	5.25	1.31	1.25
1	e	175	GLU	CD-OE1	-5.24	1.19	1.25
1	S	97	ARG	NE-CZ	5.24	1.39	1.33
1	Z	39	MET	N-CA	-5.23	1.35	1.46
1	I	102	SER	N-CA	5.23	1.56	1.46
1	i	169	TYR	CZ-OH	5.23	1.46	1.37
1	C	158	LYS	CA-CB	5.22	1.65	1.53
1	P	35	GLU	CD-OE2	5.22	1.31	1.25
1	W	76	GLU	CB-CG	5.22	1.62	1.52
1	l	229	ARG	NE-CZ	5.21	1.39	1.33
1	A	80	TRP	CD2-CE2	-5.21	1.35	1.41
1	6	184	TRP	NE1-CE2	5.21	1.44	1.37
1	5	165	VAL	CB-CG1	5.20	1.63	1.52
1	i	113	GLU	CD-OE2	-5.20	1.20	1.25
1	G	97	ARG	CD-NE	5.20	1.55	1.46
1	X	205	LEU	C-N	5.20	1.42	1.33
1	Q	169	TYR	CB-CG	5.20	1.59	1.51
1	j	191	VAL	CB-CG1	5.20	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	GLU	CG-CD	5.19	1.59	1.51
1	T	144	MET	CA-CB	5.19	1.65	1.53
1	J	182	LYS	CD-CE	5.19	1.64	1.51
1	h	229	ARG	CD-NE	5.19	1.55	1.46
1	G	55	MET	N-CA	5.16	1.56	1.46
1	g	164	TYR	CG-CD2	5.16	1.45	1.39
1	M	34	PRO	N-CD	-5.16	1.40	1.47
1	D	222	GLY	CA-C	-5.16	1.43	1.51
1	H	184	TRP	CE3-CZ3	5.16	1.47	1.38
1	N	23	TRP	CD1-NE1	-5.16	1.29	1.38
1	7	2	ILE	N-CA	5.15	1.56	1.46
1	O	145	TYR	CA-CB	5.15	1.65	1.53
1	b	169	TYR	CB-CG	5.15	1.59	1.51
1	j	105	ALA	C-N	5.15	1.42	1.33
1	R	145	TYR	CE1-CZ	5.15	1.45	1.38
1	k	145	TYR	CG-CD2	-5.15	1.32	1.39
1	e	180	GLU	CA-CB	-5.13	1.42	1.53
1	a	27	VAL	CB-CG1	5.13	1.63	1.52
1	k	164	TYR	CG-CD1	5.13	1.45	1.39
1	7	125	PRO	N-CD	5.13	1.55	1.47
1	e	76	GLU	CD-OE1	5.13	1.31	1.25
1	O	169	TYR	CE1-CZ	5.12	1.45	1.38
1	h	117	TRP	CE3-CZ3	5.12	1.47	1.38
1	Z	164	TYR	CE1-CZ	5.12	1.45	1.38
1	P	180	GLU	CG-CD	-5.12	1.44	1.51
1	k	68	MET	N-CA	-5.12	1.36	1.46
1	F	69	LEU	CA-CB	5.12	1.65	1.53
1	e	18	ARG	CD-NE	5.12	1.55	1.46
1	J	79	GLU	CB-CG	5.11	1.61	1.52
1	K	15	ILE	N-CA	-5.11	1.36	1.46
1	N	162	ARG	CD-NE	5.11	1.55	1.46
1	V	163	ASP	CA-CB	5.11	1.65	1.53
1	5	93	PRO	N-CA	5.11	1.55	1.47
1	h	115	ILE	C-N	5.11	1.42	1.33
1	E	127	GLY	CA-C	-5.11	1.43	1.51
1	l	61	GLY	CA-C	-5.11	1.43	1.51
1	g	212	GLU	CD-OE1	5.11	1.31	1.25
1	W	37	ILE	C-N	5.10	1.44	1.34
1	c	227	LYS	CD-CE	5.09	1.64	1.51
1	D	206	GLY	CA-C	5.09	1.59	1.51
1	N	222	GLY	C-N	5.09	1.42	1.33
1	N	80	TRP	CD1-NE1	5.09	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	112	GLN	CA-CB	5.09	1.65	1.53
1	j	133	TRP	CD1-NE1	5.09	1.46	1.38
1	M	84	HIS	CG-CD2	5.08	1.44	1.35
1	L	180	GLU	CD-OE1	5.08	1.31	1.25
1	f	143	ARG	CD-NE	5.08	1.55	1.46
1	T	145	TYR	CE2-CZ	5.08	1.45	1.38
1	Q	35	GLU	CG-CD	-5.08	1.44	1.51
1	V	200	THR	CA-C	5.08	1.66	1.52
1	g	23	TRP	CB-CG	5.08	1.59	1.50
1	H	223	GLY	CA-C	-5.08	1.43	1.51
1	P	156	GLY	N-CA	5.08	1.53	1.46
1	X	172	LEU	N-CA	-5.07	1.36	1.46
1	5	32	PHE	CG-CD1	5.07	1.46	1.38
1	k	97	ARG	NE-CZ	5.07	1.39	1.33
1	S	102	SER	CB-OG	5.07	1.48	1.42
1	i	162	ARG	CD-NE	5.06	1.55	1.46
1	k	24	VAL	CA-CB	-5.06	1.44	1.54
1	7	28	GLU	CD-OE1	5.06	1.31	1.25
1	m	94	GLY	N-CA	-5.06	1.38	1.46
1	X	97	ARG	NE-CZ	5.06	1.39	1.33
1	5	38	PRO	N-CD	-5.06	1.40	1.47
1	Z	1	PRO	N-CA	5.06	1.55	1.47
1	B	109	SER	CA-CB	5.05	1.60	1.52
1	O	71	GLU	CB-CG	5.05	1.61	1.52
1	a	75	GLU	CD-OE1	5.05	1.31	1.25
1	O	165	VAL	CB-CG2	5.05	1.63	1.52
1	f	132	ARG	CD-NE	5.05	1.55	1.46
1	D	164	TYR	CE1-CZ	5.05	1.45	1.38
1	7	32	PHE	CA-CB	5.04	1.65	1.53
1	U	180	GLU	CG-CD	5.04	1.59	1.51
1	d	133	TRP	CE3-CZ3	5.04	1.47	1.38
1	V	41	SER	CA-CB	5.04	1.60	1.52
1	f	71	GLU	CG-CD	5.04	1.59	1.51
1	m	218	CYS	CB-SG	-5.03	1.73	1.81
1	E	143	ARG	CA-CB	5.03	1.65	1.53
1	R	127	GLY	CA-C	-5.03	1.43	1.51
1	R	229	ARG	CD-NE	5.03	1.54	1.46
1	X	1	PRO	N-CD	5.03	1.54	1.47
1	i	219	GLN	C-N	5.02	1.42	1.33
1	6	29	GLU	CD-OE1	5.02	1.31	1.25
1	Y	183	ASN	N-CA	-5.02	1.36	1.46
1	A	79	GLU	CB-CG	5.02	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	213	GLU	CB-CG	5.02	1.61	1.52
1	V	130	TYR	CD2-CE2	5.02	1.46	1.39
1	i	37	ILE	C-N	-5.01	1.24	1.34
1	J	132	ARG	CZ-NH2	5.01	1.39	1.33
1	5	149	SER	CA-CB	5.01	1.60	1.52
1	l	98	GLU	CB-CG	5.01	1.61	1.52
1	V	143	ARG	CZ-NH1	-5.01	1.26	1.33
1	c	133	TRP	CE3-CZ3	5.01	1.47	1.38
1	7	168	PHE	CG-CD1	5.01	1.46	1.38
1	e	128	GLU	CD-OE1	5.01	1.31	1.25
1	K	174	ALA	CA-CB	5.01	1.62	1.52
1	i	184	TRP	CG-CD1	-5.01	1.29	1.36
1	F	35	GLU	CD-OE1	5.00	1.31	1.25
1	J	133	TRP	CD2-CE2	5.00	1.47	1.41
1	X	179	GLN	CB-CG	5.00	1.66	1.52
1	Z	165	VAL	N-CA	-5.00	1.36	1.46
1	e	197	ASP	CA-CB	5.00	1.65	1.53

All (1921) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	143	ARG	NE-CZ-NH2	-22.78	108.91	120.30
1	X	18	ARG	NE-CZ-NH1	22.41	131.50	120.30
1	6	82	ARG	NE-CZ-NH2	-21.88	109.36	120.30
1	k	97	ARG	NE-CZ-NH2	-19.67	110.47	120.30
1	B	18	ARG	NE-CZ-NH2	-19.43	110.59	120.30
1	h	82	ARG	NE-CZ-NH1	19.42	130.01	120.30
1	O	97	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	X	18	ARG	NE-CZ-NH2	-19.05	110.78	120.30
1	Y	97	ARG	NE-CZ-NH2	-18.90	110.85	120.30
1	O	143	ARG	NE-CZ-NH1	18.34	129.47	120.30
1	Z	18	ARG	NE-CZ-NH2	-18.05	111.28	120.30
1	V	145	TYR	CB-CG-CD1	-18.00	110.20	121.00
1	W	162	ARG	NE-CZ-NH1	17.81	129.20	120.30
1	L	173	ARG	NE-CZ-NH2	-17.75	111.43	120.30
1	g	167	ARG	NE-CZ-NH1	17.66	129.13	120.30
1	i	229	ARG	NE-CZ-NH1	17.57	129.09	120.30
1	A	173	ARG	NE-CZ-NH2	-17.27	111.67	120.30
1	X	82	ARG	NE-CZ-NH1	16.71	128.66	120.30
1	T	82	ARG	NE-CZ-NH1	16.67	128.63	120.30
1	W	229	ARG	NE-CZ-NH1	16.63	128.62	120.30
1	T	18	ARG	NE-CZ-NH1	16.39	128.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	82	ARG	NE-CZ-NH2	-16.38	112.11	120.30
1	E	173	ARG	NE-CZ-NH2	-16.35	112.13	120.30
1	T	82	ARG	NE-CZ-NH2	-16.33	112.13	120.30
1	m	97	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	6	82	ARG	NE-CZ-NH1	15.95	128.28	120.30
1	7	167	ARG	NE-CZ-NH1	15.89	128.25	120.30
1	E	162	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	7	154	ARG	NE-CZ-NH2	-15.75	112.42	120.30
1	X	167	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	h	168	PHE	CB-CG-CD1	-15.48	109.96	120.80
1	P	97	ARG	NE-CZ-NH1	15.25	127.92	120.30
1	J	145	TYR	CB-CG-CD1	14.75	129.85	121.00
1	N	100	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	h	167	ARG	NE-CZ-NH1	14.67	127.64	120.30
1	N	132	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	N	18	ARG	NE-CZ-NH1	14.30	127.45	120.30
1	6	229	ARG	NE-CZ-NH1	14.23	127.42	120.30
1	l	18	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	Z	97	ARG	NE-CZ-NH1	14.10	127.35	120.30
1	6	173	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	j	173	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	W	100	ARG	NE-CZ-NH2	13.93	127.27	120.30
1	e	132	ARG	NE-CZ-NH1	13.93	127.27	120.30
1	K	169	TYR	CB-CG-CD1	-13.83	112.70	121.00
1	h	161	PHE	CB-CG-CD1	-13.75	111.18	120.80
1	C	132	ARG	NE-CZ-NH2	-13.74	113.43	120.30
1	Y	154	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	V	18	ARG	NE-CZ-NH2	-13.69	113.46	120.30
1	Y	97	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	j	18	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	c	167	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	K	154	ARG	NE-CZ-NH1	13.45	127.03	120.30
1	A	100	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	g	32	PHE	CB-CG-CD2	13.32	130.12	120.80
1	S	154	ARG	NE-CZ-NH1	13.21	126.90	120.30
1	F	132	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	K	154	ARG	NE-CZ-NH2	-13.07	113.76	120.30
1	C	173	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	A	229	ARG	NE-CZ-NH2	12.91	126.75	120.30
1	B	96	MET	CG-SD-CE	-12.90	79.55	100.20
1	L	82	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	i	169	TYR	CB-CG-CD2	-12.80	113.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	18	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	F	169	TYR	CB-CG-CD1	-12.77	113.34	121.00
1	6	173	ARG	NE-CZ-NH2	-12.71	113.94	120.30
1	h	82	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	X	162	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	J	132	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	G	130	TYR	CB-CG-CD2	12.62	128.57	121.00
1	6	167	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	h	161	PHE	CB-CG-CD2	12.54	129.58	120.80
1	J	145	TYR	CB-CG-CD2	-12.49	113.51	121.00
1	J	132	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	d	169	TYR	CB-CG-CD2	-12.42	113.55	121.00
1	N	132	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	i	164	TYR	CB-CG-CD2	12.28	128.37	121.00
1	O	162	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	h	143	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	T	167	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	l	100	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	f	18	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	M	132	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	V	162	ARG	NE-CZ-NH2	12.11	126.36	120.30
1	c	97	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	5	100	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	c	82	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	B	18	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	m	167	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	O	130	TYR	CB-CG-CD2	-11.94	113.83	121.00
1	R	97	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	M	132	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	6	32	PHE	CB-CG-CD2	11.88	129.12	120.80
1	m	18	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	Q	173	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	j	40	PHE	CB-CG-CD1	-11.84	112.52	120.80
1	Y	82	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	T	143	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	a	173	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	6	130	TYR	CB-CG-CD1	11.73	128.04	121.00
1	H	173	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	L	168	PHE	CB-CG-CD1	-11.71	112.60	120.80
1	i	154	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	g	143	ARG	NE-CZ-NH2	11.65	126.12	120.30
1	6	229	ARG	NE-CZ-NH2	-11.61	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	18	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	i	18	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	H	167	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	L	169	TYR	CB-CG-CD2	-11.54	114.08	121.00
1	M	169	TYR	CB-CG-CD2	-11.53	114.08	121.00
1	X	154	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	c	229	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	V	173	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	j	154	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	I	18	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	a	229	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	i	164	TYR	CB-CG-CD1	-11.34	114.20	121.00
1	L	145	TYR	CB-CG-CD2	11.32	127.79	121.00
1	M	143	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	k	130	TYR	CB-CG-CD2	-11.22	114.27	121.00
1	k	143	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	N	162	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	O	132	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	Y	132	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	T	167	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	e	167	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	D	97	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	O	169	TYR	CB-CG-CD2	-10.99	114.40	121.00
1	c	18	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	M	162	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	Q	169	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	W	164	TYR	CB-CG-CD1	10.90	127.54	121.00
1	a	197	ASP	CB-CG-OD2	10.87	128.09	118.30
1	k	18	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	D	173	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	Z	164	TYR	CB-CG-CD2	-10.77	114.54	121.00
1	i	40	PHE	CB-CG-CD2	10.77	128.34	120.80
1	i	169	TYR	CB-CG-CD1	10.77	127.46	121.00
1	X	144	MET	CG-SD-CE	-10.75	83.00	100.20
1	k	130	TYR	CB-CG-CD1	10.71	127.43	121.00
1	6	143	ARG	NE-CZ-NH2	10.71	125.66	120.30
1	F	18	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	Y	229	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	O	82	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	e	97	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	P	152	ASP	CB-CG-OD2	10.59	127.83	118.30
1	D	18	ARG	NE-CZ-NH2	-10.57	115.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	143	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	R	18	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	h	100	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	M	229	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	103	ASP	CB-CG-OD2	10.51	127.76	118.30
1	R	97	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	J	97	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	k	97	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	h	167	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	B	32	PHE	CB-CG-CD2	10.45	128.11	120.80
1	6	32	PHE	CB-CG-CD1	-10.41	113.51	120.80
1	F	143	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	H	143	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	O	100	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	M	154	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	h	168	PHE	CB-CG-CD2	10.35	128.04	120.80
1	W	173	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	K	145	TYR	CB-CG-CD2	-10.28	114.83	121.00
1	Q	173	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	L	145	TYR	CB-CG-CD1	-10.26	114.84	121.00
1	I	214	MET	CG-SD-CE	-10.25	83.81	100.20
1	a	97	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	B	130	TYR	CB-CG-CD1	-10.23	114.86	121.00
1	7	79	GLU	OE1-CD-OE2	-10.23	111.02	123.30
1	N	162	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	U	132	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	K	169	TYR	CB-CG-CD2	10.22	127.13	121.00
1	E	229	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	F	82	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	7	162	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	W	166	ASP	CB-CG-OD1	10.17	127.45	118.30
1	6	132	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	X	162	ARG	NH1-CZ-NH2	-10.10	108.29	119.40
1	e	132	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	U	18	ARG	NE-CZ-NH2	10.08	125.34	120.30
1	F	81	ASP	CB-CG-OD1	10.07	127.36	118.30
1	F	143	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	6	130	TYR	CB-CG-CD2	-10.04	114.97	121.00
1	c	18	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	N	133	TRP	CB-CG-CD1	10.03	140.04	127.00
1	L	154	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	Z	82	ARG	NE-CZ-NH1	10.02	125.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	S	167	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	E	143	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	Q	164	TYR	CB-CG-CD2	-9.97	115.02	121.00
1	G	18	ARG	NE-CZ-NH2	9.95	125.28	120.30
1	h	132	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	j	143	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	E	145	TYR	CB-CG-CD1	-9.94	115.04	121.00
1	L	229	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	W	162	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	e	97	ARG	NE-CZ-NH2	-9.87	115.37	120.30
1	k	167	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	I	154	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	Y	82	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	I	130	TYR	CB-CG-CD2	9.81	126.89	121.00
1	Z	173	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	D	162	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	g	154	ARG	NE-CZ-NH1	-9.79	115.40	120.30
1	b	132	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	f	154	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	a	100	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	W	18	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	c	97	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	J	169	TYR	CB-CG-CD1	9.62	126.77	121.00
1	T	97	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	5	130	TYR	CB-CG-CD1	-9.59	115.25	121.00
1	O	143	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	5	100	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	L	130	TYR	CB-CG-CD2	-9.55	115.27	121.00
1	C	154	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	m	166	ASP	CB-CG-OD2	9.52	126.86	118.30
1	H	164	TYR	CB-CG-CD2	9.51	126.71	121.00
1	6	200	THR	CA-CB-CG2	-9.51	99.08	112.40
1	I	133	TRP	CB-CG-CD2	-9.47	114.29	126.60
1	L	169	TYR	CB-CG-CD1	9.46	126.68	121.00
1	e	182	LYS	N-CA-CB	9.46	127.63	110.60
1	E	18	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	D	82	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	G	143	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	7	161	PHE	CB-CG-CD2	-9.42	114.20	120.80
1	d	143	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	f	97	ARG	NE-CZ-NH1	9.40	125.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	154	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	Z	173	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	b	130	TYR	CB-CG-CD2	9.37	126.62	121.00
1	Y	100	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	f	154	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	F	100	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	5	132	ARG	NE-CZ-NH2	9.33	124.97	120.30
1	W	164	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	A	66	MET	CG-SD-CE	-9.31	85.30	100.20
1	Y	132	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	A	173	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	k	164	TYR	CB-CG-CD2	-9.27	115.44	121.00
1	g	229	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	162	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	a	18	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	c	82	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	F	55	MET	CG-SD-CE	-9.22	85.44	100.20
1	L	154	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	i	162	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	E	145	TYR	CB-CG-CD2	9.20	126.52	121.00
1	h	169	TYR	CB-CG-CD2	-9.20	115.48	121.00
1	R	68	MET	CG-SD-CE	-9.19	85.49	100.20
1	I	229	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	g	167	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	i	40	PHE	CB-CG-CD1	-9.18	114.38	120.80
1	7	97	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	G	169	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	T	145	TYR	CB-CG-CD2	-9.11	115.53	121.00
1	l	18	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	J	173	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	I	10	MET	CG-SD-CE	-9.07	85.69	100.20
1	i	82	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	h	100	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	E	81	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	f	18	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	H	100	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	E	173	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	5	26	VAL	CG1-CB-CG2	-9.04	96.43	110.90
1	j	184	TRP	CB-CG-CD2	-9.03	114.86	126.60
1	Q	194	ALA	N-CA-CB	-9.02	97.47	110.10
1	G	82	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	H	167	ARG	NH1-CZ-NH2	-8.98	109.52	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	29	GLU	OE1-CD-OE2	-8.96	112.55	123.30
1	W	82	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	P	164	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	L	96	MET	CG-SD-CE	-8.93	85.92	100.20
1	l	164	TYR	CB-CG-CD2	-8.91	115.66	121.00
1	N	168	PHE	CB-CG-CD1	-8.88	114.58	120.80
1	A	154	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	C	229	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	Q	82	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	51	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	G	229	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	E	162	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	U	97	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	O	185	MET	CG-SD-CE	-8.80	86.11	100.20
1	I	132	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	H	82	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	K	143	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	m	229	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	J	32	PHE	CB-CG-CD1	8.75	126.92	120.80
1	c	173	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	L	167	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	E	208	ALA	N-CA-CB	-8.72	97.90	110.10
1	P	18	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	X	162	ARG	NE-CZ-NH2	8.69	124.65	120.30
1	6	18	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	K	229	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	X	145	TYR	CB-CG-CD1	-8.64	115.81	121.00
1	k	163	ASP	CB-CG-OD2	8.64	126.08	118.30
1	J	130	TYR	CG-CD2-CE2	-8.64	114.39	121.30
1	L	130	TYR	CB-CG-CD1	8.64	126.18	121.00
1	d	162	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	K	143	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	d	130	TYR	CB-CG-CD2	-8.61	115.83	121.00
1	I	82	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	j	152	ASP	CB-CG-OD2	8.59	126.03	118.30
1	I	133	TRP	CB-CG-CD1	8.59	138.16	127.00
1	i	145	TYR	CG-CD1-CE1	-8.59	114.43	121.30
1	D	98	GLU	OE1-CD-OE2	-8.58	113.00	123.30
1	M	197	ASP	CB-CG-OD1	-8.57	110.59	118.30
1	P	132	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	T	41	SER	N-CA-CB	8.56	123.34	110.50
1	I	130	TYR	CB-CG-CD1	-8.56	115.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	145	TYR	CB-CG-CD2	-8.55	115.87	121.00
1	L	132	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	P	82	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	5	169	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	R	82	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	L	229	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	H	130	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	P	164	TYR	CG-CD2-CE2	-8.48	114.52	121.30
1	d	167	ARG	NE-CZ-NH2	8.47	124.53	120.30
1	M	152	ASP	CB-CG-OD2	8.43	125.88	118.30
1	h	164	TYR	CB-CG-CD2	8.42	126.05	121.00
1	d	130	TYR	CB-CG-CD1	8.42	126.05	121.00
1	P	130	TYR	CG-CD1-CE1	-8.41	114.57	121.30
1	O	32	PHE	CB-CG-CD1	-8.41	114.92	120.80
1	P	167	ARG	NE-CZ-NH2	8.41	124.50	120.30
1	b	143	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	S	130	TYR	CB-CG-CD1	8.38	126.03	121.00
1	k	82	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	l	96	MET	CG-SD-CE	8.37	113.59	100.20
1	j	100	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	K	208	ALA	CB-CA-C	8.36	122.64	110.10
1	N	173	ARG	NE-CZ-NH1	-8.35	116.12	120.30
1	J	197	ASP	CB-CG-OD1	-8.34	110.79	118.30
1	a	18	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	l	132	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	M	215	MET	CG-SD-CE	-8.31	86.91	100.20
1	Z	82	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	5	86	VAL	CB-CA-C	8.30	127.17	111.40
1	l	103	ASP	CB-CG-OD1	8.29	125.76	118.30
1	W	97	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	D	154	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	E	10	MET	CG-SD-CE	-8.27	86.98	100.20
1	C	166	ASP	CB-CG-OD1	8.26	125.74	118.30
1	k	184	TRP	CG-CD2-CE3	-8.26	126.47	133.90
1	k	100	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	J	66	MET	CG-SD-CE	-8.21	87.06	100.20
1	b	166	ASP	CB-CG-OD1	8.21	125.69	118.30
1	S	51	ASP	CB-CG-OD1	8.20	125.68	118.30
1	Y	18	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	J	82	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	X	100	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	U	145	TYR	CB-CG-CD1	-8.16	116.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	m	18	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	M	130	TYR	CG-CD1-CE1	-8.14	114.79	121.30
1	H	162	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	S	143	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	F	169	TYR	CB-CG-CD2	8.12	125.87	121.00
1	Y	169	TYR	CB-CG-CD1	-8.12	116.13	121.00
1	l	154	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	L	97	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	M	109	SER	N-CA-CB	8.11	122.66	110.50
1	O	154	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	82	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	M	40	PHE	CB-CG-CD2	-8.07	115.15	120.80
1	C	152	ASP	CB-CG-OD1	8.07	125.56	118.30
1	k	68	MET	CG-SD-CE	-8.06	87.30	100.20
1	V	162	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	6	132	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	18	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	P	130	TYR	CD1-CE1-CZ	8.00	127.00	119.80
1	H	167	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	J	166	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	j	145	TYR	CB-CG-CD2	7.96	125.78	121.00
1	m	173	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	U	145	TYR	CB-CG-CD2	7.95	125.77	121.00
1	j	40	PHE	CB-CG-CD2	7.94	126.36	120.80
1	j	133	TRP	CG-CD2-CE3	-7.93	126.77	133.90
1	E	130	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	6	40	PHE	CB-CG-CD1	-7.92	115.25	120.80
1	V	164	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	U	169	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	O	197	ASP	CB-CG-OD2	7.91	125.41	118.30
1	Z	162	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	D	82	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	U	169	TYR	CB-CG-CD2	7.90	125.74	121.00
1	J	130	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	k	100	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	154	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	O	130	TYR	CB-CG-CD1	7.88	125.73	121.00
1	d	168	PHE	CB-CG-CD1	-7.88	115.29	120.80
1	M	197	ASP	CB-CG-OD2	7.87	125.38	118.30
1	P	169	TYR	CZ-CE2-CD2	7.85	126.87	119.80
1	a	164	TYR	CG-CD1-CE1	-7.85	115.02	121.30
1	M	145	TYR	CB-CG-CD1	-7.85	116.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	130	TYR	CB-CG-CD1	7.85	125.71	121.00
1	Q	162	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	7	130	TYR	CB-CG-CD2	-7.84	116.29	121.00
1	Z	162	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	N	133	TRP	CB-CG-CD2	-7.82	116.44	126.60
1	H	173	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	D	96	MET	CG-SD-CE	-7.80	87.72	100.20
1	S	39	MET	CG-SD-CE	-7.80	87.72	100.20
1	W	145	TYR	CB-CG-CD1	-7.79	116.33	121.00
1	6	168	PHE	CB-CG-CD1	-7.79	115.35	120.80
1	X	167	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	d	145	TYR	CZ-CE2-CD2	-7.76	112.82	119.80
1	l	164	TYR	CB-CG-CD1	7.74	125.64	121.00
1	K	149	SER	N-CA-CB	7.73	122.10	110.50
1	R	39	MET	CG-SD-CE	-7.72	87.85	100.20
1	P	97	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	F	167	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	T	168	PHE	CB-CG-CD1	-7.71	115.40	120.80
1	J	167	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	W	19	THR	CA-CB-CG2	-7.71	101.61	112.40
1	F	82	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	J	197	ASP	CB-CG-OD2	7.70	125.23	118.30
1	A	18	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	k	145	TYR	CB-CG-CD1	-7.69	116.39	121.00
1	V	81	ASP	N-CA-CB	-7.67	96.79	110.60
1	a	82	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	i	152	ASP	CB-CG-OD1	7.66	125.20	118.30
1	I	145	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	B	32	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	H	100	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	Z	133	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	J	32	PHE	CB-CG-CD2	-7.62	115.47	120.80
1	S	164	TYR	CG-CD1-CE1	-7.61	115.21	121.30
1	U	196	PRO	N-CA-CB	7.61	112.44	103.30
1	M	145	TYR	CG-CD1-CE1	-7.61	115.21	121.30
1	J	18	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	Z	164	TYR	CB-CG-CD1	7.58	125.55	121.00
1	d	100	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	f	162	ARG	CG-CD-NE	-7.57	95.91	111.80
1	5	168	PHE	CB-CG-CD1	-7.56	115.51	120.80
1	e	229	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	e	169	TYR	CB-CG-CD1	-7.56	116.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	18	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	169	TYR	CB-CG-CD2	7.54	125.52	121.00
1	B	59	VAL	CA-CB-CG1	7.52	122.18	110.90
1	M	162	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	b	117	TRP	CB-CG-CD1	7.51	136.76	127.00
1	7	117	TRP	CG-CD2-CE3	-7.51	127.14	133.90
1	7	154	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	m	88	ALA	N-CA-CB	-7.50	99.59	110.10
1	T	185	MET	CG-SD-CE	-7.50	88.20	100.20
1	N	229	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	d	152	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	g	130	TYR	CB-CG-CD1	-7.49	116.50	121.00
1	N	154	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	g	97	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	l	162	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	E	32	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	G	143	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	J	108	THR	CA-CB-CG2	-7.45	101.97	112.40
1	T	100	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	M	18	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	132	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	G	18	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	F	154	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	b	117	TRP	CB-CG-CD2	-7.42	116.96	126.60
1	m	143	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	J	169	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	b	18	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	I	166	ASP	CB-CG-OD2	7.38	124.95	118.30
1	O	202	LEU	CB-CG-CD1	7.38	123.55	111.00
1	N	53	ASN	N-CA-CB	7.37	123.86	110.60
1	j	188	THR	CA-CB-CG2	-7.36	102.10	112.40
1	k	173	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	I	229	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	F	40	PHE	CB-CG-CD2	-7.35	115.65	120.80
1	I	197	ASP	CB-CG-OD2	7.34	124.91	118.30
1	I	18	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	T	163	ASP	CB-CG-OD2	7.34	124.90	118.30
1	5	161	PHE	CB-CG-CD1	7.34	125.94	120.80
1	7	132	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	G	154	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	P	66	MET	CG-SD-CE	-7.32	88.49	100.20
1	U	178	SER	N-CA-CB	7.32	121.47	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	100	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	G	102	SER	N-CA-CB	7.31	121.46	110.50
1	6	164	TYR	CB-CG-CD1	-7.31	116.62	121.00
1	5	164	TYR	CG-CD1-CE1	-7.29	115.47	121.30
1	W	83	LEU	CB-CG-CD2	7.28	123.37	111.00
1	d	69	LEU	CB-CG-CD2	-7.27	98.65	111.00
1	Q	18	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	X	10	MET	CG-SD-CE	-7.26	88.58	100.20
1	A	81	ASP	CB-CG-OD2	7.26	124.83	118.30
1	N	100	ARG	NH1-CZ-NH2	-7.25	111.42	119.40
1	P	79	GLU	OE1-CD-OE2	-7.25	114.60	123.30
1	Y	162	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	5	103	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	d	133	TRP	CG-CD2-CE3	-7.24	127.39	133.90
1	Z	217	ALA	CB-CA-C	-7.23	99.25	110.10
1	5	132	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	b	226	HIS	CA-CB-CG	7.23	125.89	113.60
1	A	229	ARG	NH1-CZ-NH2	-7.23	111.45	119.40
1	k	167	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	e	82	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	M	130	TYR	CD1-CE1-CZ	7.22	126.30	119.80
1	T	125	PRO	N-CD-CG	-7.21	92.38	103.20
1	L	162	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	a	173	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	V	167	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	164	TYR	CB-CG-CD2	7.18	125.31	121.00
1	c	167	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	V	173	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	7	229	ARG	CD-NE-CZ	7.18	133.65	123.60
1	R	173	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	P	229	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	H	229	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	I	164	TYR	CG-CD2-CE2	7.16	127.03	121.30
1	B	194	ALA	N-CA-CB	-7.16	100.08	110.10
1	C	80	TRP	CD1-NE1-CE2	-7.16	102.56	109.00
1	O	32	PHE	CB-CG-CD2	7.15	125.80	120.80
1	k	197	ASP	CB-CG-OD1	7.14	124.73	118.30
1	V	145	TYR	CG-CD1-CE1	-7.14	115.59	121.30
1	b	40	PHE	CB-CG-CD1	-7.14	115.80	120.80
1	O	132	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	Q	40	PHE	CG-CD1-CE1	-7.14	112.95	120.80
1	i	145	TYR	CB-CG-CD1	-7.14	116.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	197	ASP	CB-CG-OD1	7.13	124.72	118.30
1	d	103	ASP	O-C-N	-7.13	111.29	122.70
1	G	137	GLY	O-C-N	-7.12	111.31	122.70
1	F	130	TYR	CB-CG-CD1	7.11	125.26	121.00
1	6	40	PHE	CB-CG-CD2	7.10	125.77	120.80
1	i	229	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	m	40	PHE	CB-CG-CD1	7.09	125.77	120.80
1	6	16	SER	N-CA-CB	7.09	121.13	110.50
1	L	118	MET	CG-SD-CE	-7.09	88.86	100.20
1	F	168	PHE	CB-CG-CD2	-7.08	115.84	120.80
1	H	81	ASP	CB-CG-OD1	7.08	124.67	118.30
1	7	108	THR	CA-CB-CG2	-7.07	102.50	112.40
1	G	162	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	5	65	ALA	N-CA-CB	7.07	120.00	110.10
1	d	168	PHE	CB-CG-CD2	7.07	125.75	120.80
1	j	167	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	e	228	ALA	N-CA-CB	-7.06	100.21	110.10
1	f	155	GLN	CG-CD-OE1	7.06	135.73	121.60
1	C	173	ARG	NH1-CZ-NH2	7.05	127.16	119.40
1	j	178	SER	N-CA-CB	7.05	121.07	110.50
1	e	143	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	V	144	MET	CG-SD-CE	-7.04	88.93	100.20
1	I	100	ARG	CG-CD-NE	-7.04	97.01	111.80
1	N	161	PHE	CB-CG-CD2	-7.04	115.87	120.80
1	W	97	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	L	32	PHE	CB-CG-CD1	-7.03	115.88	120.80
1	Q	197	ASP	CB-CG-OD2	7.03	124.63	118.30
1	C	18	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	B	51	ASP	CB-CG-OD2	7.02	124.61	118.30
1	Q	210	THR	CA-CB-CG2	-7.01	102.58	112.40
1	h	169	TYR	CB-CG-CD1	7.01	125.21	121.00
1	N	130	TYR	CB-CG-CD1	7.00	125.20	121.00
1	l	68	MET	CG-SD-CE	-6.99	89.01	100.20
1	d	161	PHE	CB-CG-CD2	-6.99	115.91	120.80
1	S	47	ALA	N-CA-CB	-6.99	100.32	110.10
1	6	23	TRP	CB-CG-CD2	-6.99	117.52	126.60
1	k	143	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	d	96	MET	CG-SD-CE	-6.98	89.04	100.20
1	l	100	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	U	23	TRP	CH2-CZ2-CE2	6.97	124.37	117.40
1	T	6	LEU	CB-CG-CD1	6.97	122.84	111.00
1	Z	92	GLU	OE1-CD-OE2	-6.96	114.94	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	169	TYR	CZ-CE2-CD2	6.96	126.06	119.80
1	a	32	PHE	CB-CG-CD1	-6.96	115.93	120.80
1	G	55	MET	CG-SD-CE	-6.96	89.07	100.20
1	J	195	ASN	CA-CB-CG	6.95	128.70	113.40
1	N	169	TYR	CG-CD2-CE2	6.94	126.85	121.30
1	g	212	GLU	OE1-CD-OE2	-6.94	114.97	123.30
1	G	229	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	R	55	MET	CG-SD-CE	-6.94	89.10	100.20
1	R	168	PHE	CB-CG-CD2	6.94	125.66	120.80
1	d	218	CYS	N-CA-CB	6.94	123.09	110.60
1	D	130	TYR	CG-CD2-CE2	-6.94	115.75	121.30
1	N	81	ASP	CB-CG-OD2	6.94	124.54	118.30
1	U	188	THR	CA-CB-CG2	-6.93	102.69	112.40
1	W	228	ALA	N-CA-CB	-6.93	100.40	110.10
1	Y	152	ASP	CB-CG-OD2	6.93	124.53	118.30
1	S	164	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	Q	229	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	j	161	PHE	CB-CG-CD1	-6.91	115.96	120.80
1	C	76	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	F	100	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	5	108	THR	CA-CB-CG2	-6.90	102.74	112.40
1	I	96	MET	CA-CB-CG	6.90	125.03	113.30
1	g	32	PHE	CB-CG-CD1	-6.89	115.98	120.80
1	7	23	TRP	CE2-CD2-CE3	6.89	126.97	118.70
1	c	23	TRP	CD2-CE2-CZ2	-6.88	114.04	122.30
1	K	117	TRP	CG-CD2-CE3	-6.88	127.71	133.90
1	i	161	PHE	CB-CG-CD1	-6.88	115.99	120.80
1	U	97	ARG	NH1-CZ-NH2	-6.87	111.84	119.40
1	g	40	PHE	CB-CG-CD1	6.87	125.61	120.80
1	O	162	ARG	CD-NE-CZ	6.87	133.21	123.60
1	j	142	VAL	CA-CB-CG2	6.86	121.19	110.90
1	I	32	PHE	CB-CG-CD2	-6.85	116.00	120.80
1	7	161	PHE	CB-CG-CD1	6.85	125.60	120.80
1	P	32	PHE	CB-CG-CD1	6.85	125.59	120.80
1	A	23	TRP	CG-CD2-CE3	-6.85	127.74	133.90
1	R	229	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	m	162	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	L	145	TYR	CD1-CE1-CZ	6.84	125.95	119.80
1	k	169	TYR	CB-CG-CD2	6.83	125.10	121.00
1	7	217	ALA	N-CA-CB	-6.83	100.53	110.10
1	O	97	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	h	145	TYR	CB-CG-CD2	-6.83	116.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	e	185	MET	CG-SD-CE	-6.83	89.28	100.20
1	W	100	ARG	NH1-CZ-NH2	-6.83	111.89	119.40
1	j	229	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	V	143	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	O	167	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	E	118	MET	CG-SD-CE	-6.80	89.31	100.20
1	I	55	MET	CG-SD-CE	-6.80	89.32	100.20
1	B	208	ALA	N-CA-CB	-6.80	100.58	110.10
1	U	32	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	f	83	LEU	N-CA-CB	-6.79	96.81	110.40
1	K	130	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	W	74	ASN	CB-CG-OD1	6.79	135.17	121.60
1	a	164	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	I	164	TYR	CZ-CE2-CD2	-6.78	113.70	119.80
1	N	96	MET	O-C-N	-6.78	111.85	122.70
1	P	211	LEU	CB-CA-C	6.78	123.08	110.20
1	h	130	TYR	CB-CG-CD1	6.78	125.06	121.00
1	U	204	ALA	CB-CA-C	-6.77	99.95	110.10
1	A	105	ALA	CB-CA-C	-6.77	99.95	110.10
1	b	164	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	S	209	ALA	CB-CA-C	6.77	120.25	110.10
1	l	184	TRP	CH2-CZ2-CE2	6.76	124.16	117.40
1	E	144	MET	CG-SD-CE	-6.76	89.39	100.20
1	d	23	TRP	CZ3-CH2-CZ2	-6.76	113.49	121.60
1	a	167	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	32	PHE	CB-CG-CD2	6.75	125.53	120.80
1	7	143	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	I	27	VAL	CG1-CB-CG2	-6.74	100.11	110.90
1	V	168	PHE	CD1-CE1-CZ	6.74	128.19	120.10
1	a	80	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	B	180	GLU	OE1-CD-OE2	-6.73	115.22	123.30
1	C	168	PHE	CG-CD2-CE2	6.73	128.21	120.80
1	l	216	THR	OG1-CB-CG2	-6.73	94.52	110.00
1	W	130	TYR	CG-CD2-CE2	6.73	126.68	121.30
1	d	167	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	K	32	PHE	CB-CG-CD2	-6.72	116.09	120.80
1	W	48	THR	CA-CB-CG2	-6.72	102.99	112.40
1	a	229	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	K	10	MET	CG-SD-CE	-6.72	89.45	100.20
1	j	184	TRP	CB-CG-CD1	6.72	135.73	127.00
1	M	23	TRP	CB-CG-CD1	6.71	135.73	127.00
1	f	141	ILE	N-CA-CB	6.71	126.24	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	107	THR	CA-CB-CG2	-6.71	103.00	112.40
1	G	128	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	D	145	TYR	CD1-CE1-CZ	6.69	125.82	119.80
1	X	118	MET	CG-SD-CE	-6.69	89.49	100.20
1	g	166	ASP	CB-CG-OD1	6.69	124.32	118.30
1	L	32	PHE	CG-CD2-CE2	-6.69	113.44	120.80
1	W	145	TYR	CG-CD2-CE2	-6.69	115.95	121.30
1	a	231	LEU	CB-CG-CD2	-6.69	99.63	111.00
1	B	130	TYR	CG-CD1-CE1	-6.69	115.95	121.30
1	N	82	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	i	197	ASP	CB-CG-OD1	6.68	124.32	118.30
1	F	176	GLN	CA-CB-CG	6.68	128.10	113.40
1	6	3	VAL	CG1-CB-CG2	6.68	121.59	110.90
1	D	23	TRP	CE2-CD2-CE3	6.68	126.71	118.70
1	G	167	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	I	51	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	K	178	SER	N-CA-CB	6.68	120.51	110.50
1	M	23	TRP	CD1-NE1-CE2	-6.67	102.99	109.00
1	7	58	THR	CA-CB-CG2	-6.67	103.06	112.40
1	D	100	ARG	O-C-N	-6.67	111.86	123.20
1	J	152	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	133	TRP	CB-CG-CD2	-6.67	117.93	126.60
1	l	145	TYR	CZ-CE2-CD2	-6.66	113.81	119.80
1	C	229	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	W	116	GLY	O-C-N	-6.65	112.06	122.70
1	b	96	MET	CG-SD-CE	-6.65	89.56	100.20
1	K	144	MET	CG-SD-CE	-6.64	89.57	100.20
1	T	162	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	a	55	MET	CG-SD-CE	-6.64	89.57	100.20
1	B	130	TYR	CG-CD2-CE2	-6.64	115.99	121.30
1	W	65	ALA	CB-CA-C	-6.62	100.17	110.10
1	d	97	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	Y	119	THR	N-CA-CB	6.62	122.88	110.30
1	5	39	MET	CA-CB-CG	6.62	124.55	113.30
1	S	96	MET	CG-SD-CE	-6.61	89.63	100.20
1	j	138	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	b	18	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	M	82	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	W	51	ASP	CB-CG-OD1	6.58	124.23	118.30
1	X	135	ILE	O-C-N	-6.58	112.17	122.70
1	c	18	ARG	CD-NE-CZ	6.58	132.82	123.60
1	D	168	PHE	CB-CG-CD2	-6.58	116.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	152	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	Y	229	ARG	NH1-CZ-NH2	-6.58	112.16	119.40
1	a	130	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	X	161	PHE	CB-CG-CD1	6.57	125.40	120.80
1	m	82	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	V	39	MET	CG-SD-CE	-6.56	89.70	100.20
1	i	108	THR	CA-CB-CG2	-6.56	103.21	112.40
1	j	126	VAL	CG1-CB-CG2	-6.56	100.41	110.90
1	7	169	TYR	CZ-CE2-CD2	-6.55	113.90	119.80
1	g	98	GLU	OE1-CD-OE2	-6.55	115.43	123.30
1	M	65	ALA	N-CA-CB	6.55	119.27	110.10
1	b	162	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	V	142	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	J	82	ARG	CD-NE-CZ	6.54	132.75	123.60
1	S	80	TRP	CB-CG-CD1	6.54	135.50	127.00
1	7	97	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	W	229	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	G	178	SER	O-C-N	-6.53	112.26	122.70
1	B	165	VAL	O-C-N	-6.53	112.26	122.70
1	f	145	TYR	O-C-N	-6.52	112.27	122.70
1	d	100	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
1	d	145	TYR	CD1-CE1-CZ	6.52	125.67	119.80
1	K	164	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	F	184	TRP	CD1-NE1-CE2	-6.51	103.14	109.00
1	S	100	ARG	CG-CD-NE	-6.51	98.13	111.80
1	L	32	PHE	CZ-CE2-CD2	6.50	127.90	120.10
1	l	103	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	h	164	TYR	CG-CD2-CE2	6.50	126.50	121.30
1	P	158	LYS	O-C-N	-6.49	112.31	122.70
1	S	169	TYR	CB-CG-CD2	6.49	124.90	121.00
1	5	132	ARG	CD-NE-CZ	6.49	132.69	123.60
1	T	40	PHE	CB-CG-CD2	6.49	125.34	120.80
1	c	23	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	D	23	TRP	CG-CD2-CE3	-6.48	128.07	133.90
1	K	14	ALA	CB-CA-C	6.48	119.82	110.10
1	N	117	TRP	CB-CG-CD2	-6.48	118.17	126.60
1	N	169	TYR	CB-CG-CD1	6.48	124.89	121.00
1	k	222	GLY	C-N-CA	6.48	135.91	122.30
1	L	133	TRP	CB-CG-CD1	6.48	135.42	127.00
1	h	154	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	6	214	MET	CG-SD-CE	-6.47	89.84	100.20
1	V	161	PHE	CB-CG-CD1	-6.47	116.27	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	82	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	j	163	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	82	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	l	229	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	G	162	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	d	173	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	W	130	TYR	CB-CG-CD1	6.45	124.87	121.00
1	l	154	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	e	82	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	d	100	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	7	118	MET	CG-SD-CE	-6.45	89.89	100.20
1	j	209	ALA	CB-CA-C	6.44	119.76	110.10
1	5	29	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	g	132	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	c	48	THR	CA-CB-CG2	-6.43	103.39	112.40
1	G	142	VAL	CA-CB-CG2	-6.43	101.25	110.90
1	l	82	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	H	162	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	O	164	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	g	163	ASP	CB-CG-OD2	6.42	124.08	118.30
1	L	97	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	S	18	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	c	117	TRP	CE2-CD2-CG	-6.42	102.17	107.30
1	M	169	TYR	CB-CG-CD1	6.42	124.85	121.00
1	f	229	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	O	81	ASP	CB-CG-OD2	6.41	124.07	118.30
1	g	130	TYR	CG-CD2-CE2	-6.41	116.17	121.30
1	U	32	PHE	CB-CG-CD1	6.41	125.29	120.80
1	b	64	ALA	N-CA-CB	6.41	119.07	110.10
1	M	152	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	d	55	MET	CG-SD-CE	-6.40	89.95	100.20
1	A	166	ASP	CB-CG-OD1	6.40	124.06	118.30
1	G	215	MET	N-CA-CB	-6.40	99.08	110.60
1	T	169	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	g	54	THR	CA-CB-CG2	6.39	121.35	112.40
1	U	215	MET	CG-SD-CE	-6.39	89.98	100.20
1	m	105	ALA	N-CA-CB	-6.38	101.16	110.10
1	Y	146	SER	N-CA-CB	6.38	120.08	110.50
1	R	133	TRP	CG-CD2-CE3	-6.38	128.16	133.90
1	l	144	MET	CG-SD-CE	-6.38	89.99	100.20
1	f	43	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	7	161	PHE	CZ-CE2-CD2	6.37	127.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	122	PRO	O-C-N	-6.37	109.00	121.10
1	m	130	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	e	164	TYR	CG-CD1-CE1	-6.36	116.21	121.30
1	B	182	LYS	O-C-N	-6.36	112.52	122.70
1	M	23	TRP	CB-CG-CD2	-6.36	118.33	126.60
1	T	130	TYR	CB-CG-CD1	6.36	124.82	121.00
1	Y	78	ALA	N-CA-CB	-6.36	101.19	110.10
1	j	23	TRP	CD2-CE3-CZ3	-6.36	110.53	118.80
1	B	6	LEU	N-CA-CB	6.36	123.11	110.40
1	W	79	GLU	OE1-CD-OE2	-6.36	115.67	123.30
1	i	110	THR	CA-CB-CG2	-6.36	103.50	112.40
1	G	24	VAL	CA-CB-CG1	-6.36	101.37	110.90
1	d	154	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	N	134	ILE	O-C-N	-6.35	112.53	122.70
1	5	229	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	e	97	ARG	CG-CD-NE	-6.35	98.46	111.80
1	H	82	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	X	82	ARG	CD-NE-CZ	6.34	132.48	123.60
1	Y	126	VAL	O-C-N	-6.34	112.42	123.20
1	M	59	VAL	CA-CB-CG1	6.33	120.40	110.90
1	D	197	ASP	CB-CG-OD1	6.33	124.00	118.30
1	I	184	TRP	CB-CG-CD1	6.33	135.23	127.00
1	E	167	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	161	PHE	CB-CG-CD1	-6.32	116.37	120.80
1	R	18	ARG	CG-CD-NE	-6.32	98.52	111.80
1	g	212	GLU	CB-CA-C	-6.32	97.76	110.40
1	A	100	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	c	164	TYR	CD1-CE1-CZ	-6.32	114.11	119.80
1	g	126	VAL	O-C-N	-6.32	112.45	123.20
1	L	133	TRP	CB-CG-CD2	-6.32	118.39	126.60
1	W	169	TYR	CA-CB-CG	-6.31	101.40	113.40
1	X	143	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	V	23	TRP	CD1-CG-CD2	-6.31	101.25	106.30
1	H	96	MET	N-CA-CB	6.31	121.95	110.60
1	d	145	TYR	CG-CD1-CE1	-6.31	116.25	121.30
1	N	126	VAL	CG1-CB-CG2	-6.30	100.81	110.90
1	N	162	ARG	N-CA-CB	6.30	121.94	110.60
1	a	98	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	l	184	TRP	CG-CD2-CE3	-6.29	128.24	133.90
1	l	168	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	O	167	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	l	158	LYS	N-CA-CB	6.29	121.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	97	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	a	194	ALA	O-C-N	-6.28	112.65	122.70
1	M	230	VAL	CA-CB-CG2	6.28	120.31	110.90
1	A	32	PHE	CB-CG-CD2	6.27	125.19	120.80
1	e	145	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	i	132	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	g	173	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	5	97	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	C	208	ALA	N-CA-CB	-6.26	101.33	110.10
1	i	130	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	L	168	PHE	CB-CG-CD2	6.26	125.18	120.80
1	O	31	ALA	CB-CA-C	6.26	119.49	110.10
1	h	128	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	T	145	TYR	CD1-CG-CD2	6.25	124.78	117.90
1	h	14	ALA	O-C-N	-6.25	112.70	122.70
1	E	68	MET	CG-SD-CE	-6.25	90.20	100.20
1	X	187	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	m	181	VAL	CG1-CB-CG2	-6.25	100.91	110.90
1	K	229	ARG	NH1-CZ-NH2	-6.24	112.53	119.40
1	a	196	PRO	N-CA-CB	6.24	110.79	103.30
1	H	23	TRP	CE3-CZ3-CH2	-6.24	114.33	121.20
1	L	133	TRP	CG-CD2-CE3	-6.24	128.29	133.90
1	L	162	ARG	CG-CD-NE	-6.24	98.70	111.80
1	P	191	VAL	CA-CB-CG1	6.24	120.26	110.90
1	6	172	LEU	CA-CB-CG	6.24	129.65	115.30
1	b	152	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	W	135	ILE	O-C-N	-6.23	112.73	122.70
1	H	166	ASP	CB-CG-OD2	6.23	123.91	118.30
1	N	152	ASP	N-CA-CB	-6.22	99.40	110.60
1	J	229	ARG	O-C-N	-6.22	112.75	122.70
1	j	164	TYR	CD1-CE1-CZ	-6.22	114.20	119.80
1	l	148	THR	N-CA-CB	6.22	122.11	110.30
1	U	19	THR	N-CA-CB	6.21	122.11	110.30
1	P	6	LEU	CB-CA-C	-6.21	98.40	110.20
1	d	143	ARG	NH1-CZ-NH2	-6.21	112.56	119.40
1	M	130	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	R	144	MET	CG-SD-CE	-6.21	90.27	100.20
1	V	229	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	b	142	VAL	CA-CB-CG2	-6.21	101.59	110.90
1	l	42	ALA	N-CA-CB	-6.21	101.41	110.10
1	J	152	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	h	197	ASP	CB-CG-OD1	-6.20	112.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	133	TRP	NE1-CE2-CD2	6.20	113.50	107.30
1	A	184	TRP	CG-CD2-CE3	-6.20	128.32	133.90
1	M	165	VAL	CA-CB-CG1	-6.20	101.61	110.90
1	O	169	TYR	CG-CD2-CE2	-6.20	116.34	121.30
1	f	40	PHE	CB-CG-CD2	6.19	125.14	120.80
1	e	217	ALA	CB-CA-C	6.19	119.39	110.10
1	U	216	THR	CA-CB-CG2	-6.18	103.74	112.40
1	c	66	MET	CA-CB-CG	6.18	123.81	113.30
1	C	68	MET	O-C-N	-6.18	112.81	122.70
1	U	184	TRP	CE2-CD2-CG	-6.18	102.35	107.30
1	G	210	THR	CA-CB-CG2	-6.17	103.76	112.40
1	m	144	MET	N-CA-CB	-6.17	99.49	110.60
1	E	55	MET	CG-SD-CE	-6.17	90.33	100.20
1	j	229	ARG	CG-CD-NE	-6.17	98.85	111.80
1	a	164	TYR	CD1-CE1-CZ	6.16	125.35	119.80
1	e	81	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	Y	36	VAL	CA-CB-CG2	6.16	120.14	110.90
1	B	110	THR	CA-CB-CG2	-6.15	103.79	112.40
1	Q	231	LEU	CB-CA-C	6.15	121.89	110.20
1	H	142	VAL	CA-CB-CG1	6.15	120.12	110.90
1	5	143	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	I	218	CYS	CA-CB-SG	6.14	125.06	114.00
1	L	1	PRO	CA-N-CD	-6.14	102.90	111.50
1	F	133	TRP	CB-CG-CD1	6.14	134.99	127.00
1	N	66	MET	CG-SD-CE	-6.14	90.38	100.20
1	T	164	TYR	CB-CG-CD1	6.14	124.68	121.00
1	Y	86	VAL	CA-CB-CG2	-6.14	101.69	110.90
1	F	32	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	R	169	TYR	CG-CD2-CE2	-6.13	116.39	121.30
1	d	126	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	a	220	GLY	CA-C-O	-6.13	109.56	120.60
1	a	169	TYR	CB-CG-CD2	6.13	124.68	121.00
1	B	86	VAL	CA-CB-CG2	-6.13	101.71	110.90
1	C	130	TYR	CG-CD2-CE2	-6.12	116.40	121.30
1	P	162	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	M	97	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	R	205	LEU	O-C-N	-6.12	112.80	123.20
1	M	23	TRP	CD2-CE2-CZ2	-6.12	114.96	122.30
1	D	178	SER	N-CA-CB	6.11	119.66	110.50
1	6	14	ALA	CB-CA-C	6.11	119.26	110.10
1	V	23	TRP	CG-CD1-NE1	6.10	116.20	110.10
1	g	163	ASP	CB-CG-OD1	-6.10	112.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	80	TRP	CB-CG-CD2	-6.10	118.67	126.60
1	E	166	ASP	N-CA-CB	-6.10	99.63	110.60
1	7	167	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	C	164	TYR	CB-CG-CD1	6.09	124.65	121.00
1	G	51	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	L	113	GLU	CG-CD-OE1	6.09	130.47	118.30
1	i	55	MET	CG-SD-CE	-6.08	90.47	100.20
1	B	145	TYR	CZ-CE2-CD2	6.08	125.27	119.80
1	E	184	TRP	CA-CB-CG	6.08	125.25	113.70
1	6	133	TRP	CD1-NE1-CE2	-6.08	103.53	109.00
1	Q	100	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	X	217	ALA	N-CA-CB	-6.08	101.59	110.10
1	R	169	TYR	CZ-CE2-CD2	6.08	125.27	119.80
1	W	212	GLU	O-C-N	-6.07	112.98	122.70
1	P	214	MET	CG-SD-CE	6.07	109.91	100.20
1	C	55	MET	CG-SD-CE	-6.07	90.49	100.20
1	X	148	THR	OG1-CB-CG2	-6.07	96.04	110.00
1	Z	167	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	P	184	TRP	CG-CD2-CE3	-6.07	128.44	133.90
1	S	40	PHE	CB-CG-CD1	-6.07	116.55	120.80
1	6	54	THR	CA-CB-CG2	-6.07	103.90	112.40
1	N	168	PHE	CD1-CG-CD2	6.07	126.19	118.30
1	k	215	MET	CG-SD-CE	-6.07	90.50	100.20
1	k	82	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	e	68	MET	CG-SD-CE	6.06	109.89	100.20
1	f	130	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	l	161	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	I	86	VAL	CA-CB-CG2	-6.05	101.82	110.90
1	O	97	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
1	G	164	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	a	226	HIS	O-C-N	-6.05	113.02	122.70
1	B	58	THR	OG1-CB-CG2	-6.05	96.09	110.00
1	A	133	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	B	130	TYR	CD1-CG-CD2	6.05	124.55	117.90
1	C	162	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	5	185	MET	N-CA-CB	-6.04	99.72	110.60
1	G	169	TYR	CG-CD2-CE2	-6.04	116.47	121.30
1	K	168	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	J	158	LYS	CA-CB-CG	6.04	126.68	113.40
1	a	162	ARG	CD-NE-CZ	-6.04	115.15	123.60
1	i	197	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	Z	154	ARG	NE-CZ-NH2	-6.04	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	23	TRP	CA-CB-CG	6.03	125.16	113.70
1	L	213	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	I	191	VAL	CG1-CB-CG2	-6.03	101.25	110.90
1	B	109	SER	N-CA-CB	6.02	119.54	110.50
1	l	169	TYR	CB-CG-CD1	6.02	124.61	121.00
1	h	56	LEU	CB-CG-CD2	6.02	121.23	111.00
1	L	66	MET	CG-SD-CE	-6.02	90.57	100.20
1	W	212	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	B	68	MET	CG-SD-CE	-6.01	90.58	100.20
1	I	161	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	e	143	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	168	PHE	CZ-CE2-CD2	-6.00	112.89	120.10
1	W	68	MET	CA-CB-CG	-6.00	103.09	113.30
1	A	184	TRP	CE2-CD2-CE3	6.00	125.91	118.70
1	I	212	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	P	117	TRP	CH2-CZ2-CE2	6.00	123.40	117.40
1	Y	199	LYS	O-C-N	-6.00	113.09	122.70
1	k	132	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	M	76	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	O	161	PHE	CB-CG-CD2	6.00	125.00	120.80
1	6	93	PRO	O-C-N	-6.00	113.00	123.20
1	h	166	ASP	CB-CG-OD2	6.00	123.69	118.30
1	b	82	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	7	23	TRP	CG-CD2-CE3	-5.99	128.51	133.90
1	c	103	ASP	CB-CG-OD2	5.99	123.69	118.30
1	F	40	PHE	CB-CG-CD1	5.99	124.99	120.80
1	P	154	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	L	159	GLU	CA-C-N	5.99	133.87	117.10
1	a	152	ASP	CB-CG-OD1	5.99	123.69	118.30
1	Z	166	ASP	CB-CG-OD1	5.98	123.68	118.30
1	6	18	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
1	C	32	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	D	39	MET	CG-SD-CE	5.97	109.76	100.20
1	7	229	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	77	ALA	O-C-N	-5.97	113.15	122.70
1	G	130	TYR	CG-CD2-CE2	5.97	126.08	121.30
1	Q	145	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	Q	154	ARG	CB-CA-C	-5.97	98.46	110.40
1	l	77	ALA	N-CA-CB	5.97	118.46	110.10
1	C	167	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	G	142	VAL	CA-CB-CG1	5.96	119.84	110.90
1	j	185	MET	CA-CB-CG	5.96	123.43	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	97	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	S	80	TRP	CB-CG-CD2	-5.96	118.86	126.60
1	W	47	ALA	O-C-N	-5.96	113.17	122.70
1	7	173	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	6	143	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	m	161	PHE	CD1-CE1-CZ	-5.95	112.96	120.10
1	f	80	TRP	CB-CG-CD2	-5.95	118.87	126.60
1	P	3	VAL	CB-CA-C	-5.94	100.11	111.40
1	a	42	ALA	N-CA-CB	5.94	118.42	110.10
1	k	230	VAL	CB-CA-C	-5.94	100.11	111.40
1	L	164	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	R	34	PRO	O-C-N	-5.93	113.20	122.70
1	F	44	SER	CB-CA-C	-5.93	98.83	110.10
1	L	185	MET	CG-SD-CE	-5.93	90.71	100.20
1	N	40	PHE	CB-CG-CD1	5.93	124.95	120.80
1	A	209	ALA	O-C-N	-5.93	113.21	122.70
1	g	88	ALA	N-CA-CB	-5.93	101.80	110.10
1	G	69	LEU	CB-CG-CD1	5.93	121.07	111.00
1	T	145	TYR	CG-CD2-CE2	-5.93	116.56	121.30
1	h	101	GLY	O-C-N	-5.93	113.22	122.70
1	e	105	ALA	N-CA-CB	-5.92	101.81	110.10
1	c	145	TYR	CA-CB-CG	-5.92	102.15	113.40
1	U	190	LEU	CB-CG-CD1	5.92	121.06	111.00
1	5	167	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	7	33	SER	N-CA-CB	-5.92	101.62	110.50
1	m	3	VAL	CA-CB-CG2	5.92	119.78	110.90
1	a	100	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	U	142	VAL	O-C-N	-5.92	113.24	122.70
1	5	83	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	h	152	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	C	130	TYR	O-C-N	-5.91	113.25	122.70
1	Y	145	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
1	g	169	TYR	CG-CD2-CE2	-5.91	116.58	121.30
1	J	161	PHE	CZ-CE2-CD2	-5.90	113.02	120.10
1	A	40	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	5	177	ALA	N-CA-CB	5.90	118.36	110.10
1	D	10	MET	CG-SD-CE	-5.90	90.76	100.20
1	J	40	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	J	171	THR	CA-CB-CG2	-5.90	104.14	112.40
1	D	97	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	144	MET	CB-CA-C	5.89	122.19	110.40
1	a	31	ALA	O-C-N	-5.89	113.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	103	ASP	CB-CG-OD1	5.89	123.60	118.30
1	X	229	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	V	24	VAL	CA-CB-CG2	-5.89	102.07	110.90
1	7	226	HIS	CA-CB-CG	5.89	123.61	113.60
1	e	170	LYS	O-C-N	-5.88	113.28	122.70
1	j	209	ALA	O-C-N	-5.88	113.29	122.70
1	j	199	LYS	O-C-N	-5.88	113.29	122.70
1	k	69	LEU	O-C-N	-5.88	113.29	122.70
1	X	132	ARG	CD-NE-CZ	5.88	131.83	123.60
1	H	174	ALA	N-CA-CB	-5.88	101.87	110.10
1	V	80	TRP	CZ3-CH2-CZ2	-5.88	114.55	121.60
1	e	162	ARG	CA-CB-CG	5.88	126.33	113.40
1	V	68	MET	CG-SD-CE	-5.87	90.80	100.20
1	6	97	ARG	O-C-N	-5.87	113.30	122.70
1	F	11	VAL	O-C-N	-5.87	113.31	122.70
1	F	23	TRP	CB-CG-CD2	-5.87	118.97	126.60
1	U	175	GLU	CB-CG-CD	-5.87	98.35	114.20
1	Z	18	ARG	NH1-CZ-NH2	5.87	125.85	119.40
1	g	154	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	D	144	MET	CG-SD-CE	-5.86	90.82	100.20
1	L	130	TYR	O-C-N	-5.86	113.32	122.70
1	S	32	PHE	CB-CA-C	5.86	122.12	110.40
1	N	64	ALA	N-CA-CB	5.86	118.30	110.10
1	M	124	ILE	CG1-CB-CG2	5.86	124.28	111.40
1	N	117	TRP	CE2-CD2-CG	-5.85	102.62	107.30
1	W	108	THR	N-CA-CB	5.85	121.42	110.30
1	G	23	TRP	CZ3-CH2-CZ2	-5.85	114.58	121.60
1	5	66	MET	CG-SD-CE	-5.85	90.83	100.20
1	Q	142	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	m	97	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	d	44	SER	N-CA-CB	5.85	119.28	110.50
1	X	82	ARG	NH1-CZ-NH2	-5.85	112.97	119.40
1	C	97	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	M	124	ILE	O-C-N	-5.84	110.00	121.10
1	O	229	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	I	199	LYS	N-CA-CB	-5.84	100.09	110.60
1	b	88	ALA	O-C-N	-5.84	113.27	123.20
1	P	145	TYR	CA-CB-CG	-5.84	102.31	113.40
1	h	152	ASP	CB-CG-OD2	5.84	123.55	118.30
1	j	88	ALA	CB-CA-C	-5.83	101.35	110.10
1	P	110	THR	CA-CB-CG2	-5.83	104.23	112.40
1	6	111	LEU	CB-CG-CD2	5.83	120.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	154	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	K	100	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	O	194	ALA	C-N-CA	5.83	136.28	121.70
1	Q	103	ASP	CB-CA-C	-5.83	98.74	110.40
1	E	169	TYR	CG-CD2-CE2	-5.83	116.64	121.30
1	g	163	ASP	CA-CB-CG	-5.83	100.58	113.40
1	H	82	ARG	CG-CD-NE	-5.83	99.57	111.80
1	B	229	ARG	CD-NE-CZ	5.82	131.75	123.60
1	G	132	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	K	27	VAL	CA-CB-CG1	-5.82	102.17	110.90
1	Q	152	ASP	CB-CG-OD1	-5.82	113.07	118.30
1	K	110	THR	CA-CB-CG2	-5.81	104.26	112.40
1	f	218	CYS	CA-CB-SG	5.81	124.47	114.00
1	b	177	ALA	CB-CA-C	5.81	118.82	110.10
1	l	132	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	h	14	ALA	N-CA-CB	5.81	118.24	110.10
1	G	178	SER	CB-CA-C	-5.81	99.06	110.10
1	5	208	ALA	N-CA-CB	5.81	118.23	110.10
1	l	26	VAL	CA-C-O	5.81	132.30	120.10
1	V	4	GLN	N-CA-C	5.81	126.68	111.00
1	J	164	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	R	20	LEU	CB-CG-CD1	5.80	120.87	111.00
1	R	126	VAL	CB-CA-C	-5.80	100.38	111.40
1	h	96	MET	CG-SD-CE	-5.80	90.92	100.20
1	T	18	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	a	40	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	i	130	TYR	CG-CD1-CE1	-5.80	116.66	121.30
1	Q	228	ALA	N-CA-CB	5.80	118.22	110.10
1	U	214	MET	CG-SD-CE	-5.80	90.92	100.20
1	i	2	ILE	O-C-N	-5.80	113.42	122.70
1	Z	65	ALA	N-CA-CB	-5.79	101.99	110.10
1	G	11	VAL	CA-CB-CG2	5.79	119.59	110.90
1	C	31	ALA	CB-CA-C	-5.79	101.42	110.10
1	K	25	LYS	O-C-N	-5.79	113.44	122.70
1	c	86	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	k	188	THR	CA-CB-CG2	-5.79	104.30	112.40
1	U	18	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
1	j	28	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	V	82	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	F	10	MET	N-CA-CB	5.78	121.00	110.60
1	Y	136	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	l	173	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	218	CYS	CA-CB-SG	5.78	124.40	114.00
1	P	82	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	R	133	TRP	CE2-CD2-CE3	5.78	125.63	118.70
1	F	51	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	G	144	MET	O-C-N	-5.77	113.47	122.70
1	U	97	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	6	214	MET	CA-CB-CG	-5.77	103.49	113.30
1	h	105	ALA	N-CA-CB	-5.77	102.02	110.10
1	e	79	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	D	167	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	F	130	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	Y	227	LYS	N-CA-CB	5.76	120.97	110.60
1	Q	82	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	V	218	CYS	N-CA-CB	5.76	120.97	110.60
1	D	173	ARG	NH1-CZ-NH2	-5.76	113.07	119.40
1	R	18	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	a	108	THR	CA-CB-CG2	-5.76	104.34	112.40
1	b	144	MET	CG-SD-CE	-5.76	90.99	100.20
1	f	130	TYR	CG-CD2-CE2	-5.76	116.69	121.30
1	A	82	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
1	I	204	ALA	CB-CA-C	-5.75	101.47	110.10
1	V	166	ASP	CB-CG-OD1	5.75	123.48	118.30
1	k	126	VAL	CA-CB-CG2	5.75	119.53	110.90
1	M	96	MET	CG-SD-CE	-5.75	91.00	100.20
1	c	188	THR	CA-CB-CG2	5.75	120.45	112.40
1	C	64	ALA	O-C-N	-5.75	113.50	122.70
1	i	37	ILE	CA-CB-CG2	-5.75	99.41	110.90
1	Z	100	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	m	163	ASP	CB-CG-OD2	5.75	123.47	118.30
1	N	11	VAL	N-CA-CB	-5.74	98.87	111.50
1	W	117	TRP	N-CA-CB	-5.74	100.27	110.60
1	A	169	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	O	100	ARG	CD-NE-CZ	5.74	131.63	123.60
1	Q	202	LEU	CB-CA-C	-5.74	99.30	110.20
1	b	40	PHE	CB-CG-CD2	5.74	124.81	120.80
1	A	204	ALA	O-C-N	-5.73	113.53	122.70
1	j	23	TRP	CG-CD2-CE3	-5.73	128.74	133.90
1	f	159	GLU	N-CA-CB	-5.73	100.29	110.60
1	H	97	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	N	23	TRP	CD2-CE3-CZ3	-5.73	111.36	118.80
1	a	38	PRO	N-CA-CB	-5.73	96.30	102.60
1	f	137	GLY	O-C-N	-5.73	113.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	GLU	CA-C-N	5.72	129.79	117.20
1	m	184	TRP	CG-CD2-CE3	-5.72	128.75	133.90
1	g	140	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	k	184	TRP	CE2-CD2-CE3	5.72	125.56	118.70
1	E	17	PRO	O-C-N	5.71	131.84	122.70
1	T	128	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	5	82	ARG	CG-CD-NE	-5.71	99.81	111.80
1	U	186	THR	CA-CB-CG2	-5.71	104.41	112.40
1	W	59	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	c	31	ALA	N-CA-CB	-5.71	102.11	110.10
1	k	55	MET	CA-CB-CG	5.71	123.00	113.30
1	L	131	LYS	N-CA-CB	5.70	120.86	110.60
1	5	191	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	7	45	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	E	107	THR	CA-CB-CG2	-5.70	104.42	112.40
1	N	200	THR	CA-CB-CG2	-5.70	104.42	112.40
1	D	140	LYS	CB-CA-C	-5.70	99.00	110.40
1	T	71	GLU	O-C-N	-5.70	113.58	122.70
1	6	218	CYS	O-C-N	-5.70	113.58	122.70
1	L	132	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	O	82	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	6	118	MET	CG-SD-CE	-5.69	91.09	100.20
1	U	82	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	k	173	ARG	O-C-N	-5.69	113.59	122.70
1	S	130	TYR	CB-CG-CD2	-5.69	117.58	121.00
1	5	51	ASP	CB-CG-OD2	5.69	123.42	118.30
1	M	10	MET	CG-SD-CE	-5.69	91.10	100.20
1	l	161	PHE	CB-CG-CD1	5.69	124.78	120.80
1	A	28	GLU	OE1-CD-OE2	-5.69	116.48	123.30
1	B	133	TRP	CB-CG-CD1	5.69	134.39	127.00
1	T	214	MET	O-C-N	-5.68	113.60	122.70
1	R	161	PHE	C-N-CA	5.68	135.90	121.70
1	N	208	ALA	N-CA-CB	-5.68	102.15	110.10
1	U	35	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	V	147	PRO	O-C-N	5.68	131.78	122.70
1	f	169	TYR	CG-CD1-CE1	-5.68	116.76	121.30
1	h	162	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	40	PHE	CG-CD2-CE2	-5.67	114.56	120.80
1	E	145	TYR	CZ-CE2-CD2	5.67	124.90	119.80
1	i	143	ARG	N-CA-CB	5.67	120.81	110.60
1	N	18	ARG	NH1-CZ-NH2	-5.67	113.17	119.40
1	a	80	TRP	NE1-CE2-CD2	5.67	112.97	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	67	GLN	O-C-N	-5.67	113.63	122.70
1	f	11	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	L	113	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	P	19	THR	CA-CB-CG2	5.67	120.33	112.40
1	C	133	TRP	CG-CD2-CE3	-5.66	128.80	133.90
1	W	209	ALA	N-CA-CB	-5.66	102.18	110.10
1	l	91	ILE	CA-CB-CG1	5.66	121.75	111.00
1	U	82	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	V	30	LYS	O-C-N	-5.65	113.66	122.70
1	P	145	TYR	CB-CG-CD1	5.65	124.39	121.00
1	7	23	TRP	NE1-CE2-CD2	5.65	112.95	107.30
1	O	172	LEU	CB-CG-CD2	5.65	120.60	111.00
1	M	164	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	Z	24	VAL	O-C-N	-5.64	113.67	122.70
1	l	181	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	I	166	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	M	153	ILE	O-C-N	-5.64	113.67	122.70
1	X	28	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	Z	215	MET	CG-SD-CE	-5.64	91.18	100.20
1	k	152	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	m	13	GLN	CB-CA-C	-5.64	99.13	110.40
1	g	144	MET	CG-SD-CE	5.63	109.21	100.20
1	6	152	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	H	147	PRO	O-C-N	5.63	131.70	122.70
1	P	213	GLU	OE1-CD-OE2	-5.63	116.55	123.30
1	R	163	ASP	CB-CA-C	5.63	121.65	110.40
1	U	173	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	6	186	THR	O-C-N	-5.63	113.70	122.70
1	X	217	ALA	CB-CA-C	-5.62	101.67	110.10
1	E	215	MET	CG-SD-CE	-5.62	91.20	100.20
1	6	23	TRP	CB-CG-CD1	5.62	134.31	127.00
1	F	142	VAL	CA-CB-CG1	5.62	119.33	110.90
1	b	97	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	F	56	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	L	1	PRO	N-CA-CB	5.62	110.04	103.30
1	B	100	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	L	145	TYR	CG-CD1-CE1	-5.61	116.81	121.30
1	U	10	MET	CG-SD-CE	-5.61	91.23	100.20
1	Z	188	THR	CA-CB-CG2	5.61	120.25	112.40
1	A	196	PRO	N-CA-CB	5.61	110.03	103.30
1	D	161	PHE	CG-CD1-CE1	-5.60	114.64	120.80
1	J	164	TYR	CD1-CE1-CZ	-5.60	114.76	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	108	THR	CA-CB-CG2	-5.60	104.56	112.40
1	S	154	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	l	47	ALA	CB-CA-C	-5.60	101.69	110.10
1	D	51	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	X	68	MET	O-C-N	-5.60	113.74	122.70
1	a	81	ASP	CB-CA-C	-5.59	99.21	110.40
1	j	115	ILE	CB-CA-C	-5.59	100.41	111.60
1	i	143	ARG	CG-CD-NE	-5.59	100.06	111.80
1	D	81	ASP	CB-CG-OD1	5.59	123.33	118.30
1	K	154	ARG	CG-CD-NE	-5.59	100.07	111.80
1	S	163	ASP	CB-CG-OD2	5.59	123.33	118.30
1	X	143	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	d	23	TRP	CG-CD2-CE3	-5.59	128.87	133.90
1	T	82	ARG	CD-NE-CZ	5.58	131.41	123.60
1	E	10	MET	O-C-N	-5.58	113.78	122.70
1	J	103	ASP	CB-CG-OD2	5.58	123.32	118.30
1	O	140	LYS	N-CA-CB	5.58	120.64	110.60
1	6	68	MET	CG-SD-CE	-5.58	91.28	100.20
1	W	3	VAL	CG1-CB-CG2	-5.58	101.98	110.90
1	Z	75	GLU	O-C-N	-5.58	113.78	122.70
1	F	181	VAL	O-C-N	-5.57	113.78	122.70
1	a	95	GLN	O-C-N	-5.57	113.78	122.70
1	F	161	PHE	CB-CG-CD1	5.57	124.70	120.80
1	h	150	ILE	CA-CB-CG1	5.57	121.58	111.00
1	6	133	TRP	NE1-CE2-CD2	5.57	112.87	107.30
1	C	117	TRP	CG-CD2-CE3	-5.57	128.89	133.90
1	G	19	THR	O-C-N	-5.57	113.80	122.70
1	J	67	GLN	O-C-N	-5.57	113.80	122.70
1	Q	226	HIS	CA-CB-CG	5.57	123.06	113.60
1	m	216	THR	CA-CB-CG2	-5.57	104.61	112.40
1	A	48	THR	CA-CB-CG2	-5.56	104.61	112.40
1	N	188	THR	N-CA-CB	5.56	120.87	110.30
1	P	164	TYR	CD1-CG-CD2	5.56	124.02	117.90
1	N	143	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	f	31	ALA	CB-CA-C	5.56	118.44	110.10
1	G	51	ASP	CB-CG-OD2	5.56	123.30	118.30
1	7	117	TRP	CD2-CE3-CZ3	-5.56	111.57	118.80
1	A	58	THR	CA-CB-CG2	-5.56	104.62	112.40
1	M	167	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	a	145	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	k	121	ASN	N-CA-CB	-5.55	100.60	110.60
1	S	228	ALA	O-C-N	-5.55	113.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	230	VAL	CA-CB-CG2	5.55	119.23	110.90
1	c	23	TRP	NE1-CE2-CD2	5.55	112.85	107.30
1	G	43	LEU	O-C-N	-5.55	113.83	122.70
1	Y	154	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	Y	168	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	A	10	MET	CG-SD-CE	-5.54	91.33	100.20
1	B	159	GLU	N-CA-CB	-5.54	100.62	110.60
1	Y	39	MET	CG-SD-CE	-5.54	91.33	100.20
1	X	124	ILE	O-C-N	-5.54	110.57	121.10
1	i	219	GLN	CB-CA-C	5.54	121.48	110.40
1	N	130	TYR	CA-CB-CG	5.54	123.93	113.40
1	c	144	MET	CG-SD-CE	-5.54	91.34	100.20
1	W	194	ALA	O-C-N	-5.54	113.84	122.70
1	F	1	PRO	N-CA-CB	5.54	109.94	103.30
1	K	208	ALA	N-CA-CB	-5.54	102.35	110.10
1	M	32	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	b	126	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	k	82	ARG	CD-NE-CZ	5.53	131.35	123.60
1	g	229	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	F	161	PHE	CG-CD1-CE1	5.53	126.89	120.80
1	F	86	VAL	O-C-N	-5.53	113.85	122.70
1	j	180	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	c	23	TRP	CH2-CZ2-CE2	5.53	122.92	117.40
1	7	47	ALA	N-CA-CB	-5.53	102.36	110.10
1	P	167	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	c	32	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	K	43	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	P	126	VAL	CA-CB-CG1	-5.52	102.62	110.90
1	V	167	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	X	134	ILE	O-C-N	-5.52	113.87	122.70
1	G	23	TRP	CH2-CZ2-CE2	5.52	122.92	117.40
1	I	24	VAL	CG1-CB-CG2	-5.52	102.08	110.90
1	c	23	TRP	CE2-CD2-CE3	5.52	125.32	118.70
1	J	168	PHE	CB-CA-C	-5.51	99.37	110.40
1	L	100	ARG	O-C-N	-5.51	113.83	123.20
1	D	162	ARG	O-C-N	-5.51	113.88	122.70
1	L	204	ALA	N-CA-CB	5.51	117.81	110.10
1	6	198	CYS	O-C-N	-5.51	113.89	122.70
1	g	182	LYS	N-CA-CB	5.51	120.51	110.60
1	F	202	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	K	56	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	D	192	GLN	CB-CA-C	5.50	121.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	36	VAL	CG1-CB-CG2	-5.50	102.11	110.90
1	S	221	VAL	O-C-N	-5.50	113.86	123.20
1	I	145	TYR	CB-CG-CD1	5.49	124.30	121.00
1	R	209	ALA	CB-CA-C	5.49	118.34	110.10
1	W	185	MET	CG-SD-CE	-5.49	91.42	100.20
1	L	164	TYR	CB-CG-CD1	5.49	124.29	121.00
1	f	144	MET	CG-SD-CE	-5.49	91.42	100.20
1	N	118	MET	CG-SD-CE	-5.49	91.42	100.20
1	S	185	MET	O-C-N	-5.49	113.92	122.70
1	Z	48	THR	CA-CB-CG2	-5.49	104.72	112.40
1	h	215	MET	CG-SD-CE	-5.49	91.42	100.20
1	j	48	THR	CA-CB-CG2	-5.49	104.72	112.40
1	k	27	VAL	CG1-CB-CG2	-5.48	102.12	110.90
1	F	161	PHE	CD1-CG-CD2	-5.48	111.17	118.30
1	I	189	LEU	CB-CG-CD2	5.48	120.32	111.00
1	b	145	TYR	CG-CD2-CE2	5.48	125.69	121.30
1	c	27	VAL	O-C-N	-5.48	113.93	122.70
1	a	197	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	h	226	HIS	CA-CB-CG	-5.48	104.29	113.60
1	N	119	THR	CA-CB-OG1	5.48	120.50	109.00
1	Q	64	ALA	CA-C-O	5.48	131.60	120.10
1	j	163	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	118	MET	CA-CB-CG	-5.47	104.00	113.30
1	j	180	GLU	O-C-N	-5.47	113.94	122.70
1	U	132	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	17	PRO	N-CA-CB	5.47	109.86	103.30
1	D	154	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	170	LYS	O-C-N	-5.47	113.95	122.70
1	H	151	LEU	CB-CG-CD2	5.47	120.30	111.00
1	L	103	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	N	117	TRP	CB-CG-CD1	5.47	134.11	127.00
1	U	154	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	164	TYR	N-CA-CB	-5.47	100.76	110.60
1	Y	185	MET	CG-SD-CE	-5.46	91.46	100.20
1	D	164	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	J	117	TRP	NE1-CE2-CZ2	5.46	136.41	130.40
1	Y	59	VAL	CA-CB-CG2	5.46	119.09	110.90
1	d	23	TRP	CE3-CZ3-CH2	5.46	127.21	121.20
1	B	123	PRO	N-CD-CG	5.46	111.39	103.20
1	D	152	ASP	CB-CG-OD2	5.46	123.21	118.30
1	N	80	TRP	CG-CD2-CE3	-5.46	128.99	133.90
1	Y	215	MET	CG-SD-CE	5.46	108.93	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	104	ILE	CB-CA-C	5.45	122.51	111.60
1	Q	40	PHE	CB-CG-CD1	-5.45	116.98	120.80
1	I	169	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	O	229	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	g	164	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	H	184	TRP	CD1-NE1-CE2	-5.45	104.10	109.00
1	P	18	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	V	130	TYR	CB-CG-CD2	5.45	124.27	121.00
1	W	162	ARG	N-CA-CB	-5.45	100.79	110.60
1	X	69	LEU	N-CA-CB	-5.45	99.50	110.40
1	d	35	GLU	O-C-N	-5.45	113.98	122.70
1	m	154	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	m	182	LYS	O-C-N	-5.45	113.99	122.70
1	Z	186	THR	O-C-N	-5.44	113.99	122.70
1	b	13	GLN	N-CA-CB	5.44	120.39	110.60
1	b	87	HIS	CA-C-O	5.44	131.53	120.10
1	C	97	ARG	CG-CD-NE	-5.44	100.37	111.80
1	Y	72	THR	N-CA-CB	5.44	120.64	110.30
1	J	118	MET	CG-SD-CE	-5.44	91.50	100.20
1	7	100	ARG	O-C-N	-5.44	113.96	123.20
1	A	152	ASP	CB-CG-OD2	5.43	123.19	118.30
1	X	167	ARG	CG-CD-NE	-5.43	100.39	111.80
1	h	22	ALA	CB-CA-C	-5.43	101.95	110.10
1	Z	208	ALA	N-CA-CB	-5.43	102.50	110.10
1	5	107	THR	OG1-CB-CG2	-5.43	97.51	110.00
1	L	145	TYR	CG-CD2-CE2	5.43	125.64	121.30
1	Q	76	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	W	188	THR	O-C-N	-5.42	114.02	122.70
1	W	143	ARG	CD-NE-CZ	5.42	131.19	123.60
1	C	122	PRO	CA-C-N	5.42	132.28	117.10
1	E	170	LYS	O-C-N	-5.42	114.03	122.70
1	I	173	ARG	N-CA-CB	-5.42	100.84	110.60
1	B	64	ALA	CB-CA-C	-5.42	101.97	110.10
1	K	169	TYR	CG-CD1-CE1	-5.42	116.96	121.30
1	H	133	TRP	CE2-CD2-CG	-5.42	102.97	107.30
1	i	80	TRP	CG-CD2-CE3	-5.42	129.03	133.90
1	e	200	THR	O-C-N	-5.42	114.03	122.70
1	6	197	ASP	CB-CG-OD2	5.42	123.17	118.30
1	5	149	SER	N-CA-CB	5.41	118.62	110.50
1	Y	117	TRP	CG-CD2-CE3	-5.41	129.03	133.90
1	B	51	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	Z	31	ALA	O-C-N	-5.41	114.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	7	1	PRO	N-CD-CG	-5.41	95.09	103.20
1	a	168	PHE	CB-CG-CD1	5.41	124.58	120.80
1	A	100	ARG	CG-CD-NE	-5.41	100.45	111.80
1	A	133	TRP	CD1-NE1-CE2	5.41	113.86	109.00
1	M	167	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	P	31	ALA	CB-CA-C	5.40	118.20	110.10
1	K	163	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	L	54	THR	CA-CB-CG2	5.40	119.96	112.40
1	N	52	LEU	O-C-N	-5.40	114.06	122.70
1	W	86	VAL	CA-CB-CG1	-5.40	102.80	110.90
1	a	145	TYR	CB-CG-CD1	5.40	124.24	121.00
1	j	107	THR	O-C-N	-5.40	114.06	122.70
1	d	229	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	L	169	TYR	CG-CD2-CE2	-5.40	116.98	121.30
1	e	96	MET	CA-CB-CG	5.40	122.47	113.30
1	6	193	ASN	N-CA-CB	5.39	120.31	110.60
1	g	219	GLN	CB-CA-C	-5.39	99.62	110.40
1	K	161	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	a	188	THR	O-C-N	-5.39	114.08	122.70
1	G	130	TYR	CZ-CE2-CD2	-5.38	114.95	119.80
1	U	212	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	a	202	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	N	210	THR	O-C-N	-5.38	114.09	122.70
1	c	161	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	Y	145	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	d	125	PRO	N-CA-C	-5.38	98.11	112.10
1	T	73	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	Z	78	ALA	CB-CA-C	5.38	118.17	110.10
1	c	117	TRP	O-C-N	-5.38	114.09	122.70
1	7	53	ASN	CB-CA-C	-5.38	99.64	110.40
1	f	178	SER	N-CA-C	5.38	125.53	111.00
1	5	51	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	5	164	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
1	m	154	ARG	CG-CD-NE	-5.38	100.51	111.80
1	d	213	GLU	N-CA-CB	-5.38	100.92	110.60
1	E	100	ARG	CG-CD-NE	-5.38	100.51	111.80
1	E	229	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	R	23	TRP	CZ3-CH2-CZ2	-5.37	115.16	121.60
1	U	26	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	Z	207	PRO	N-CD-CG	5.37	111.26	103.20
1	N	165	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	D	47	ALA	N-CA-CB	-5.37	102.59	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	183	ASN	CB-CG-OD1	5.37	132.33	121.60
1	N	82	ARG	CG-CD-NE	-5.36	100.54	111.80
1	X	100	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	f	38	PRO	N-CA-CB	5.36	109.74	103.30
1	h	88	ALA	N-CA-CB	5.36	117.61	110.10
1	b	97	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	F	92	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	H	120	HIS	CA-CB-CG	5.36	122.71	113.60
1	T	154	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	f	54	THR	CA-CB-CG2	-5.36	104.90	112.40
1	V	179	GLN	CG-CD-OE1	-5.35	110.89	121.60
1	j	23	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	7	41	SER	N-CA-CB	-5.35	102.47	110.50
1	W	27	VAL	CA-CB-CG2	-5.35	102.87	110.90
1	W	108	THR	CA-CB-CG2	-5.35	104.91	112.40
1	d	27	VAL	CG1-CB-CG2	-5.35	102.33	110.90
1	D	60	GLY	C-N-CA	5.35	133.54	122.30
1	N	24	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	7	143	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	K	144	MET	CA-CB-CG	5.35	122.40	113.30
1	X	169	TYR	CB-CG-CD2	5.35	124.21	121.00
1	B	199	LYS	O-C-N	-5.35	114.14	122.70
1	M	157	PRO	N-CA-CB	5.35	109.72	103.30
1	7	79	GLU	CG-CD-OE1	5.35	129.00	118.30
1	I	165	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	N	55	MET	CG-SD-CE	5.35	108.75	100.20
1	U	53	ASN	O-C-N	-5.34	114.15	122.70
1	U	72	THR	CA-CB-CG2	-5.34	104.92	112.40
1	P	169	TYR	CE1-CZ-CE2	-5.34	111.25	119.80
1	R	168	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	k	16	SER	N-CA-CB	5.34	118.51	110.50
1	g	105	ALA	O-C-N	-5.34	114.12	123.20
1	g	105	ALA	CB-CA-C	-5.34	102.09	110.10
1	D	58	THR	OG1-CB-CG2	-5.34	97.72	110.00
1	c	143	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	d	53	ASN	O-C-N	-5.34	114.16	122.70
1	Y	96	MET	CG-SD-CE	-5.34	91.66	100.20
1	c	56	LEU	N-CA-CB	5.34	121.07	110.40
1	7	19	THR	CA-CB-CG2	-5.34	104.93	112.40
1	h	145	TYR	CB-CG-CD1	5.34	124.20	121.00
1	h	164	TYR	CZ-CE2-CD2	-5.33	115.00	119.80
1	Z	113	GLU	OE1-CD-OE2	-5.33	116.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	176	GLN	N-CA-CB	5.33	120.20	110.60
1	S	167	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	c	117	TRP	CE2-CD2-CE3	5.33	125.10	118.70
1	6	189	LEU	CB-CG-CD2	5.33	120.06	111.00
1	7	161	PHE	N-CA-CB	-5.33	101.01	110.60
1	A	186	THR	N-CA-CB	5.33	120.42	110.30
1	H	164	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	J	126	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	R	229	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	C	181	VAL	O-C-N	-5.33	114.18	122.70
1	D	32	PHE	CZ-CE2-CD2	-5.32	113.71	120.10
1	F	110	THR	CA-C-O	5.32	131.28	120.10
1	5	80	TRP	CE3-CZ3-CH2	5.32	127.06	121.20
1	c	117	TRP	CH2-CZ2-CE2	5.32	122.72	117.40
1	j	224	PRO	N-CA-CB	5.32	109.69	103.30
1	d	71	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	Y	173	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	F	25	LYS	CD-CE-NZ	5.32	123.94	111.70
1	J	117	TRP	CD2-CE2-CZ2	-5.32	115.92	122.30
1	K	80	TRP	CD2-CE3-CZ3	-5.32	111.88	118.80
1	S	52	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	e	118	MET	CG-SD-CE	-5.32	91.69	100.20
1	m	172	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	e	229	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	g	141	ILE	C-N-CA	5.32	135.00	121.70
1	B	54	THR	N-CA-CB	5.31	120.39	110.30
1	b	143	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	O	154	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	T	40	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	a	124	ILE	O-C-N	-5.31	111.01	121.10
1	L	119	THR	CA-CB-OG1	5.31	120.14	109.00
1	X	79	GLU	CA-CB-CG	5.31	125.08	113.40
1	6	212	GLU	O-C-N	-5.31	114.21	122.70
1	k	87	HIS	O-C-N	-5.31	114.21	122.70
1	W	230	VAL	CG1-CB-CG2	-5.30	102.41	110.90
1	5	133	TRP	CB-CG-CD2	-5.30	119.70	126.60
1	i	23	TRP	CD1-NE1-CE2	5.30	113.77	109.00
1	e	61	GLY	O-C-N	-5.30	114.21	122.70
1	E	169	TYR	CZ-CE2-CD2	5.30	124.57	119.80
1	X	142	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	g	26	VAL	CA-CB-CG1	5.30	118.85	110.90
1	M	4	GLN	C-N-CA	5.29	134.94	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	97	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	l	145	TYR	CB-CG-CD1	5.29	124.18	121.00
1	K	176	GLN	N-CA-CB	-5.29	101.07	110.60
1	P	78	ALA	O-C-N	-5.29	114.23	122.70
1	Q	118	MET	CG-SD-CE	-5.29	91.73	100.20
1	R	58	THR	O-C-N	-5.29	114.23	122.70
1	m	167	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	K	214	MET	O-C-N	-5.29	114.24	122.70
1	l	62	HIS	CB-CG-ND1	-5.29	109.98	123.20
1	7	23	TRP	CD1-NE1-CE2	-5.29	104.24	109.00
1	F	186	THR	CA-CB-CG2	-5.29	105.00	112.40
1	e	90	PRO	CA-N-CD	-5.28	104.10	111.50
1	N	145	TYR	CG-CD1-CE1	-5.28	117.07	121.30
1	A	215	MET	CG-SD-CE	-5.28	91.75	100.20
1	H	110	THR	CA-CB-CG2	-5.28	105.01	112.40
1	M	51	ASP	CB-CG-OD1	5.28	123.05	118.30
1	M	164	TYR	CG-CD2-CE2	-5.28	117.08	121.30
1	P	48	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	132	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	d	178	SER	N-CA-CB	5.28	118.42	110.50
1	D	13	GLN	CG-CD-OE1	5.27	132.14	121.60
1	P	173	ARG	CA-CB-CG	5.27	125.00	113.40
1	d	82	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	6	10	MET	N-CA-CB	-5.27	101.11	110.60
1	Y	164	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	m	151	LEU	CB-CG-CD2	5.27	119.96	111.00
1	D	200	THR	CA-CB-CG2	-5.27	105.02	112.40
1	E	47	ALA	CA-C-N	-5.27	105.61	117.20
1	G	184	TRP	CB-CA-C	5.26	120.93	110.40
1	L	173	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	N	58	THR	CA-CB-CG2	5.26	119.77	112.40
1	N	175	GLU	CG-CD-OE1	5.26	128.83	118.30
1	e	39	MET	CG-SD-CE	-5.26	91.78	100.20
1	6	70	LYS	N-CA-CB	-5.26	101.13	110.60
1	h	156	GLY	O-C-N	-5.26	111.11	121.10
1	R	200	THR	N-CA-CB	5.26	120.29	110.30
1	d	229	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	N	18	ARG	CB-CA-C	5.25	120.91	110.40
1	P	85	PRO	N-CA-CB	5.25	109.61	103.30
1	U	3	VAL	CG1-CB-CG2	-5.25	102.49	110.90
1	7	184	TRP	CZ3-CH2-CZ2	-5.25	115.30	121.60
1	h	181	VAL	CA-CB-CG1	-5.25	103.02	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	164	TYR	CG-CD1-CE1	-5.25	117.10	121.30
1	h	164	TYR	CD1-CG-CD2	-5.25	112.12	117.90
1	a	22	ALA	N-CA-CB	-5.25	102.75	110.10
1	G	72	THR	CA-CB-CG2	5.25	119.75	112.40
1	Z	105	ALA	N-CA-CB	-5.25	102.75	110.10
1	j	172	LEU	CB-CG-CD2	5.25	119.92	111.00
1	S	44	SER	O-C-N	-5.25	114.31	122.70
1	5	167	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
1	b	145	TYR	CZ-CE2-CD2	-5.25	115.08	119.80
1	B	113	GLU	CB-CA-C	5.24	120.89	110.40
1	F	145	TYR	CD1-CE1-CZ	5.24	124.52	119.80
1	N	159	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	m	208	ALA	CB-CA-C	5.24	117.96	110.10
1	A	30	LYS	CA-CB-CG	5.24	124.93	113.40
1	L	217	ALA	N-CA-CB	5.24	117.44	110.10
1	T	32	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	l	166	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	b	164	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	5	19	THR	N-CA-CB	5.24	120.25	110.30
1	K	110	THR	N-CA-CB	5.24	120.25	110.30
1	Q	20	LEU	CB-CG-CD2	5.24	119.90	111.00
1	i	142	VAL	CA-CB-CG2	-5.24	103.05	110.90
1	f	217	ALA	N-CA-CB	5.24	117.43	110.10
1	g	52	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	C	96	MET	C-N-CA	5.23	134.78	121.70
1	V	100	ARG	CG-CD-NE	-5.23	100.81	111.80
1	7	3	VAL	CB-CA-C	-5.23	101.46	111.40
1	H	210	THR	CA-CB-CG2	-5.23	105.08	112.40
1	Q	229	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	Z	32	PHE	CZ-CE2-CD2	-5.23	113.82	120.10
1	A	135	ILE	O-C-N	-5.23	114.33	122.70
1	G	215	MET	CG-SD-CE	-5.23	91.84	100.20
1	S	68	MET	CG-SD-CE	-5.23	91.84	100.20
1	S	158	LYS	O-C-N	5.23	131.06	122.70
1	e	229	ARG	CB-CA-C	5.23	120.85	110.40
1	S	183	ASN	CA-CB-CG	5.23	124.90	113.40
1	T	143	ARG	C-N-CA	5.23	134.77	121.70
1	W	214	MET	CG-SD-CE	-5.23	91.84	100.20
1	j	17	PRO	N-CA-CB	5.23	109.57	103.30
1	J	133	TRP	CB-CG-CD1	5.22	133.79	127.00
1	6	29	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	f	229	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	l	175	GLU	N-CA-CB	-5.22	101.20	110.60
1	h	140	LYS	N-CA-CB	-5.22	101.20	110.60
1	C	17	PRO	N-CA-CB	5.22	109.56	103.30
1	D	154	ARG	CG-CD-NE	-5.22	100.84	111.80
1	W	23	TRP	CE3-CZ3-CH2	-5.22	115.46	121.20
1	S	155	GLN	O-C-N	-5.21	114.34	123.20
1	c	105	ALA	CB-CA-C	-5.21	102.28	110.10
1	e	11	VAL	O-C-N	-5.21	114.36	122.70
1	g	64	ALA	N-CA-CB	-5.21	102.80	110.10
1	N	143	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	i	31	ALA	N-CA-C	5.21	125.08	111.00
1	D	83	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	M	187	GLU	O-C-N	-5.21	114.36	122.70
1	6	214	MET	C-N-CA	5.21	134.73	121.70
1	h	84	HIS	N-CA-CB	5.21	119.98	110.60
1	X	124	ILE	CA-C-N	5.21	131.69	117.10
1	b	35	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	M	208	ALA	N-CA-CB	-5.21	102.81	110.10
1	P	188	THR	OG1-CB-CG2	-5.21	98.02	110.00
1	h	108	THR	CA-CB-CG2	-5.21	105.11	112.40
1	G	76	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	A	209	ALA	N-CA-CB	5.21	117.39	110.10
1	Q	130	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
1	a	162	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	l	148	THR	C-N-CA	5.21	134.71	121.70
1	A	67	GLN	O-C-N	-5.20	114.38	122.70
1	N	92	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	j	78	ALA	O-C-N	-5.20	114.38	122.70
1	I	215	MET	CA-CB-CG	5.20	122.14	113.30
1	Z	2	ILE	O-C-N	-5.20	114.38	122.70
1	b	152	ASP	CB-CG-OD1	5.20	122.98	118.30
1	I	161	PHE	O-C-N	-5.20	114.38	122.70
1	T	141	ILE	O-C-N	-5.20	114.38	122.70
1	k	65	ALA	N-CA-CB	-5.20	102.82	110.10
1	A	51	ASP	OD1-CG-OD2	5.20	133.18	123.30
1	T	111	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	U	184	TRP	CE2-CD2-CE3	5.20	124.94	118.70
1	V	95	GLN	O-C-N	-5.20	114.38	122.70
1	W	229	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	Y	66	MET	CG-SD-CE	-5.20	91.88	100.20
1	Y	80	TRP	NE1-CE2-CZ2	5.20	136.12	130.40
1	K	97	ARG	CD-NE-CZ	5.20	130.88	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	7	148	THR	OG1-CB-CG2	-5.20	98.05	110.00
1	6	97	ARG	CD-NE-CZ	5.20	130.87	123.60
1	g	189	LEU	CB-CG-CD1	-5.20	102.17	111.00
1	J	12	HIS	CA-CB-CG	5.19	122.43	113.60
1	l	147	PRO	O-C-N	-5.19	114.39	122.70
1	U	171	THR	CA-CB-CG2	-5.19	105.13	112.40
1	d	184	TRP	O-C-N	-5.19	114.40	122.70
1	C	187	GLU	O-C-N	-5.19	114.40	122.70
1	F	162	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	G	152	ASP	CB-CG-OD2	5.19	122.97	118.30
1	Q	138	LEU	CB-CG-CD1	5.19	119.82	111.00
1	B	107	THR	CA-CB-CG2	-5.19	105.14	112.40
1	V	111	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	5	169	TYR	CB-CG-CD2	5.19	124.11	121.00
1	5	223	GLY	CA-C-O	5.19	129.94	120.60
1	d	118	MET	CG-SD-CE	-5.19	91.90	100.20
1	Y	174	ALA	N-CA-CB	5.19	117.36	110.10
1	6	186	THR	CA-CB-CG2	-5.19	105.14	112.40
1	b	107	THR	CA-CB-CG2	-5.18	105.14	112.40
1	i	151	LEU	CA-CB-CG	5.18	127.22	115.30
1	I	40	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	J	180	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	Q	152	ASP	C-N-CA	5.18	134.65	121.70
1	Z	88	ALA	CB-CA-C	-5.18	102.33	110.10
1	f	98	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	g	86	VAL	CA-CB-CG2	-5.18	103.13	110.90
1	M	143	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	P	75	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	T	186	THR	O-C-N	-5.18	114.42	122.70
1	7	133	TRP	CE3-CZ3-CH2	5.18	126.89	121.20
1	H	154	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	P	54	THR	O-C-N	-5.17	114.42	122.70
1	e	154	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	V	188	THR	O-C-N	-5.17	114.42	122.70
1	j	106	GLY	O-C-N	5.17	130.98	122.70
1	C	117	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	R	37	ILE	CA-C-N	5.17	131.57	117.10
1	J	197	ASP	N-CA-C	5.17	124.96	111.00
1	R	114	GLN	O-C-N	-5.17	114.43	122.70
1	J	18	ARG	CA-CB-CG	-5.17	102.04	113.40
1	c	139	ASN	CA-CB-CG	-5.17	102.03	113.40
1	d	169	TYR	N-CA-CB	5.17	119.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	e	86	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	k	165	VAL	CA-CB-CG2	5.17	118.65	110.90
1	T	142	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	R	97	ARG	CB-CA-C	-5.16	100.08	110.40
1	S	210	THR	CA-CB-CG2	-5.16	105.18	112.40
1	k	95	GLN	N-CA-CB	5.16	119.89	110.60
1	G	23	TRP	CE3-CZ3-CH2	5.16	126.87	121.20
1	L	50	GLN	N-CA-CB	5.16	119.89	110.60
1	L	69	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	L	117	TRP	CB-CG-CD2	-5.16	119.89	126.60
1	O	133	TRP	O-C-N	-5.16	114.45	122.70
1	c	174	ALA	CB-CA-C	5.16	117.84	110.10
1	h	210	THR	N-CA-CB	5.16	120.09	110.30
1	T	43	LEU	CB-CA-C	-5.15	100.41	110.20
1	7	80	TRP	CG-CD2-CE3	-5.15	129.26	133.90
1	C	168	PHE	CB-CG-CD1	5.15	124.41	120.80
1	G	24	VAL	CA-CB-CG2	5.15	118.63	110.90
1	J	174	ALA	CB-CA-C	5.15	117.83	110.10
1	5	170	LYS	CB-CA-C	-5.15	100.09	110.40
1	a	133	TRP	N-CA-CB	5.15	119.87	110.60
1	N	136	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	W	66	MET	CG-SD-CE	-5.15	91.96	100.20
1	F	26	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	I	66	MET	CG-SD-CE	-5.15	91.96	100.20
1	F	145	TYR	C-N-CA	5.15	134.57	121.70
1	H	133	TRP	CB-CG-CD2	-5.15	119.91	126.60
1	Q	6	LEU	O-C-N	-5.15	114.46	122.70
1	M	165	VAL	CA-CB-CG2	5.15	118.62	110.90
1	m	92	GLU	CB-CA-C	-5.14	100.11	110.40
1	H	38	PRO	N-CA-C	5.14	125.47	112.10
1	d	228	ALA	N-CA-CB	-5.14	102.90	110.10
1	6	142	VAL	CA-CB-CG1	5.14	118.61	110.90
1	V	97	ARG	CD-NE-CZ	5.14	130.79	123.60
1	b	136	LEU	CA-C-N	5.14	126.48	116.20
1	G	169	TYR	CD1-CG-CD2	5.14	123.55	117.90
1	d	51	ASP	O-C-N	-5.14	114.48	122.70
1	Z	113	GLU	N-CA-CB	-5.13	101.36	110.60
1	c	30	LYS	O-C-N	-5.13	114.48	122.70
1	7	75	GLU	O-C-N	5.13	130.91	122.70
1	i	26	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	H	229	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	U	37	ILE	CA-C-N	5.13	131.47	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	11	VAL	CA-CB-CG1	5.13	118.60	110.90
1	B	117	TRP	CE2-CD2-CG	-5.13	103.20	107.30
1	D	65	ALA	N-CA-CB	-5.13	102.92	110.10
1	G	63	GLN	CG-CD-OE1	-5.13	111.34	121.60
1	J	143	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	b	180	GLU	O-C-N	-5.13	114.50	122.70
1	J	133	TRP	CB-CG-CD2	-5.12	119.94	126.60
1	5	42	ALA	N-CA-CB	-5.12	102.92	110.10
1	l	80	TRP	NE1-CE2-CD2	5.12	112.42	107.30
1	O	163	ASP	CB-CG-OD2	5.12	122.91	118.30
1	Z	52	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	5	59	VAL	CA-CB-CG2	5.12	118.58	110.90
1	Q	68	MET	CA-CB-CG	5.12	122.00	113.30
1	e	203	LYS	CB-CA-C	-5.12	100.16	110.40
1	R	220	GLY	O-C-N	-5.12	114.51	122.70
1	D	49	PRO	CB-CA-C	5.12	124.80	112.00
1	a	66	MET	CG-SD-CE	-5.12	92.01	100.20
1	7	23	TRP	CD2-CE2-CZ2	-5.12	116.16	122.30
1	I	108	THR	CA-CB-CG2	-5.12	105.24	112.40
1	W	144	MET	CG-SD-CE	-5.12	92.02	100.20
1	A	144	MET	CG-SD-CE	-5.11	92.02	100.20
1	7	132	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	66	MET	CG-SD-CE	-5.11	92.02	100.20
1	O	161	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	W	168	PHE	CG-CD2-CE2	5.11	126.42	120.80
1	l	125	PRO	O-C-N	-5.11	114.52	122.70
1	c	173	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	174	ALA	CB-CA-C	-5.11	102.44	110.10
1	U	51	ASP	CB-CG-OD1	5.11	122.89	118.30
1	W	96	MET	CG-SD-CE	-5.11	92.03	100.20
1	5	145	TYR	CG-CD1-CE1	-5.11	117.22	121.30
1	m	3	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	N	24	VAL	O-C-N	-5.10	114.53	122.70
1	P	173	ARG	N-CA-CB	-5.10	101.41	110.60
1	B	229	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	S	216	THR	CA-CB-CG2	-5.10	105.26	112.40
1	T	164	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	Y	40	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	m	135	ILE	O-C-N	-5.10	114.54	122.70
1	C	157	PRO	N-CA-CB	5.10	109.42	103.30
1	T	105	ALA	N-CA-CB	-5.10	102.96	110.10
1	V	210	THR	CA-CB-CG2	5.10	119.54	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	53	ASN	CB-CG-ND2	5.10	128.93	116.70
1	M	198	CYS	CA-CB-SG	-5.10	104.83	114.00
1	m	198	CYS	C-N-CA	5.10	134.44	121.70
1	i	46	GLY	O-C-N	-5.10	114.55	122.70
1	F	117	TRP	CD1-CG-CD2	-5.09	102.22	106.30
1	Y	28	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	i	100	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	E	99	PRO	N-CA-CB	-5.09	97.00	102.60
1	6	23	TRP	CD1-NE1-CE2	5.09	113.58	109.00
1	O	181	VAL	N-CA-C	5.09	124.74	111.00
1	B	169	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	g	139	ASN	N-CA-CB	-5.09	101.44	110.60
1	H	82	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	S	154	ARG	CB-CG-CD	5.09	124.82	111.60
1	X	130	TYR	CB-CG-CD2	5.09	124.05	121.00
1	a	169	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	a	166	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	c	54	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	G	100	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	P	161	PHE	CD1-CE1-CZ	-5.08	114.00	120.10
1	Y	121	ASN	CB-CA-C	-5.08	100.23	110.40
1	5	90	PRO	N-CD-CG	5.08	110.83	103.20
1	J	171	THR	O-C-N	-5.08	114.57	122.70
1	W	77	ALA	N-CA-CB	-5.08	102.99	110.10
1	F	47	ALA	CB-CA-C	5.08	117.72	110.10
1	M	130	TYR	O-C-N	-5.08	114.57	122.70
1	g	65	ALA	CB-CA-C	5.08	117.72	110.10
1	W	219	GLN	N-CA-CB	5.08	119.73	110.60
1	b	136	LEU	O-C-N	-5.08	114.57	123.20
1	e	126	VAL	CA-CB-CG1	-5.08	103.29	110.90
1	j	132	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	7	55	MET	CG-SD-CE	-5.07	92.08	100.20
1	L	159	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	P	63	GLN	O-C-N	-5.07	114.59	122.70
1	U	10	MET	CA-CB-CG	-5.07	104.68	113.30
1	D	64	ALA	N-CA-CB	-5.07	103.00	110.10
1	k	231	LEU	CB-CG-CD2	5.07	119.62	111.00
1	E	48	THR	N-CA-CB	5.07	119.93	110.30
1	b	76	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	e	133	TRP	O-C-N	-5.07	114.59	122.70
1	K	86	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	U	197	ASP	CB-CG-OD2	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	154	ARG	NH1-CZ-NH2	5.07	124.97	119.40
1	P	190	LEU	N-CA-CB	5.06	120.53	110.40
1	c	121	ASN	N-CA-CB	-5.06	101.48	110.60
1	L	139	ASN	C-N-CA	5.06	134.36	121.70
1	P	29	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	j	213	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	f	70	LYS	O-C-N	-5.06	114.60	122.70
1	d	153	ILE	CA-CB-CG1	5.06	120.62	111.00
1	O	144	MET	CG-SD-CE	-5.06	92.11	100.20
1	6	7	GLN	CG-CD-OE1	5.06	131.71	121.60
1	i	147	PRO	N-CA-CB	5.06	109.37	103.30
1	i	148	THR	CA-CB-CG2	5.06	119.48	112.40
1	i	229	ARG	NH1-CZ-NH2	-5.06	113.84	119.40
1	H	146	SER	N-CA-C	5.05	124.65	111.00
1	X	50	GLN	N-CA-CB	5.05	119.70	110.60
1	F	11	VAL	CA-C-O	5.05	130.71	120.10
1	U	229	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	V	144	MET	CA-CB-CG	5.05	121.89	113.30
1	b	198	CYS	CB-CA-C	-5.05	100.30	110.40
1	h	40	PHE	CG-CD2-CE2	-5.05	115.24	120.80
1	m	132	ARG	O-C-N	-5.05	114.62	122.70
1	F	145	TYR	CA-CB-CG	-5.05	103.81	113.40
1	X	37	ILE	O-C-N	-5.05	111.51	121.10
1	5	104	ILE	CB-CA-C	-5.05	101.50	111.60
1	c	117	TRP	CD2-CE2-CZ2	-5.05	116.24	122.30
1	l	197	ASP	CB-CG-OD2	5.05	122.84	118.30
1	M	169	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	b	120	HIS	CA-CB-CG	-5.05	105.02	113.60
1	e	115	ILE	O-C-N	-5.05	114.62	123.20
1	C	84	HIS	N-CA-CB	5.04	119.68	110.60
1	b	207	PRO	N-CD-CG	5.04	110.77	103.20
1	K	39	MET	CG-SD-CE	-5.04	92.13	100.20
1	b	185	MET	CG-SD-CE	-5.04	92.13	100.20
1	6	228	ALA	CB-CA-C	5.04	117.67	110.10
1	7	229	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	6	203	LYS	O-C-N	-5.04	114.63	122.70
1	m	169	TYR	CG-CD1-CE1	-5.04	117.27	121.30
1	N	168	PHE	CG-CD1-CE1	-5.04	115.26	120.80
1	V	34	PRO	C-N-CA	5.04	134.30	121.70
1	i	231	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	j	229	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	e	164	TYR	CZ-CE2-CD2	-5.04	115.27	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	155	GLN	CA-CB-CG	5.04	124.48	113.40
1	c	29	GLU	CB-CA-C	-5.04	100.33	110.40
1	l	213	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	e	190	LEU	CB-CG-CD2	5.04	119.56	111.00
1	f	188	THR	CA-CB-CG2	-5.04	105.35	112.40
1	C	97	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	143	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	F	133	TRP	NE1-CE2-CD2	5.03	112.33	107.30
1	k	23	TRP	CA-CB-CG	5.03	123.26	113.70
1	D	40	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	E	182	LYS	N-CA-CB	5.03	119.66	110.60
1	H	103	ASP	CB-CG-OD1	5.03	122.83	118.30
1	m	230	VAL	N-CA-C	5.03	124.58	111.00
1	7	26	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	D	65	ALA	CB-CA-C	5.03	117.64	110.10
1	H	49	PRO	N-CD-CG	5.03	110.74	103.20
1	J	97	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	G	40	PHE	CB-CG-CD1	5.02	124.32	120.80
1	m	164	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	108	THR	CA-CB-CG2	-5.02	105.37	112.40
1	F	144	MET	CA-CB-CG	5.02	121.84	113.30
1	L	195	ASN	CB-CG-OD1	5.02	131.65	121.60
1	M	83	LEU	O-C-N	-5.02	114.66	122.70
1	N	133	TRP	CG-CD1-NE1	5.02	115.12	110.10
1	5	167	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	U	107	THR	CA-CB-CG2	-5.02	105.37	112.40
1	6	124	ILE	CA-CB-CG2	-5.02	100.86	110.90
1	B	136	LEU	O-C-N	-5.02	114.67	123.20
1	J	131	LYS	N-CA-CB	-5.02	101.56	110.60
1	6	148	THR	N-CA-CB	5.02	119.84	110.30
1	I	103	ASP	CB-CG-OD2	5.02	122.82	118.30
1	J	23	TRP	CD1-NE1-CE2	-5.02	104.48	109.00
1	e	103	ASP	CB-CG-OD1	5.02	122.81	118.30
1	B	31	ALA	N-CA-CB	5.01	117.12	110.10
1	H	62	HIS	C-N-CA	5.01	134.24	121.70
1	K	32	PHE	CB-CG-CD1	5.01	124.31	120.80
1	P	125	PRO	N-CD-CG	5.01	110.72	103.20
1	S	82	ARG	O-C-N	-5.01	114.68	122.70
1	C	74	ASN	O-C-N	-5.01	114.69	122.70
1	V	187	GLU	O-C-N	-5.01	114.68	122.70
1	Y	210	THR	CA-CB-CG2	-5.01	105.39	112.40
1	Z	181	VAL	CG1-CB-CG2	-5.01	102.89	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	118	MET	CB-CA-C	-5.00	100.39	110.40
1	A	111	LEU	CB-CG-CD1	5.00	119.51	111.00
1	F	37	ILE	CA-CB-CG1	-5.00	101.49	111.00
1	H	229	ARG	N-CA-C	5.00	124.51	111.00
1	J	68	MET	CG-SD-CE	-5.00	92.19	100.20
1	M	82	ARG	NH1-CZ-NH2	-5.00	113.90	119.40
1	R	162	ARG	N-CA-CB	-5.00	101.59	110.60
1	k	154	ARG	O-C-N	-5.00	114.70	122.70
1	B	91	ILE	O-C-N	-5.00	114.70	122.70
1	d	199	LYS	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (251) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	132	ARG	Sidechain
1	5	143	ARG	Sidechain
1	5	62	HIS	Sidechain
1	5	97	ARG	Sidechain
1	6	132	ARG	Sidechain
1	6	143	ARG	Sidechain
1	6	169	TYR	Sidechain
1	6	18	ARG	Sidechain
1	6	229	ARG	Sidechain
1	7	121	ASN	Peptide
1	7	167	ARG	Sidechain
1	7	18	ARG	Sidechain
1	7	97	ARG	Sidechain
1	A	145	TYR	Sidechain
1	A	162	ARG	Sidechain
1	A	164	TYR	Sidechain
1	A	18	ARG	Sidechain
1	B	130	TYR	Sidechain
1	B	132	ARG	Sidechain
1	B	162	ARG	Sidechain
1	B	32	PHE	Sidechain
1	B	48	THR	Peptide
1	C	100	ARG	Sidechain
1	C	114	GLN	Mainchain
1	C	132	ARG	Sidechain
1	C	145	TYR	Sidechain
1	C	169	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	173	ARG	Sidechain
1	D	121	ASN	Peptide
1	D	124	ILE	Peptide
1	D	130	TYR	Sidechain
1	D	132	ARG	Sidechain
1	D	154	ARG	Sidechain
1	D	206	GLY	Peptide
1	D	229	ARG	Sidechain
1	D	62	HIS	Sidechain
1	E	100	ARG	Sidechain
1	E	124	ILE	Peptide
1	E	132	ARG	Sidechain
1	E	226	HIS	Sidechain
1	F	143	ARG	Sidechain
1	F	154	ARG	Sidechain
1	F	173	ARG	Sidechain
1	G	100	ARG	Sidechain
1	G	120	HIS	Sidechain
1	G	154	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	173	ARG	Sidechain
1	G	40	PHE	Sidechain
1	G	97	ARG	Sidechain
1	H	124	ILE	Peptide
1	H	132	ARG	Sidechain
1	H	164	TYR	Sidechain
1	H	173	ARG	Sidechain
1	H	40	PHE	Sidechain
1	I	100	ARG	Sidechain
1	I	145	TYR	Sidechain
1	I	97	ARG	Sidechain
1	J	100	ARG	Sidechain
1	J	120	HIS	Sidechain
1	J	130	TYR	Sidechain
1	J	132	ARG	Sidechain
1	J	145	TYR	Sidechain
1	J	162	ARG	Sidechain
1	J	164	TYR	Sidechain
1	J	169	TYR	Sidechain
1	J	173	ARG	Sidechain
1	J	18	ARG	Sidechain
1	K	121	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	K	130	TYR	Sidechain
1	K	145	TYR	Sidechain
1	K	164	TYR	Sidechain
1	K	169	TYR	Sidechain
1	K	173	ARG	Sidechain
1	K	18	ARG	Sidechain
1	K	223	GLY	Peptide
1	K	229	ARG	Sidechain
1	K	40	PHE	Sidechain
1	K	82	ARG	Sidechain
1	L	121	ASN	Peptide
1	L	143	ARG	Sidechain
1	L	145	TYR	Sidechain
1	L	162	ARG	Sidechain
1	L	164	TYR	Sidechain
1	L	229	ARG	Sidechain
1	M	123	PRO	Peptide
1	M	130	TYR	Sidechain
1	M	132	ARG	Sidechain
1	M	143	ARG	Sidechain
1	N	132	ARG	Sidechain
1	N	14	ALA	Peptide
1	N	161	PHE	Sidechain
1	N	164	TYR	Sidechain
1	N	173	ARG	Sidechain
1	N	82	ARG	Sidechain
1	O	169	TYR	Sidechain
1	O	226	HIS	Sidechain
1	O	82	ARG	Sidechain
1	O	84	HIS	Sidechain
1	P	124	ILE	Peptide
1	P	130	TYR	Sidechain
1	P	132	ARG	Sidechain
1	P	145	TYR	Sidechain
1	P	162	ARG	Sidechain
1	Q	164	TYR	Sidechain
1	Q	167	ARG	Sidechain
1	Q	82	ARG	Sidechain
1	R	143	ARG	Sidechain
1	R	167	ARG	Sidechain
1	R	211	LEU	Mainchain
1	S	100	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	S	121	ASN	Peptide
1	S	145	TYR	Sidechain
1	S	162	ARG	Sidechain
1	S	164	TYR	Sidechain
1	S	169	TYR	Sidechain
1	T	124	ILE	Peptide
1	T	164	TYR	Sidechain
1	T	229	ARG	Sidechain
1	U	130	TYR	Sidechain
1	U	132	ARG	Sidechain
1	U	145	TYR	Sidechain
1	U	18	ARG	Sidechain
1	U	206	GLY	Peptide
1	U	229	ARG	Sidechain
1	U	40	PHE	Sidechain
1	V	145	TYR	Sidechain
1	V	154	ARG	Sidechain
1	V	164	TYR	Sidechain
1	V	169	TYR	Sidechain
1	V	173	ARG	Sidechain
1	V	18	ARG	Sidechain
1	V	229	ARG	Sidechain
1	V	40	PHE	Sidechain
1	V	82	ARG	Sidechain
1	W	120	HIS	Sidechain
1	W	124	ILE	Peptide
1	W	173	ARG	Sidechain
1	W	229	ARG	Sidechain
1	W	50	GLN	Mainchain
1	X	164	TYR	Sidechain
1	X	168	PHE	Sidechain
1	X	40	PHE	Sidechain
1	Y	100	ARG	Sidechain
1	Y	124	ILE	Peptide
1	Y	130	TYR	Sidechain
1	Y	145	TYR	Sidechain
1	Y	161	PHE	Sidechain
1	Y	162	ARG	Sidechain
1	Y	167	ARG	Sidechain
1	Y	169	TYR	Sidechain
1	Y	32	PHE	Sidechain
1	Z	100	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Z	120	HIS	Sidechain
1	Z	130	TYR	Sidechain
1	Z	132	ARG	Sidechain
1	Z	162	ARG	Sidechain
1	Z	164	TYR	Sidechain
1	Z	173	ARG	Sidechain
1	Z	190	LEU	Peptide
1	Z	229	ARG	Sidechain
1	Z	75	GLU	Mainchain
1	a	121	ASN	Peptide
1	a	130	TYR	Sidechain
1	a	162	ARG	Sidechain
1	a	18	ARG	Sidechain
1	a	229	ARG	Sidechain
1	b	124	ILE	Peptide
1	b	130	TYR	Sidechain
1	b	143	ARG	Sidechain
1	b	167	ARG	Sidechain
1	b	173	ARG	Sidechain
1	b	18	ARG	Sidechain
1	b	5	ASN	Mainchain
1	b	82	ARG	Sidechain
1	b	87	HIS	Sidechain
1	c	100	ARG	Sidechain
1	c	132	ARG	Sidechain
1	c	143	ARG	Sidechain
1	c	145	TYR	Sidechain
1	c	162	ARG	Sidechain
1	c	164	TYR	Sidechain
1	c	169	TYR	Sidechain
1	c	229	ARG	Sidechain
1	c	82	ARG	Sidechain
1	c	92	GLU	Peptide
1	d	100	ARG	Sidechain
1	d	132	ARG	Sidechain
1	d	145	TYR	Sidechain
1	d	164	TYR	Sidechain
1	d	167	ARG	Sidechain
1	d	200	THR	Mainchain
1	e	145	TYR	Sidechain
1	e	154	ARG	Sidechain
1	e	162	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	e	167	ARG	Sidechain
1	e	169	TYR	Sidechain
1	e	18	ARG	Sidechain
1	f	143	ARG	Sidechain
1	f	145	TYR	Sidechain
1	f	154	ARG	Sidechain
1	f	167	ARG	Sidechain
1	f	229	ARG	Sidechain
1	f	84	HIS	Peptide
1	f	85	PRO	Peptide
1	f	97	ARG	Sidechain
1	g	130	TYR	Sidechain
1	g	154	ARG	Sidechain
1	g	167	ARG	Sidechain
1	g	97	ARG	Sidechain
1	h	121	ASN	Peptide
1	h	154	ARG	Sidechain
1	h	162	ARG	Sidechain
1	h	164	TYR	Sidechain
1	h	167	ARG	Sidechain
1	h	18	ARG	Sidechain
1	h	82	ARG	Sidechain
1	i	100	ARG	Sidechain
1	i	160	PRO	Peptide
1	i	162	ARG	Sidechain
1	i	167	ARG	Sidechain
1	i	226	HIS	Sidechain
1	i	229	ARG	Sidechain
1	j	120	HIS	Sidechain
1	j	130	TYR	Sidechain
1	j	143	ARG	Sidechain
1	j	147	PRO	Peptide
1	j	164	TYR	Sidechain
1	j	173	ARG	Sidechain
1	j	176	GLN	Mainchain,Peptide
1	j	82	ARG	Sidechain
1	k	143	ARG	Sidechain
1	k	161	PHE	Sidechain
1	k	169	TYR	Sidechain
1	k	173	ARG	Sidechain
1	k	229	ARG	Sidechain
1	k	5	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	k	82	ARG	Sidechain
1	l	120	HIS	Sidechain
1	l	130	TYR	Sidechain
1	l	143	ARG	Sidechain
1	l	164	TYR	Sidechain
1	l	173	ARG	Sidechain
1	l	97	ARG	Sidechain
1	m	124	ILE	Peptide
1	m	143	ARG	Sidechain
1	m	146	SER	Peptide
1	m	154	ARG	Sidechain
1	m	229	ARG	Sidechain
1	m	97	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1800	0	1802	0	0
1	6	1800	0	1802	0	0
1	7	1800	0	1802	0	0
1	A	1800	0	1802	0	0
1	B	1800	0	1802	0	0
1	C	1800	0	1802	0	0
1	D	1800	0	1802	0	0
1	E	1800	0	1802	0	0
1	F	1800	0	1802	0	0
1	G	1800	0	1802	0	0
1	H	1800	0	1802	0	0
1	I	1800	0	1802	0	0
1	J	1800	0	1802	0	0
1	K	1800	0	1802	0	0
1	L	1800	0	1802	0	0
1	M	1800	0	1802	0	0
1	N	1800	0	1802	0	0
1	O	1800	0	1802	0	0
1	P	1800	0	1802	0	0
1	Q	1800	0	1802	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1800	0	1802	0	0
1	S	1800	0	1802	0	0
1	T	1800	0	1802	0	0
1	U	1800	0	1802	0	0
1	V	1800	0	1802	0	0
1	W	1800	0	1802	0	0
1	X	1800	0	1802	0	0
1	Y	1800	0	1802	0	0
1	Z	1800	0	1802	0	0
1	a	1800	0	1802	0	0
1	b	1800	0	1802	0	0
1	c	1800	0	1802	0	0
1	d	1800	0	1802	0	0
1	e	1800	0	1802	0	0
1	f	1800	0	1802	0	0
1	g	1800	0	1802	0	0
1	h	1800	0	1802	0	0
1	i	1800	0	1802	0	0
1	j	1800	0	1802	0	0
1	k	1800	0	1802	0	0
1	l	1800	0	1802	0	0
1	m	1800	0	1802	0	0
All	All	75600	0	75684	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	5	229/231 (99%)	214 (93%)	12 (5%)	3 (1%)	15 60
1	6	229/231 (99%)	220 (96%)	8 (4%)	1 (0%)	39 80
1	7	229/231 (99%)	216 (94%)	8 (4%)	5 (2%)	8 49
1	A	229/231 (99%)	220 (96%)	7 (3%)	2 (1%)	21 67
1	B	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	5 42
1	C	229/231 (99%)	217 (95%)	10 (4%)	2 (1%)	21 67
1	D	229/231 (99%)	217 (95%)	9 (4%)	3 (1%)	15 60
1	E	229/231 (99%)	213 (93%)	10 (4%)	6 (3%)	7 45
1	F	229/231 (99%)	218 (95%)	10 (4%)	1 (0%)	39 80
1	G	229/231 (99%)	222 (97%)	6 (3%)	1 (0%)	39 80
1	H	229/231 (99%)	218 (95%)	9 (4%)	2 (1%)	21 67
1	I	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	15 60
1	J	229/231 (99%)	214 (93%)	14 (6%)	1 (0%)	39 80
1	K	229/231 (99%)	220 (96%)	7 (3%)	2 (1%)	21 67
1	L	229/231 (99%)	216 (94%)	11 (5%)	2 (1%)	21 67
1	M	229/231 (99%)	216 (94%)	10 (4%)	3 (1%)	15 60
1	N	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	11 55
1	O	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	11 55
1	P	229/231 (99%)	217 (95%)	10 (4%)	2 (1%)	21 67
1	Q	229/231 (99%)	218 (95%)	8 (4%)	3 (1%)	15 60
1	R	229/231 (99%)	224 (98%)	5 (2%)	0	100 100
1	S	229/231 (99%)	215 (94%)	12 (5%)	2 (1%)	21 67
1	T	229/231 (99%)	219 (96%)	9 (4%)	1 (0%)	39 80
1	U	229/231 (99%)	218 (95%)	6 (3%)	5 (2%)	8 49
1	V	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	15 60
1	W	229/231 (99%)	216 (94%)	11 (5%)	2 (1%)	21 67
1	X	229/231 (99%)	217 (95%)	12 (5%)	0	100 100
1	Y	229/231 (99%)	213 (93%)	12 (5%)	4 (2%)	11 55
1	Z	229/231 (99%)	216 (94%)	12 (5%)	1 (0%)	39 80
1	a	229/231 (99%)	217 (95%)	7 (3%)	5 (2%)	8 49
1	b	229/231 (99%)	216 (94%)	8 (4%)	5 (2%)	8 49
1	c	229/231 (99%)	218 (95%)	10 (4%)	1 (0%)	39 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	d	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	8 49
1	e	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	7 45
1	f	229/231 (99%)	218 (95%)	11 (5%)	0	100 100
1	g	229/231 (99%)	209 (91%)	18 (8%)	2 (1%)	21 67
1	h	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	7 45
1	i	229/231 (99%)	218 (95%)	9 (4%)	2 (1%)	21 67
1	j	229/231 (99%)	217 (95%)	9 (4%)	3 (1%)	15 60
1	k	229/231 (99%)	218 (95%)	7 (3%)	4 (2%)	11 55
1	l	229/231 (99%)	218 (95%)	9 (4%)	2 (1%)	21 67
1	m	229/231 (99%)	217 (95%)	8 (4%)	4 (2%)	11 55
All	All	9618/9702 (99%)	9072 (94%)	426 (4%)	120 (1%)	21 61

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	LEU
1	B	209	ALA
1	B	224	PRO
1	K	177	ALA
1	L	97	ARG
1	M	91	ILE
1	U	120	HIS
1	Y	120	HIS
1	d	88	ALA
1	d	218	CYS
1	D	218	CYS
1	K	149	SER
1	M	9	GLN
1	P	125	PRO
1	P	194	ALA
1	Q	194	ALA
1	T	125	PRO
1	U	178	SER
1	U	206	GLY
1	V	125	PRO
1	W	125	PRO
1	Y	125	PRO
1	k	177	ALA

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Mol	Chain	Res	Type
1	m	125	PRO
1	7	62	HIS
1	7	223	GLY
1	d	125	PRO
1	e	61	GLY
1	e	147	PRO
1	g	125	PRO
1	h	160	PRO
1	A	97	ARG
1	B	222	GLY
1	D	125	PRO
1	I	206	GLY
1	J	125	PRO
1	M	125	PRO
1	N	4	GLN
1	N	125	PRO
1	N	209	ALA
1	Q	125	PRO
1	U	125	PRO
1	Y	177	ALA
1	5	125	PRO
1	b	91	ILE
1	j	90	PRO
1	m	177	ALA
1	7	222	GLY
1	d	209	ALA
1	h	31	ALA
1	A	125	PRO
1	B	220	GLY
1	C	222	GLY
1	D	86	VAL
1	E	30	LYS
1	E	97	ARG
1	E	125	PRO
1	E	148	THR
1	F	125	PRO
1	H	6	LEU
1	H	125	PRO
1	I	125	PRO
1	O	218	CYS
1	S	96	MET
1	S	125	PRO

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Mol	Chain	Res	Type
1	Z	45	GLU
1	a	230	VAL
1	b	97	ARG
1	b	125	PRO
1	b	149	SER
1	i	125	PRO
1	j	125	PRO
1	k	217	ALA
1	d	31	ALA
1	e	178	SER
1	e	218	CYS
1	B	147	PRO
1	B	149	SER
1	L	179	GLN
1	O	157	PRO
1	O	222	GLY
1	Q	142	VAL
1	U	34	PRO
1	a	10	MET
1	6	125	PRO
1	i	218	CYS
1	j	218	CYS
1	k	15	ILE
1	k	125	PRO
1	l	96	MET
1	m	208	ALA
1	e	160	PRO
1	g	86	VAL
1	h	89	GLY
1	h	125	PRO
1	E	93	PRO
1	N	217	ALA
1	c	31	ALA
1	l	125	PRO
1	7	87	HIS
1	h	90	PRO
1	C	125	PRO
1	G	125	PRO
1	W	8	GLY
1	a	85	PRO
1	a	125	PRO
1	m	85	PRO

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Mol	Chain	Res	Type
1	7	125	PRO
1	e	125	PRO
1	a	15	ILE
1	b	147	PRO
1	h	116	GLY
1	E	157	PRO
1	V	34	PRO
1	Y	49	PRO
1	5	34	PRO
1	5	207	PRO
1	O	125	PRO
1	V	153	ILE
1	I	122	PRO

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	5	195/195 (100%)	190 (97%)	5 (3%)	54 80
1	6	195/195 (100%)	187 (96%)	8 (4%)	37 71
1	7	195/195 (100%)	187 (96%)	8 (4%)	37 71
1	A	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	B	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	C	195/195 (100%)	188 (96%)	7 (4%)	42 74
1	D	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	E	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	F	195/195 (100%)	190 (97%)	5 (3%)	54 80
1	G	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	H	195/195 (100%)	194 (100%)	1 (0%)	92 96
1	I	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	J	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	K	195/195 (100%)	190 (97%)	5 (3%)	54 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	M	195/195 (100%)	188 (96%)	7 (4%)	42 74
1	N	195/195 (100%)	188 (96%)	7 (4%)	42 74
1	O	195/195 (100%)	190 (97%)	5 (3%)	54 80
1	P	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	Q	195/195 (100%)	187 (96%)	8 (4%)	37 71
1	R	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	S	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	T	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	U	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	V	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	W	195/195 (100%)	193 (99%)	2 (1%)	82 92
1	X	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	Y	195/195 (100%)	189 (97%)	6 (3%)	47 77
1	Z	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	a	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	b	195/195 (100%)	188 (96%)	7 (4%)	42 74
1	c	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	d	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	e	195/195 (100%)	189 (97%)	6 (3%)	47 77
1	f	195/195 (100%)	189 (97%)	6 (3%)	47 77
1	g	195/195 (100%)	192 (98%)	3 (2%)	72 88
1	h	195/195 (100%)	190 (97%)	5 (3%)	54 80
1	i	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	j	195/195 (100%)	191 (98%)	4 (2%)	61 84
1	k	195/195 (100%)	190 (97%)	5 (3%)	54 80
1	l	195/195 (100%)	189 (97%)	6 (3%)	47 77
1	m	195/195 (100%)	191 (98%)	4 (2%)	61 84
All	All	8190/8190 (100%)	7999 (98%)	191 (2%)	61 83

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	107	THR
1	A	122	PRO
1	A	163	ASP
1	B	4	GLN
1	B	83	LEU
1	B	224	PRO
1	C	81	ASP
1	C	82	ARG
1	C	98	GLU
1	C	115	ILE
1	C	128	GLU
1	C	130	TYR
1	C	189	LEU
1	D	150	ILE
1	D	163	ASP
1	D	183	ASN
1	E	39	MET
1	E	90	PRO
1	E	93	PRO
1	E	161	PHE
1	F	25	LYS
1	F	74	ASN
1	F	85	PRO
1	F	138	LEU
1	F	196	PRO
1	G	7	GLN
1	G	21	ASN
1	G	58	THR
1	H	188	THR
1	I	5	ASN
1	I	119	THR
1	I	157	PRO
1	I	162	ARG
1	J	81	ASP
1	J	163	ASP
1	J	172	LEU
1	J	213	GLU
1	K	1	PRO
1	K	10	MET
1	K	69	LEU
1	K	122	PRO
1	K	153	ILE

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Mol	Chain	Res	Type
1	L	130	TYR
1	L	186	THR
1	L	207	PRO
1	M	27	VAL
1	M	112	GLN
1	M	123	PRO
1	M	124	ILE
1	M	146	SER
1	M	195	ASN
1	M	211	LEU
1	N	7	GLN
1	N	50	GLN
1	N	69	LEU
1	N	81	ASP
1	N	146	SER
1	N	147	PRO
1	N	210	THR
1	O	26	VAL
1	O	155	GLN
1	O	163	ASP
1	O	196	PRO
1	O	205	LEU
1	P	11	VAL
1	P	112	GLN
1	P	166	ASP
1	Q	4	GLN
1	Q	17	PRO
1	Q	34	PRO
1	Q	82	ARG
1	Q	91	ILE
1	Q	108	THR
1	Q	115	ILE
1	Q	123	PRO
1	R	17	PRO
1	R	91	ILE
1	R	110	THR
1	R	200	THR
1	S	81	ASP
1	S	164	TYR
1	S	212	GLU
1	T	163	ASP
1	T	169	TYR

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Mol	Chain	Res	Type
1	T	224	PRO
1	T	227	LYS
1	U	49	PRO
1	U	81	ASP
1	U	168	PHE
1	U	186	THR
1	V	24	VAL
1	V	93	PRO
1	V	186	THR
1	W	81	ASP
1	W	91	ILE
1	X	25	LYS
1	X	58	THR
1	X	181	VAL
1	X	196	PRO
1	Y	4	GLN
1	Y	21	ASN
1	Y	24	VAL
1	Y	139	ASN
1	Y	166	ASP
1	Y	188	THR
1	Z	1	PRO
1	Z	38	PRO
1	Z	195	ASN
1	5	1	PRO
1	5	49	PRO
1	5	162	ARG
1	5	195	ASN
1	5	212	GLU
1	a	13	GLN
1	a	49	PRO
1	a	130	TYR
1	a	160	PRO
1	b	1	PRO
1	b	17	PRO
1	b	34	PRO
1	b	50	GLN
1	b	69	LEU
1	b	90	PRO
1	b	130	TYR
1	c	26	VAL
1	c	153	ILE

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Mol	Chain	Res	Type
1	c	210	THR
1	6	3	VAL
1	6	69	LEU
1	6	98	GLU
1	6	111	LEU
1	6	130	TYR
1	6	160	PRO
1	6	195	ASN
1	6	229	ARG
1	i	1	PRO
1	i	34	PRO
1	i	160	PRO
1	i	197	ASP
1	j	39	MET
1	j	119	THR
1	j	185	MET
1	j	190	LEU
1	k	7	GLN
1	k	85	PRO
1	k	157	PRO
1	k	179	GLN
1	k	198	CYS
1	l	34	PRO
1	l	49	PRO
1	l	56	LEU
1	l	86	VAL
1	l	196	PRO
1	l	197	ASP
1	m	130	TYR
1	m	207	PRO
1	m	215	MET
1	m	224	PRO
1	7	19	THR
1	7	40	PHE
1	7	69	LEU
1	7	107	THR
1	7	149	SER
1	7	161	PHE
1	7	196	PRO
1	7	230	VAL
1	d	3	VAL
1	d	40	PHE

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Mol	Chain	Res	Type
1	d	41	SER
1	d	115	ILE
1	e	85	PRO
1	e	90	PRO
1	e	130	TYR
1	e	146	SER
1	e	224	PRO
1	e	230	VAL
1	f	2	ILE
1	f	122	PRO
1	f	143	ARG
1	f	144	MET
1	f	200	THR
1	f	207	PRO
1	g	90	PRO
1	g	148	THR
1	g	230	VAL
1	h	2	ILE
1	h	10	MET
1	h	69	LEU
1	h	81	ASP
1	h	165	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.