



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 04:50 AM UTC

PDB ID : 6X63 / pdb_00006x63
BMRB ID : 30741
Title : Atomic-Resolution Structure of HIV-1 Capsid Tubes by Magic Angle Spinning NMR
Authors : Lu, M.; Russell, R.W.; Bryer, A.; Quinn, C.M.; Hou, G.; Zhang, H.; Schwitters, C.D.; Perilla, J.R.; Gronenborn, A.M.; Polenova, T.
Deposited on : 2020-05-27

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

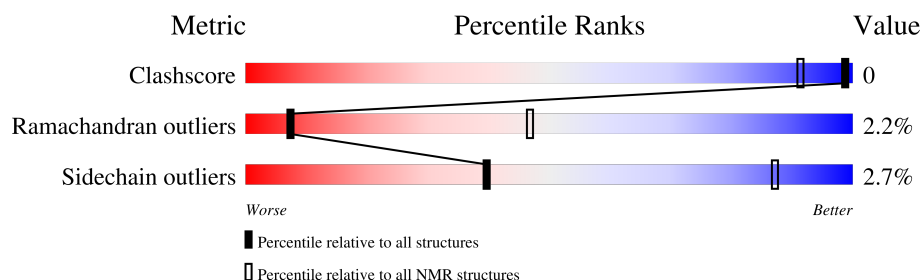
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 0%.

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.



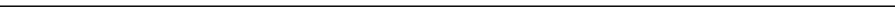
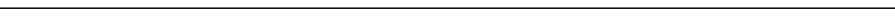
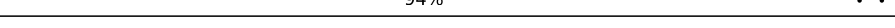
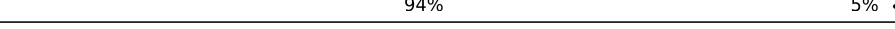
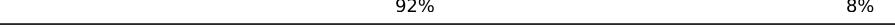
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	231	94% 6%
1	0A	231	91% 7% .
1	0B	231	90% 8% .
1	0C	231	92% 8%
1	0D	231	92% 6% .
1	0E	231	91% 7% .
1	1	231	89% 11%
1	1A	231	90% 10%

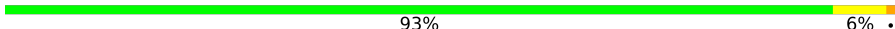
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Mol	Chain	Length	Quality of chain
1	1B	231	 90% 9% .
1	1C	231	 90% 9% .
1	1D	231	 91% 8% .
1	1E	231	 90% 9% .
1	2	231	 89% 11%
1	2A	231	 93% 6% .
1	2B	231	 90% 8% .
1	2C	231	 91% 8% .
1	2D	231	 91% 6% .
1	2E	231	 92% 8%
1	3	231	 88% 11%
1	3A	231	 90% 9% .
1	3B	231	 93% 7%
1	3C	231	 91% 9%
1	3D	231	 90% 10%
1	3E	231	 94% . .
1	4	231	 91% 9%
1	4A	231	 94% 5% .
1	4B	231	 92% 8%
1	4C	231	 90% 7% .
1	4D	231	 91% 7% .
1	4E	231	 93% 6% .
1	5	231	 92% 6% .
1	5A	231	 91% 7% .
1	5B	231	 91% 8% .

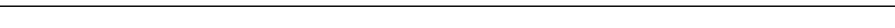
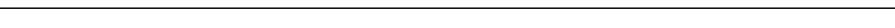
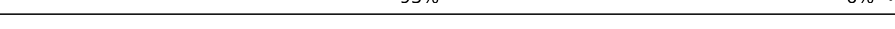
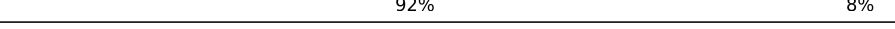
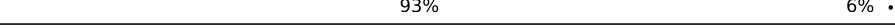
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Mol	Chain	Length	Quality of chain
1	5C	231	 90% 8% .
1	5D	231	 93% 6% .
1	5E	231	 90% 9% .
1	6	231	 91% 8% .
1	6A	231	 91% 8% .
1	6B	231	 92% 7% .
1	6C	231	 93% 6% .
1	6D	231	 91% 7% .
1	6E	231	 93% 6% .
1	7	231	 90% 8% .
1	7A	231	 92% 8% .
1	7B	231	 92% 8% .
1	7C	231	 89% 10% .
1	7D	231	 90% 8% .
1	7E	231	 90% 9% .
1	8	231	 89% 10% .
1	8A	231	 92% 6% .
1	8B	231	 90% 9% .
1	8C	231	 92% 7% .
1	8D	231	 92% 7% .
1	8E	231	 90% 10% .
1	9	231	 89% 10% .
1	9A	231	 91% 7% .
1	9B	231	 92% 6% .
1	9C	231	 93% 6% .

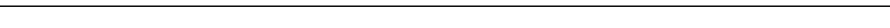
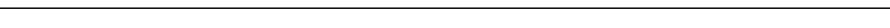
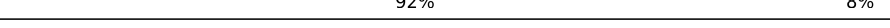
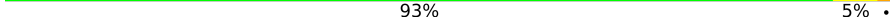
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Mol	Chain	Length	Quality of chain
1	9D	231	 92% 7% .
1	9E	231	 91% 8% .
1	A	231	 90% 8% .
1	AA	231	 94% 5% .
1	AB	231	 90% 9% .
1	AC	231	 93% 6% .
1	AD	231	 91% 8% .
1	AE	231	 89% 11% .
1	AF	231	 91% 8% .
1	B	231	 94% 6% .
1	BA	231	 91% 8% .
1	BB	231	 93% 6% .
1	BC	231	 91% 8% .
1	BD	231	 92% 6% .
1	BE	231	 93% 6% .
1	BF	231	 91% 9% .
1	C	231	 90% 8% ..
1	CA	231	 92% 8% .
1	CB	231	 93% 6% .
1	CC	231	 90% 7% .
1	CD	231	 92% 6% .
1	CE	231	 91% 8% .
1	CF	231	 90% 8% .
1	D	231	 90% 10% .
1	DA	231	 91% 7% .

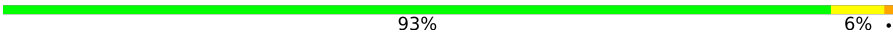
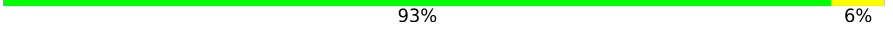
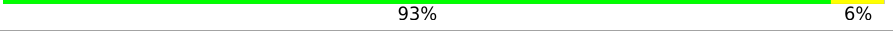
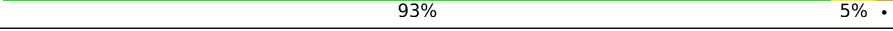
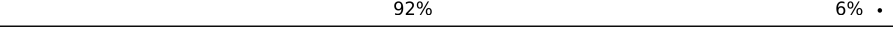
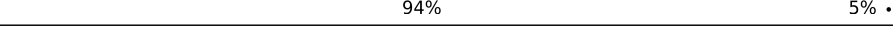
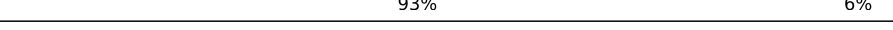
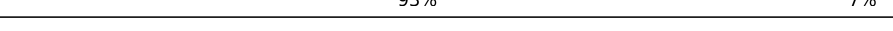
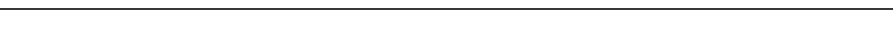
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Mol	Chain	Length	Quality of chain
1	DB	231	 91% 7% .
1	DC	231	 91% 8% .
1	DD	231	 90% 8% ..
1	DE	231	 92% 8%
1	DF	231	 88% 10% .
1	E	231	 91% 8% .
1	EA	231	 92% 6% .
1	EB	231	 92% 7% .
1	EC	231	 90% 8% .
1	ED	231	 90% 8% .
1	EE	231	 91% 7% .
1	EF	231	 93% 6%
1	F	231	 91% 9%
1	FA	231	 91% 8% .
1	FB	231	 90% 8% .
1	FC	231	 90% 8% .
1	FD	231	 92% 8%
1	FE	231	 91% 8% .
1	FF	231	 90% 8% .
1	G	231	 92% 6% .
1	GA	231	 93% 5% .
1	GB	231	 91% 8%
1	GC	231	 91% 8%
1	GD	231	 89% 8% .
1	GE	231	 92% 8%

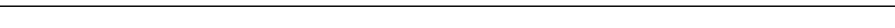
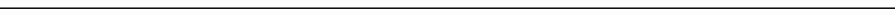
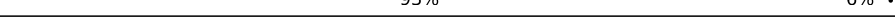
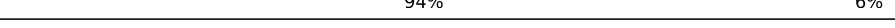
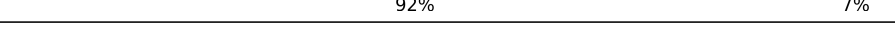
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Mol	Chain	Length	Quality of chain
1	H	231	 91% 8% .
1	HA	231	 93% 6% .
1	HB	231	 91% 7% .
1	HC	231	 92% 8%
1	HD	231	 87% 11% .
1	HE	231	 92% 6% .
1	I	231	 93% 6%
1	IA	231	 93% 6%
1	IB	231	 92% 6% .
1	IC	231	 93% 5% .
1	ID	231	 92% 6% .
1	IE	231	 94% 5% .
1	J	231	 90% 9% .
1	JA	231	 93% 6%
1	JB	231	 90% 9% .
1	JC	231	 89% 10%
1	JD	231	 93% 7%
1	JE	231	 91% 7% .
1	K	231	 90% 9%
1	KA	231	 90% 8% .
1	KB	231	 93% 6% .
1	KC	231	 91% 8% .
1	KD	231	 93% 7%
1	KE	231	 91% 8% .
1	L	231	 91% 8%

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Mol	Chain	Length	Quality of chain
1	LA	231	 92% 7% .
1	LB	231	 89% 9% .
1	LC	231	 90% 10% .
1	LD	231	 91% 8% .
1	LE	231	 91% 7% .
1	M	231	 92% 8%
1	MA	231	 90% 9% .
1	MB	231	 91% 8% .
1	MC	231	 92% 6% .
1	MD	231	 90% 8% .
1	ME	231	 91% 9%
1	N	231	 91% 8% .
1	NA	231	 91% 9%
1	NB	231	 90% 10%
1	NC	231	 90% 10%
1	ND	231	 93% 6% .
1	NE	231	 94% 6%
1	O	231	 92% 7%
1	OA	231	 90% 8% .
1	OB	231	 90% 10%
1	OC	231	 91% 7% .
1	OD	231	 92% 7%
1	OE	231	 94% . .
1	P	231	 91% 9%
1	PA	231	 91% 8%

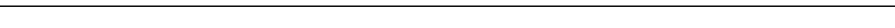
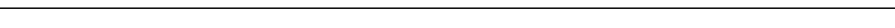
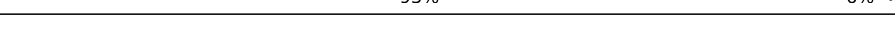
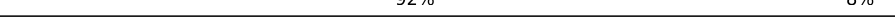
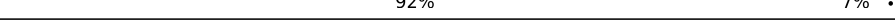
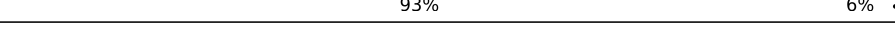
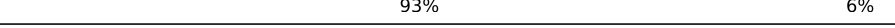
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Mol	Chain	Length	Quality of chain
1	PB	231	 91% 7% .
1	PC	231	 90% 8% .
1	PD	231	 91% 8% .
1	PE	231	 92% 7% .
1	Q	231	 91% 8% .
1	QA	231	 92% 7% .
1	QB	231	 90% 8% .
1	QC	231	 91% 8% .
1	QD	231	 90% 8% .
1	QE	231	 90% 9% .
1	R	231	 88% 12% .
1	RA	231	 91% 8% .
1	RB	231	 91% 8% .
1	RC	231	 91% 8% .
1	RD	231	 91% 9% .
1	RE	231	 91% 7% .
1	S	231	 91% 7% .
1	SA	231	 91% 7% .
1	SB	231	 91% 9% .
1	SC	231	 92% 7% .
1	SD	231	 90% 7% .
1	SE	231	 91% 8% .
1	T	231	 94% 5% .
1	TA	231	 93% 6% .
1	TB	231	 91% 7% .

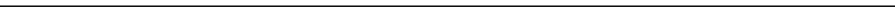
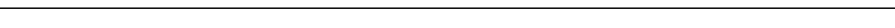
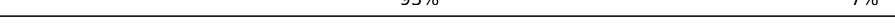
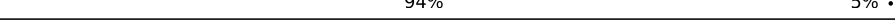
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Mol	Chain	Length	Quality of chain
1	TC	231	 91% 9%
1	TD	231	 92% 7% .
1	TE	231	 92% 8%
1	U	231	 92% 7%
1	UA	231	 92% 8%
1	UB	231	 92% 7% .
1	UC	231	 91% 6% .
1	UD	231	 90% 9% .
1	UE	231	 93% 6% .
1	V	231	 88% 11% .
1	VA	231	 88% 11% .
1	VB	231	 94% 5% .
1	VC	231	 89% 9% .
1	VD	231	 91% 7% .
1	VE	231	 93% 6% .
1	W	231	 92% 8%
1	WA	231	 92% 7% .
1	WB	231	 93% 6% .
1	WC	231	 93% 6%
1	WD	231	 92% 7% .
1	WE	231	 90% 8% .
1	X	231	 90% 10%
1	XA	231	 91% 8% .
1	XB	231	 92% 7% .
1	XC	231	 91% 8% .

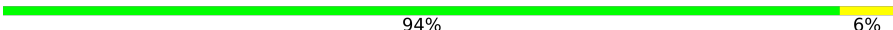
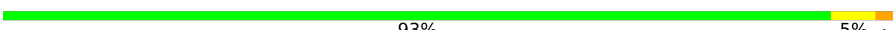
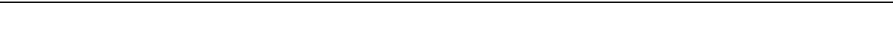
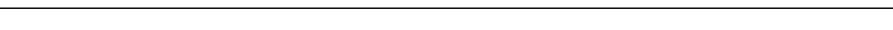
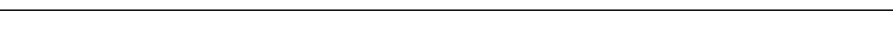
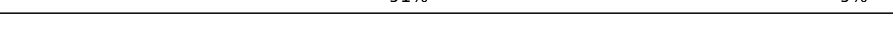
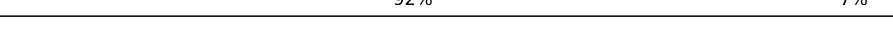
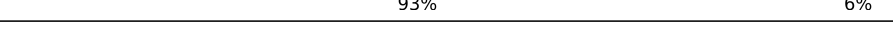
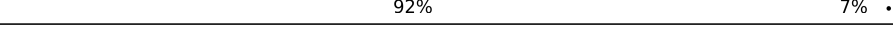
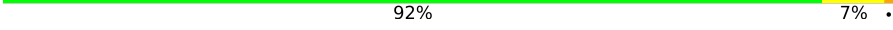
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Mol	Chain	Length	Quality of chain
1	XD	231	 92% 7% .
1	XE	231	 90% 10%
1	Y	231	 91% 9%
1	YA	231	 93% 5% ..
1	YB	231	 90% 10%
1	YC	231	 89% 11%
1	YD	231	 91% 6% .
1	YE	231	 91% 7% .
1	Z	231	 93% 6% .
1	ZA	231	 91% 7% .
1	ZB	231	 92% 6% .
1	ZC	231	 93% 5% .
1	ZD	231	 90% 9%
1	ZE	231	 90% 10%
1	a	231	 91% 7% .
1	aA	231	 93% 7%
1	aB	231	 94% 5% .
1	aC	231	 91% 6% .
1	aD	231	 88% 11%
1	aE	231	 92% 7% .
1	b	231	 87% 11% .
1	bA	231	 91% 8%
1	bB	231	 91% 8% .
1	bC	231	 90% 10% .
1	bD	231	 93% 5% .

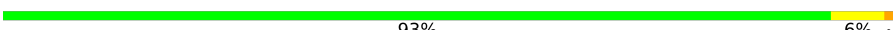
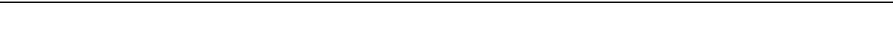
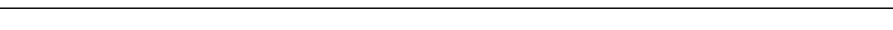
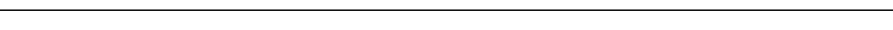
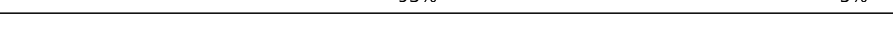
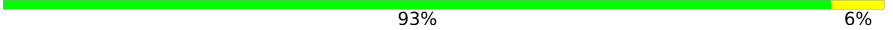
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Mol	Chain	Length	Quality of chain
1	bE	231	 94% 6%
1	c	231	 91% 9%
1	cA	231	 93% 5% .
1	cB	231	 91% 7% .
1	cC	231	 92% 7% .
1	cD	231	 92% 7% .
1	cE	231	 92% 6% .
1	d	231	 92% 8%
1	dA	231	 91% 9%
1	dB	231	 92% 7% .
1	dC	231	 93% 6% .
1	dD	231	 90% 9% .
1	dE	231	 92% 7% .
1	e	231	 91% 9%
1	eA	231	 92% 7%
1	eB	231	 91% 8% .
1	eC	231	 93% 6%
1	eD	231	 92% 7% .
1	eE	231	 91% 8% .
1	f	231	 89% 11%
1	fA	231	 92% 7% .
1	fB	231	 91% 7% .
1	fC	231	 91% 8% .
1	fD	231	 90% 9% .
1	fE	231	 92% 6% .

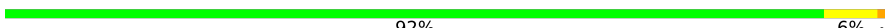
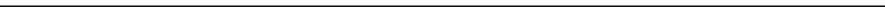
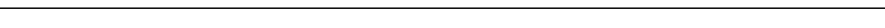
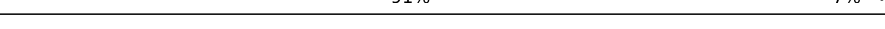
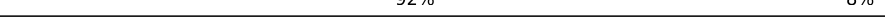
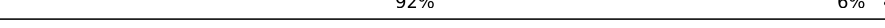
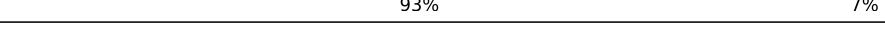
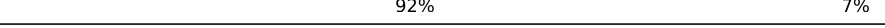
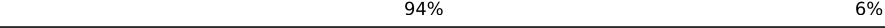
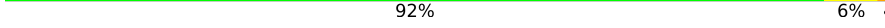
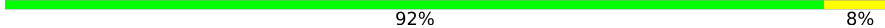
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Mol	Chain	Length	Quality of chain
1	g	231	 90% 10%
1	gA	231	 91% 9%
1	gB	231	 93% 6% .
1	gC	231	 92% 6% .
1	gD	231	 88% 11% .
1	gE	231	 91% 7% .
1	h	231	 90% 9% .
1	hA	231	 91% 8% .
1	hB	231	 92% 6% .
1	hC	231	 93% 7%
1	hD	231	 92% 6% .
1	hE	231	 92% 8%
1	i	231	 92% 7% .
1	iA	231	 93% 5% .
1	iB	231	 91% 7% ..
1	iC	231	 90% 7% .
1	iD	231	 91% 6% .
1	iE	231	 91% 8% .
1	j	231	 89% 11%
1	jA	231	 90% 9% .
1	jB	231	 90% 9% .
1	jC	231	 92% 6% .
1	jD	231	 93% 6%
1	jE	231	 92% 7% .
1	k	231	 90% 9% .

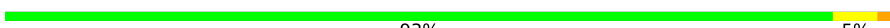
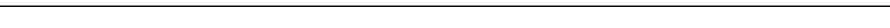
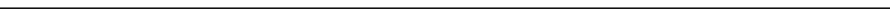
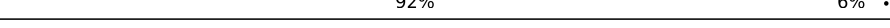
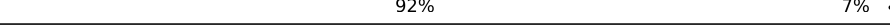
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Mol	Chain	Length	Quality of chain
1	kA	231	 91% 6% .
1	kB	231	 91% 7% .
1	kC	231	 92% 6% .
1	kD	231	 92% 6% .
1	kE	231	 91% 6% .
1	l	231	 91% 9%
1	lA	231	 92% 7% .
1	lB	231	 90% 10% .
1	lC	231	 92% 5% .
1	lD	231	 91% 9%
1	lE	231	 91% 7% .
1	m	231	 90% 8% .
1	mA	231	 92% 8%
1	mB	231	 91% 8% .
1	mC	231	 91% 7% .
1	mD	231	 92% 8%
1	mE	231	 92% 6% .
1	n	231	 93% 7%
1	nA	231	 92% 7% .
1	nB	231	 94% 6%
1	nC	231	 92% 6% .
1	nD	231	 92% 6% .
1	nE	231	 90% 9%
1	o	231	 92% 8%
1	oA	231	 94% 6% .

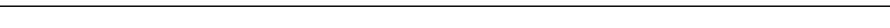
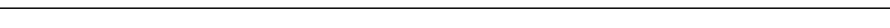
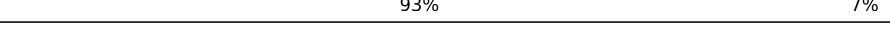
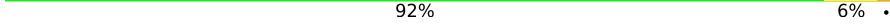
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Mol	Chain	Length	Quality of chain
1	oB	231	 90% 8% .
1	oC	231	 92% 6% .
1	oD	231	 93% 6% .
1	oE	231	 93% 5% .
1	p	231	 92% 7% .
1	pA	231	 92% 6% .
1	pB	231	 91% 8% .
1	pC	231	 92% 7% .
1	pD	231	 92% 7% .
1	pE	231	 89% 8% .
1	q	231	 89% 10% .
1	qA	231	 91% 7% .
1	qB	231	 91% 8% .
1	qC	231	 92% 8% .
1	qD	231	 90% 9% .
1	qE	231	 91% 7% .
1	r	231	 92% 6% .
1	rA	231	 90% 9% .
1	rB	231	 92% 7% .
1	rC	231	 92% 7% .
1	rD	231	 90% 9% .
1	rE	231	 91% 8% .
1	s	231	 93% 6% .
1	sA	231	 90% 10% .
1	sB	231	 91% 7% .

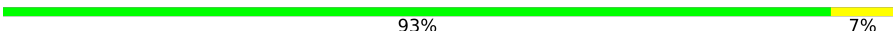
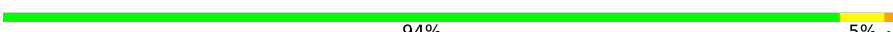
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Mol	Chain	Length	Quality of chain
1	sC	231	 92% 6% .
1	sD	231	 93% 6%
1	sE	231	 92% 6% .
1	t	231	 90% 8% .
1	tA	231	 91% 9%
1	tB	231	 90% 9% .
1	tC	231	 90% 10%
1	tD	231	 90% 7% .
1	tE	231	 92% 8%
1	u	231	 94% 6%
1	uA	231	 92% 6% .
1	uB	231	 90% 8% .
1	uC	231	 91% 7% .
1	uD	231	 91% 7% .
1	uE	231	 91% 7% .
1	v	231	 90% 9% .
1	vA	231	 91% 8%
1	vB	231	 93% 7%
1	vC	231	 90% 9% .
1	vD	231	 89% 9% .
1	vE	231	 92% 6% .
1	w	231	 92% 8%
1	wA	231	 90% 9% .
1	wB	231	 92% 7% .
1	wC	231	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	wD	231	 90% 9% .
1	wE	231	 92% 7% .
1	x	231	 93% 7%
1	xA	231	 91% 9%
1	xB	231	 90% 10%
1	xC	231	 93% 6% .
1	xD	231	 91% 9%
1	xE	231	 92% 6% .
1	y	231	 91% 7% .
1	yA	231	 90% 9% .
1	yB	231	 91% 7% .
1	yC	231	 92% 6% .
1	yD	231	 94% 5% .
1	yE	231	 93% 6% .
1	z	231	 92% 7%
1	zA	231	 94% 5% .
1	zB	231	 92% 6% .
1	zC	231	 90% 9% .
1	zD	231	 91% 8%
1	zE	231	 90% 10%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1359288 atoms, of which 680778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HIV-1 capsid protein.

Mol	Chain	Residues	Atoms						Trace
1	A	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	C	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	D	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	E	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	F	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	G	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	H	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	I	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	J	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	K	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	L	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	M	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	N	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	O	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	P	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	Q	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	R	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	S	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	T	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	U	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	V	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	W	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	X	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	Y	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	Z	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	a	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	b	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	c	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	d	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	e	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	f	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	g	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	h	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	i	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	j	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	k	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	l	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	m	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	n	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	o	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	p	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	q	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	r	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	s	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	t	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	u	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	v	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	w	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	x	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	y	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	z	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	9	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	AA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	BA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	CA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	DA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	EA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	FA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	GA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	HA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	IA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	JA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	KA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	LA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	MA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	NA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	OA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	PA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	QA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	RA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	SA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	TA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	UA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	pA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	AB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	VB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	WB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	XB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	YB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	ZB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	aB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	bB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	cB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	dB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	eB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	fB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	gB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	hB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	iB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	jB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	kB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	lB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	mB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	nB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	oB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	pB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	qB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9B	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	BC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	WC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	rC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	CD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ED	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ID	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ND	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	XD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	sD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	DE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ME	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	YE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	tE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	EF	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	FF	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

4 Residue-property plots [i](#)

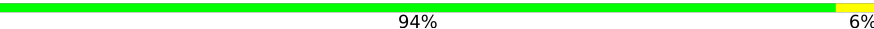
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: HIV-1 capsid protein

Chain A:  90% 8% .



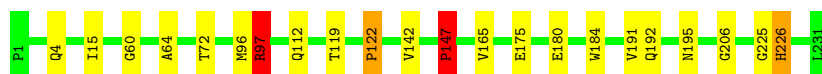
- Molecule 1: HIV-1 capsid protein

Chain B:  94% 6%



- Molecule 1: HIV-1 capsid protein

Chain C:  90% 8% ..



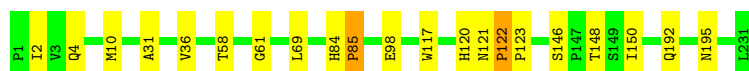
- Molecule 1: HIV-1 capsid protein

Chain D:  90% 10%



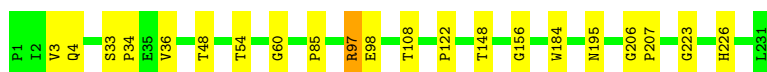
- Molecule 1: HIV-1 capsid protein

Chain E:  91% 8% .



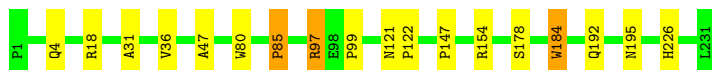
- Molecule 1: HIV-1 capsid protein

Chain F:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain G: 92% 6%



- Molecule 1: HIV-1 capsid protein

Chain H: 91% 8%



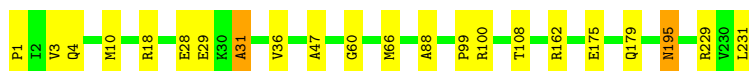
- Molecule 1: HIV-1 capsid protein

Chain I: 93% 6%



- Molecule 1: HIV-1 capsid protein

Chain J: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain K: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain L: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain M: 92% 8%



- Molecule 1: HIV-1 capsid protein

Chain N:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain O:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain P:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain Q:  91% 8%



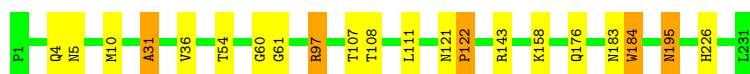
- Molecule 1: HIV-1 capsid protein

Chain R:  88% 12%



- Molecule 1: HIV-1 capsid protein

Chain S:  91% 7%

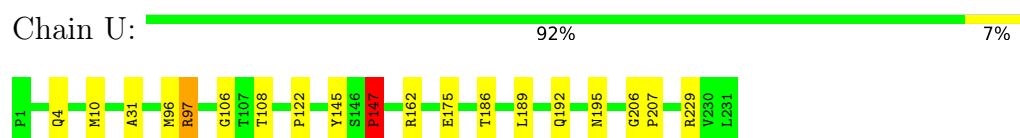


- Molecule 1: HIV-1 capsid protein

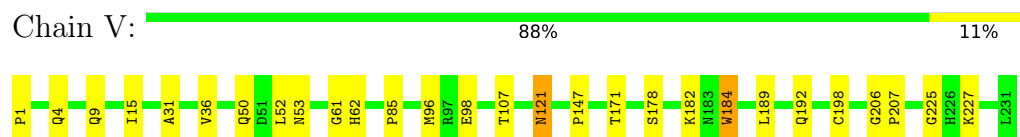
Chain T:  94% 5%



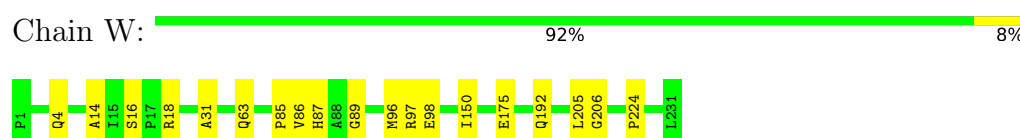
- Molecule 1: HIV-1 capsid protein



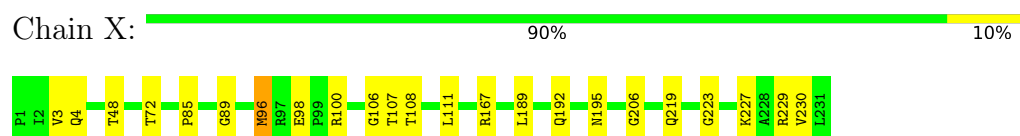
- Molecule 1: HIV-1 capsid protein



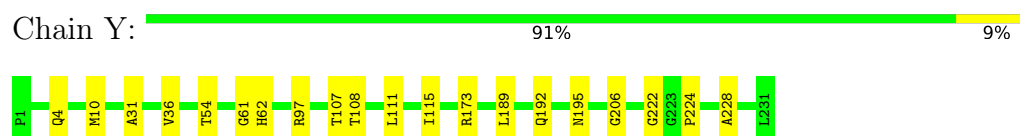
- Molecule 1: HIV-1 capsid protein



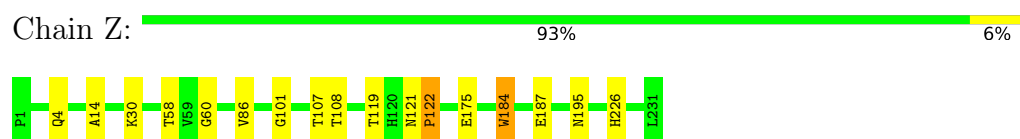
- Molecule 1: HIV-1 capsid protein



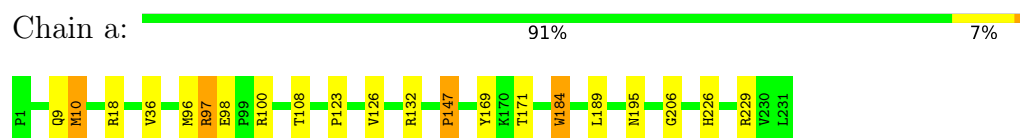
- Molecule 1: HIV-1 capsid protein



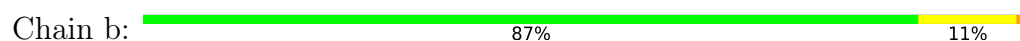
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein





- Molecule 1: HIV-1 capsid protein



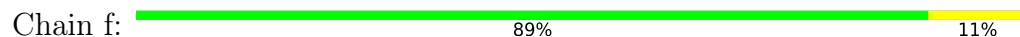
- Molecule 1: HIV-1 capsid protein



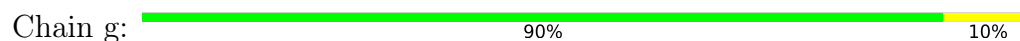
- Molecule 1: HIV-1 capsid protein



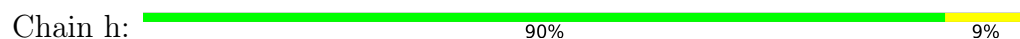
- Molecule 1: HIV-1 capsid protein



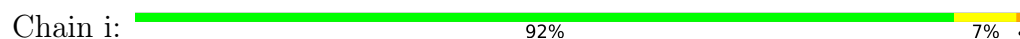
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain j:  89% 11%



- Molecule 1: HIV-1 capsid protein

Chain k:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain l:  91% 9%

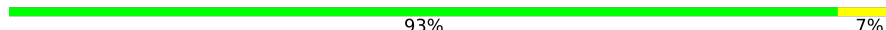


- Molecule 1: HIV-1 capsid protein

Chain m:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain n:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain o:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain p:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain q:  89% 10%

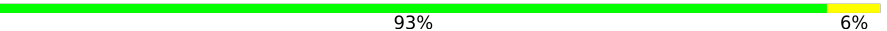


- Molecule 1: HIV-1 capsid protein

Chain r:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain s:  93% 6%

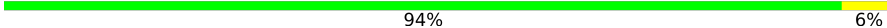


- Molecule 1: HIV-1 capsid protein

Chain t:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain u:  94% 6%



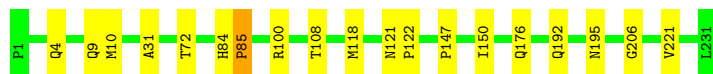
- Molecule 1: HIV-1 capsid protein

Chain v:  90% 9%

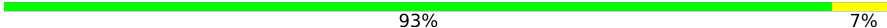


- Molecule 1: HIV-1 capsid protein

Chain w:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain x:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain y: 91% 7%



- Molecule 1: HIV-1 capsid protein

Chain z: 92% 7%



- Molecule 1: HIV-1 capsid protein

Chain 0: 94% 6%



- Molecule 1: HIV-1 capsid protein

Chain 1: 89% 11%



- Molecule 1: HIV-1 capsid protein

Chain 2: 89% 11%



- Molecule 1: HIV-1 capsid protein

Chain 3: 88% 11%

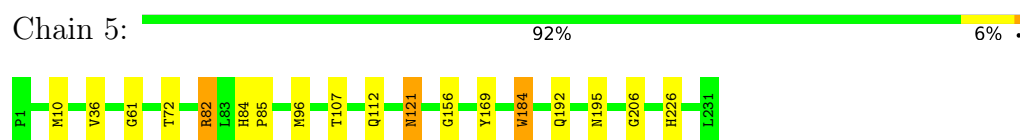


- Molecule 1: HIV-1 capsid protein

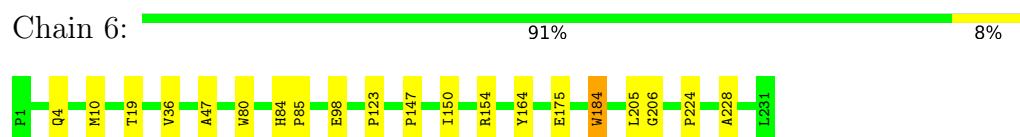
Chain 4: 91% 9%



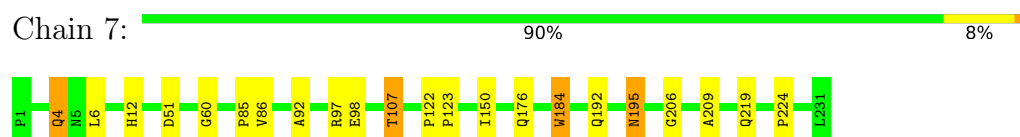
- Molecule 1: HIV-1 capsid protein



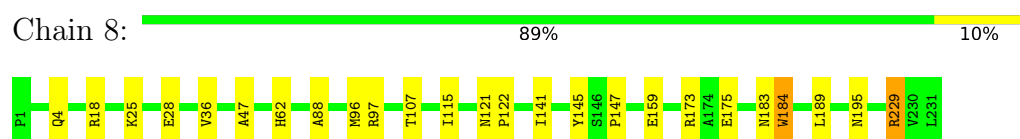
- Molecule 1: HIV-1 capsid protein



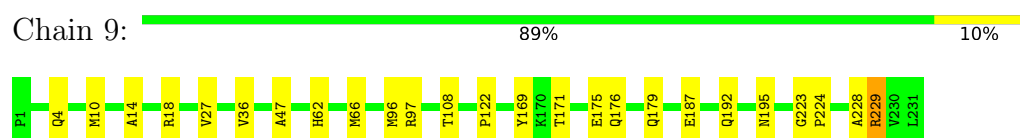
- Molecule 1: HIV-1 capsid protein



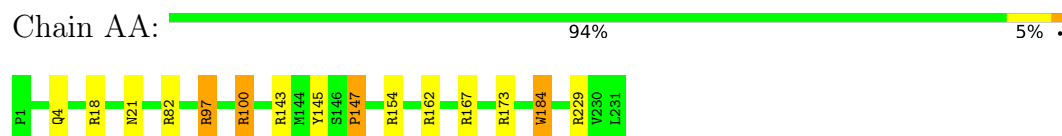
- Molecule 1: HIV-1 capsid protein



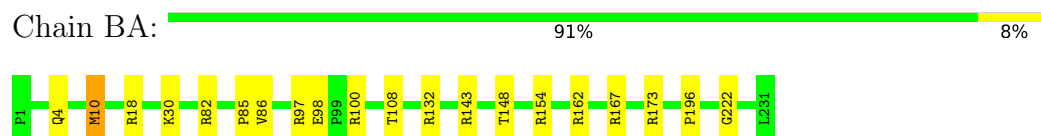
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

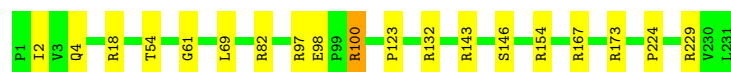


- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain CA:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain DA:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain EA:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain FA:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain GA:  93% 5%



- Molecule 1: HIV-1 capsid protein

Chain HA:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain IA:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain JA:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain KA:
90% 8%



- Molecule 1: HIV-1 capsid protein

Chain LA:
92% 7%



- Molecule 1: HIV-1 capsid protein

Chain MA:
90% 9%



- Molecule 1: HIV-1 capsid protein

Chain NA:
91% 9%



- Molecule 1: HIV-1 capsid protein

Chain OA:
90% 8%



- Molecule 1: HIV-1 capsid protein

Chain PA:
91% 8%



- Molecule 1: HIV-1 capsid protein

Chain QA:
92% 7%



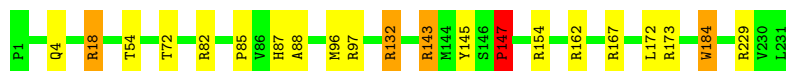
- Molecule 1: HIV-1 capsid protein

Chain RA:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain SA:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain TA:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain UA:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain VA:  88% 11%



- Molecule 1: HIV-1 capsid protein

Chain WA:  92% 7%

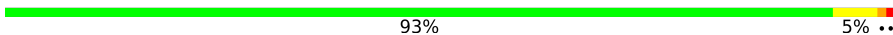


- Molecule 1: HIV-1 capsid protein

Chain XA:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain YA:  93% 5% ..



- Molecule 1: HIV-1 capsid protein

Chain ZA:  91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain aA:  93% 7%

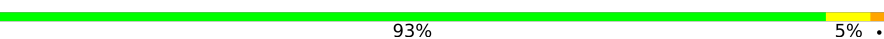


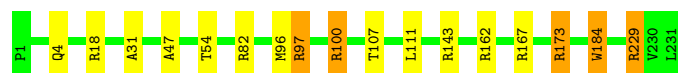
- Molecule 1: HIV-1 capsid protein

Chain bA:  91% 8%



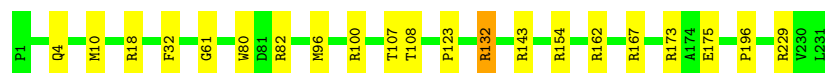
- Molecule 1: HIV-1 capsid protein

Chain cA:  93% 5% .



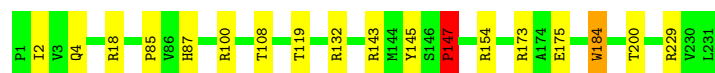
- Molecule 1: HIV-1 capsid protein

Chain dA:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain eA:  92% 7%



- Molecule 1: HIV-1 capsid protein

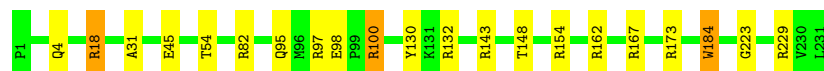
Chain fA:  92% 7% .



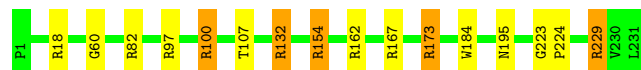
- Molecule 1: HIV-1 capsid protein



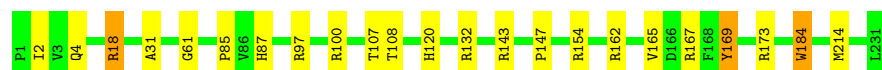
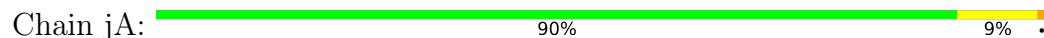
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

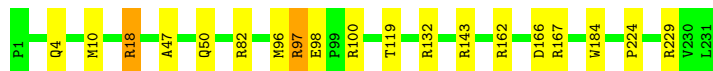


- Molecule 1: HIV-1 capsid protein

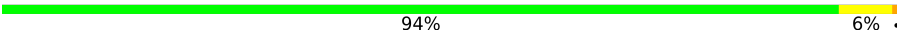


- Molecule 1: HIV-1 capsid protein

Chain nA:  92% 7%

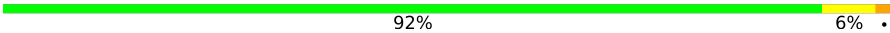


- Molecule 1: HIV-1 capsid protein

Chain oA:  94% 6%



- Molecule 1: HIV-1 capsid protein

Chain pA:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain qA:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain rA:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain sA:  90% 10%

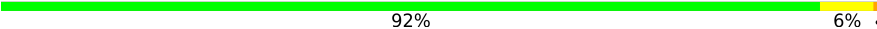


- Molecule 1: HIV-1 capsid protein

Chain tA:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain uA:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain vA:  91% 8%



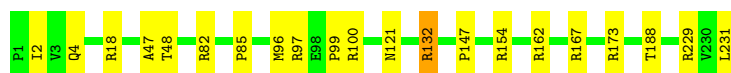
- Molecule 1: HIV-1 capsid protein

Chain wA:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain xA:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain yA:  90% 9%



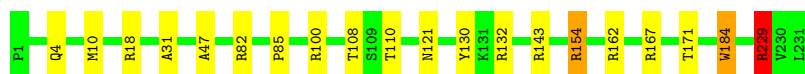
- Molecule 1: HIV-1 capsid protein

Chain zA:  94% 5%



- Molecule 1: HIV-1 capsid protein

Chain 0A:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain 1A:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain 2A: 93% 6%



- Molecule 1: HIV-1 capsid protein

Chain 3A: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 4A: 94% 5%



- Molecule 1: HIV-1 capsid protein

Chain 5A: 91% 7%



- Molecule 1: HIV-1 capsid protein

Chain 6A: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain 7A: 92% 8%

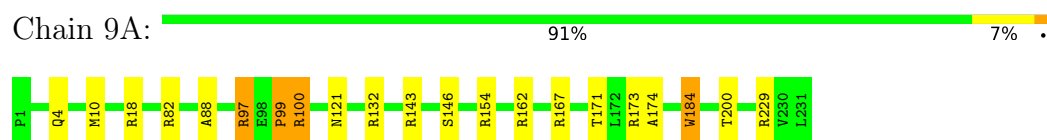


- Molecule 1: HIV-1 capsid protein

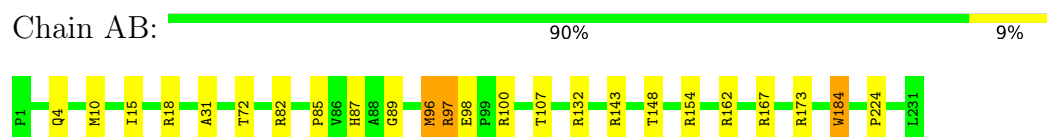
Chain 8A: 92% 6%



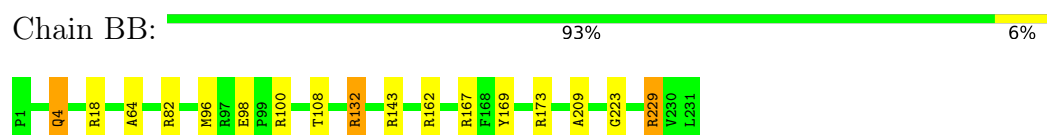
- Molecule 1: HIV-1 capsid protein



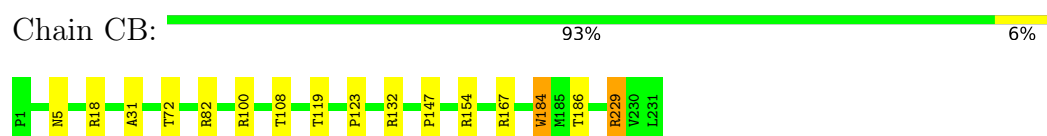
- Molecule 1: HIV-1 capsid protein



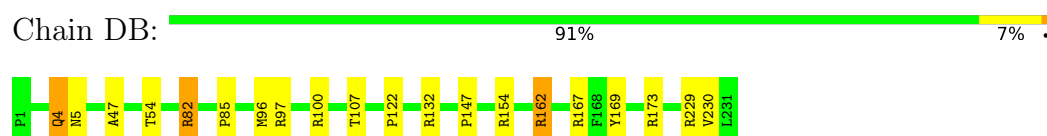
- Molecule 1: HIV-1 capsid protein



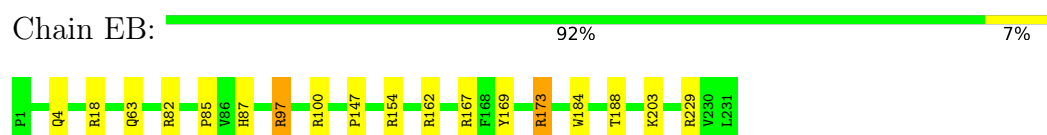
- Molecule 1: HIV-1 capsid protein



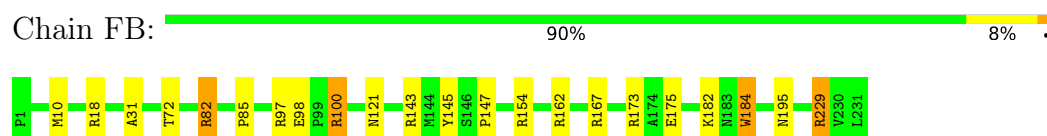
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

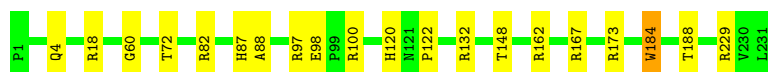


- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain GB:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain HB:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain IB:  92% 6%



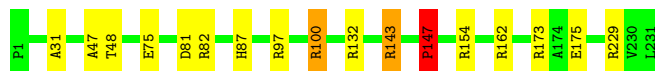
- Molecule 1: HIV-1 capsid protein

Chain JB:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain KB:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain LB:  89% 9%



- Molecule 1: HIV-1 capsid protein

Chain MB:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain NB:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain OB: 90% 10%



- Molecule 1: HIV-1 capsid protein

Chain PB: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain QB: 90% 8% .



- Molecule 1: HIV-1 capsid protein

Chain RB: 91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain SB: 91% 9% .



- Molecule 1: HIV-1 capsid protein

Chain TB: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain UB: 92% 7% .



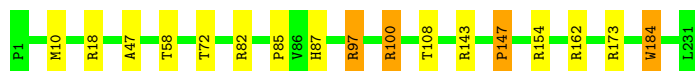
- Molecule 1: HIV-1 capsid protein

Chain VB:  94% 5%



- Molecule 1: HIV-1 capsid protein

Chain WB:  93% 6%



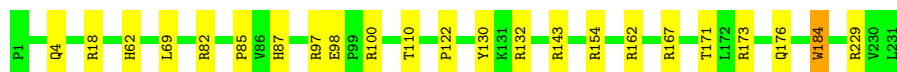
- Molecule 1: HIV-1 capsid protein

Chain XB:  92% 7%



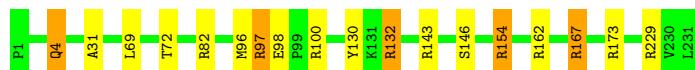
- Molecule 1: HIV-1 capsid protein

Chain YB:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain ZB:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain aB:  94% 5%



- Molecule 1: HIV-1 capsid protein

Chain bB:  91% 8%

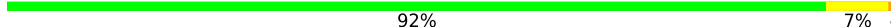


- Molecule 1: HIV-1 capsid protein

Chain cB:  91% 7% .



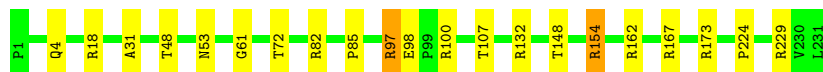
- Molecule 1: HIV-1 capsid protein

Chain dB:  92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain eB:  91% 8% .

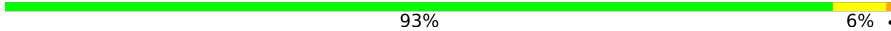


- Molecule 1: HIV-1 capsid protein

Chain fB:  91% 7% .

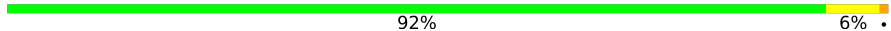


- Molecule 1: HIV-1 capsid protein

Chain gB:  93% 6% .



- Molecule 1: HIV-1 capsid protein

Chain hB:  92% 6% .



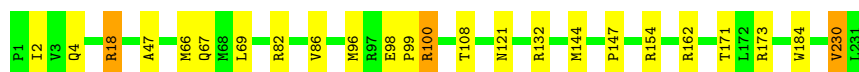
- Molecule 1: HIV-1 capsid protein

Chain iB:  91% 7% ..



- Molecule 1: HIV-1 capsid protein

Chain jB:  90% 9% .



- Molecule 1: HIV-1 capsid protein

Chain kA: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain lA: 90% 10% .



- Molecule 1: HIV-1 capsid protein

Chain mB: 91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain nB: 94% 6% .



- Molecule 1: HIV-1 capsid protein

Chain oB: 90% 8% .



- Molecule 1: HIV-1 capsid protein

Chain pB: 91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain qB: 91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain rB:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain sB:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain tB:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain uB:  90% 8%

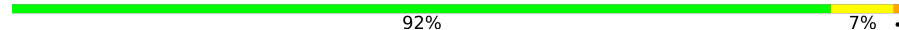


- Molecule 1: HIV-1 capsid protein

Chain vB:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain wB:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain xB:  90% 10%



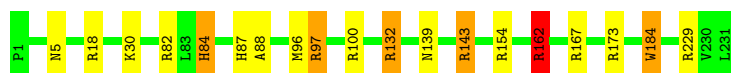
- Molecule 1: HIV-1 capsid protein

Chain yB:  91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain zB:  92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain 0B:  90% 8% .



- Molecule 1: HIV-1 capsid protein

Chain 1B:  90% 9% .



- Molecule 1: HIV-1 capsid protein

Chain 2B:  90% 8% .



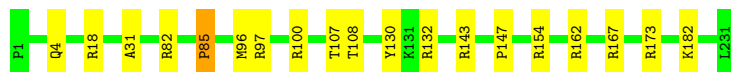
- Molecule 1: HIV-1 capsid protein

Chain 3B:  93% 7% .



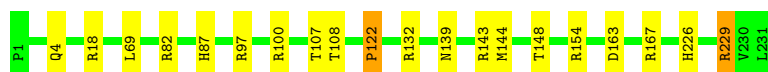
- Molecule 1: HIV-1 capsid protein

Chain 4B:  92% 8% .



- Molecule 1: HIV-1 capsid protein

Chain 5B:  91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain 6B: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain 7B: 92% 8% .



- Molecule 1: HIV-1 capsid protein

Chain 8B: 90% 9% .



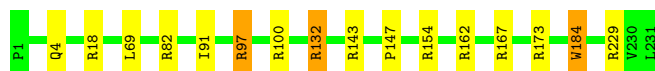
- Molecule 1: HIV-1 capsid protein

Chain 9B: 92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain AC: 93% 6% .



- Molecule 1: HIV-1 capsid protein

Chain BC: 91% 8% .



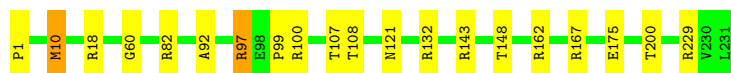
- Molecule 1: HIV-1 capsid protein

Chain CC: 90% 7% .



- Molecule 1: HIV-1 capsid protein

Chain DC:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain EC:  90% 8%



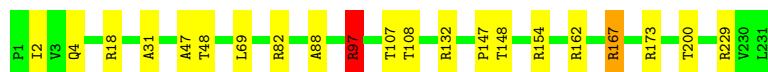
- Molecule 1: HIV-1 capsid protein

Chain FC:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain GC:  91% 8%



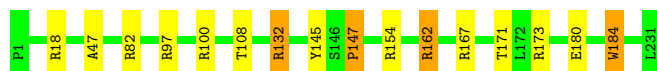
- Molecule 1: HIV-1 capsid protein

Chain HC:  92% 8%



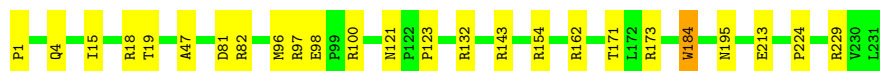
- Molecule 1: HIV-1 capsid protein

Chain IC:  93% 5%



- Molecule 1: HIV-1 capsid protein

Chain JC:  89% 10%



- Molecule 1: HIV-1 capsid protein

Chain KC:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain LC:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain MC:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain NC:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain OC:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain PC:  90% 8%



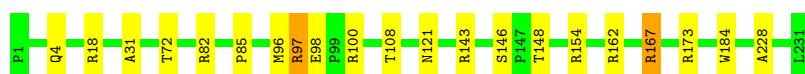
- Molecule 1: HIV-1 capsid protein

Chain QC:  91% 8%



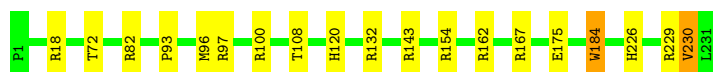
- Molecule 1: HIV-1 capsid protein

Chain RC:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain SC: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain TC: 91% 9% .



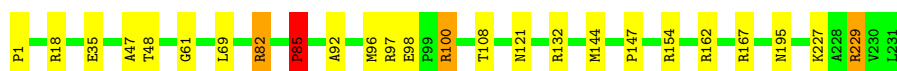
- Molecule 1: HIV-1 capsid protein

Chain UC: 91% 6% .



- Molecule 1: HIV-1 capsid protein

Chain VC: 89% 9% .



- Molecule 1: HIV-1 capsid protein

Chain WC: 93% 6% .



- Molecule 1: HIV-1 capsid protein

Chain XC: 91% 8% .

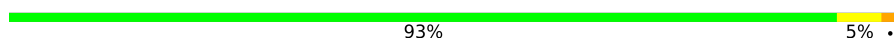


- Molecule 1: HIV-1 capsid protein

Chain YC: 89% 11% .



- Molecule 1: HIV-1 capsid protein

Chain ZC:  93% 5%



- Molecule 1: HIV-1 capsid protein

Chain aC:  91% 6%

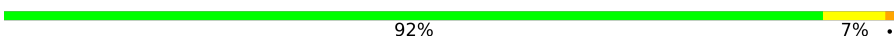


- Molecule 1: HIV-1 capsid protein

Chain bC:  90% 10%

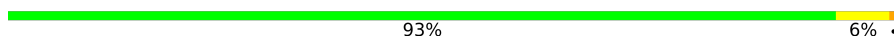


- Molecule 1: HIV-1 capsid protein

Chain cC:  92% 7%

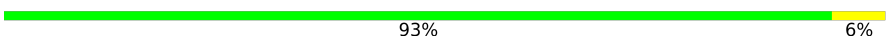


- Molecule 1: HIV-1 capsid protein

Chain dC:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain eC:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain fC:  91% 8%

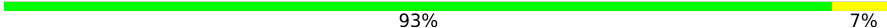


- Molecule 1: HIV-1 capsid protein

Chain gC:  92% 6% .



• Molecule 1: HIV-1 capsid protein

Chain hC:  93% 7% .



• Molecule 1: HIV-1 capsid protein

Chain iC:  90% 7% .



• Molecule 1: HIV-1 capsid protein

Chain jC:  92% 6% .



• Molecule 1: HIV-1 capsid protein

Chain kC:  92% 6% .

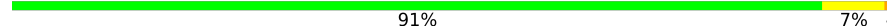


• Molecule 1: HIV-1 capsid protein

Chain lC:  92% 5% .



• Molecule 1: HIV-1 capsid protein

Chain mC:  91% 7% .



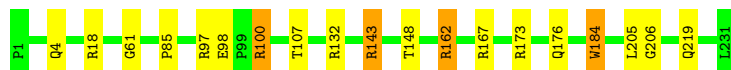
• Molecule 1: HIV-1 capsid protein

Chain nC:  92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain oC: 92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain pC: 92% 7% .



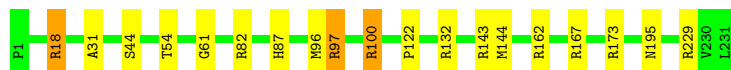
- Molecule 1: HIV-1 capsid protein

Chain qC: 92% 8% .



- Molecule 1: HIV-1 capsid protein

Chain rC: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain sC: 92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain tC: 90% 10% .



- Molecule 1: HIV-1 capsid protein

Chain uC: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain vC:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain wC:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain xC:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain yC:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain zC:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 0C:  92% 8%



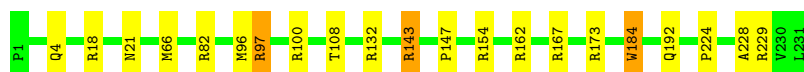
- Molecule 1: HIV-1 capsid protein

Chain 1C:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 2C:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain 3C:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain 4C:  90% 7%

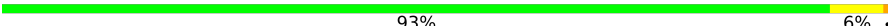


- Molecule 1: HIV-1 capsid protein

Chain 5C:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain 6C:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain 7C:  89% 10%



- Molecule 1: HIV-1 capsid protein

Chain 8C:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain 9C:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain AD: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain BD: 92% 6%



- Molecule 1: HIV-1 capsid protein

Chain CD: 92% 6%



- Molecule 1: HIV-1 capsid protein

Chain DD: 90% 8%



- Molecule 1: HIV-1 capsid protein

Chain ED: 90% 8%



- Molecule 1: HIV-1 capsid protein

Chain FD: 92% 8%



- Molecule 1: HIV-1 capsid protein

Chain GD: 89% 8%



- Molecule 1: HIV-1 capsid protein

Chain HD:  87% 11%



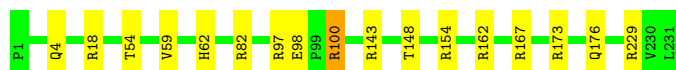
- Molecule 1: HIV-1 capsid protein

Chain ID:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain JD:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain KD:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain LD:  91% 8%

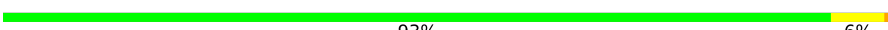


- Molecule 1: HIV-1 capsid protein

Chain MD:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain ND:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain OD:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain PD:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain QD:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain RD:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain SD:  90% 7%



- Molecule 1: HIV-1 capsid protein

Chain TD:  92% 7%



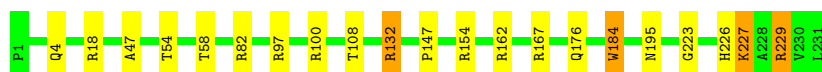
- Molecule 1: HIV-1 capsid protein

Chain UD:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain VD:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain WD: 92% 7%



- Molecule 1: HIV-1 capsid protein

Chain XD: 92% 7%



- Molecule 1: HIV-1 capsid protein

Chain YD: 91% 6%



- Molecule 1: HIV-1 capsid protein

Chain ZD: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain aD: 88% 11%



- Molecule 1: HIV-1 capsid protein

Chain bD: 93% 5%



- Molecule 1: HIV-1 capsid protein

Chain cD: 92% 7%

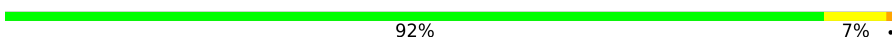


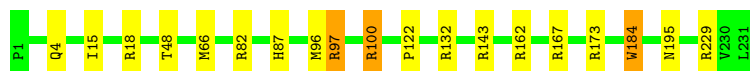
- Molecule 1: HIV-1 capsid protein

Chain dD:  90% 9% .



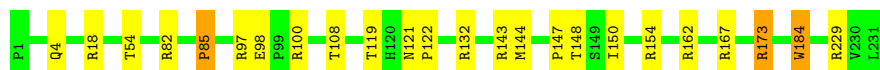
- Molecule 1: HIV-1 capsid protein

Chain eD:  92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain fD:  90% 9% .

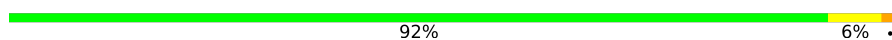


- Molecule 1: HIV-1 capsid protein

Chain gD:  88% 11% .



- Molecule 1: HIV-1 capsid protein

Chain hD:  92% 6% .

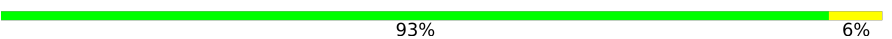


- Molecule 1: HIV-1 capsid protein

Chain iD:  91% 6% .

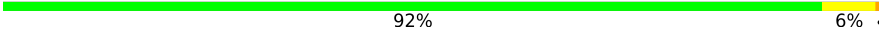


- Molecule 1: HIV-1 capsid protein

Chain jD:  93% 6% .



- Molecule 1: HIV-1 capsid protein

Chain kD:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain lD:  91% 9%

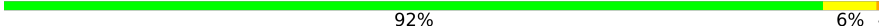


- Molecule 1: HIV-1 capsid protein

Chain mD:  92% 8%

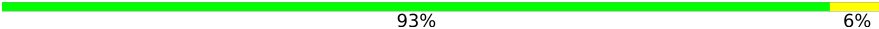


- Molecule 1: HIV-1 capsid protein

Chain nD:  92% 6%

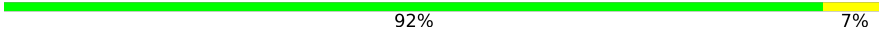


- Molecule 1: HIV-1 capsid protein

Chain oD:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain pD:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain qD:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain rD:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain sD: 93% 6%



- Molecule 1: HIV-1 capsid protein

Chain tD: 90% 7%



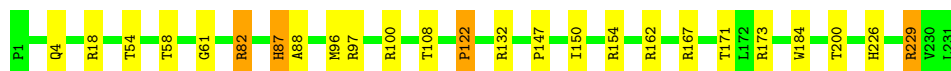
- Molecule 1: HIV-1 capsid protein

Chain uD: 91% 7%



- Molecule 1: HIV-1 capsid protein

Chain vD: 89% 9%



- Molecule 1: HIV-1 capsid protein

Chain wD: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain xD: 91% 9%

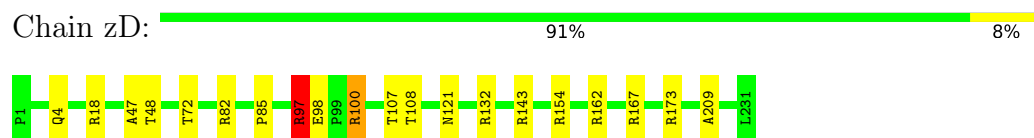


- Molecule 1: HIV-1 capsid protein

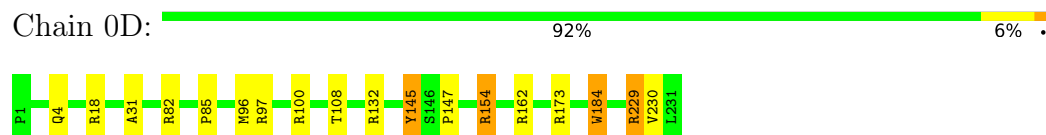
Chain yD: 94% 5%



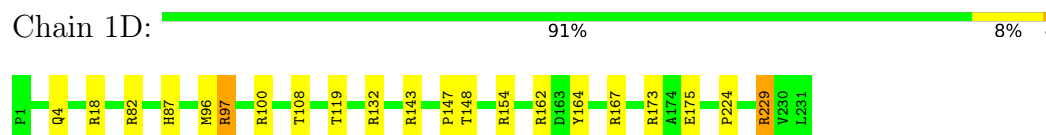
- Molecule 1: HIV-1 capsid protein



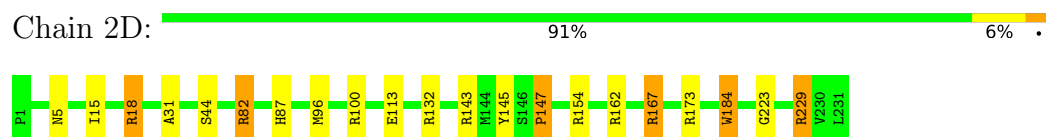
- Molecule 1: HIV-1 capsid protein



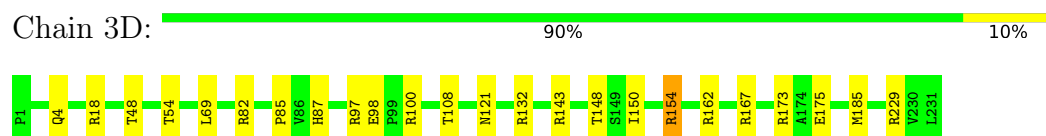
- Molecule 1: HIV-1 capsid protein



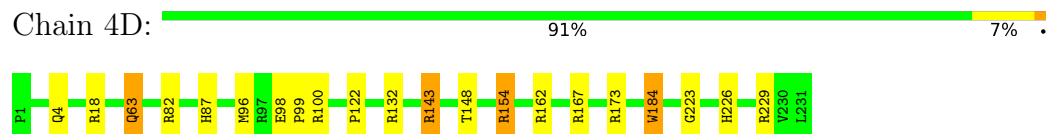
- Molecule 1: HIV-1 capsid protein



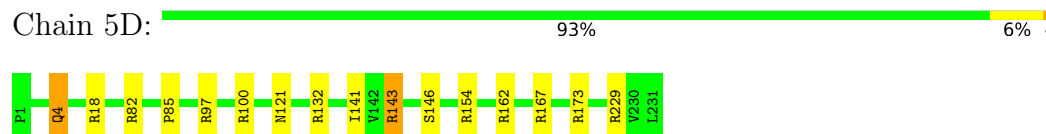
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain 6D:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain 7D:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain 8D:  92% 7%



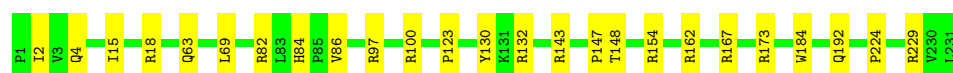
- Molecule 1: HIV-1 capsid protein

Chain 9D:  92% 7%

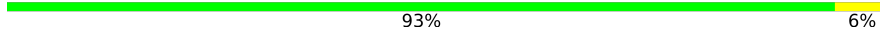


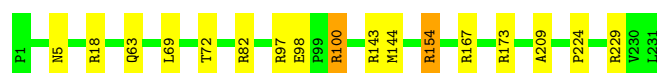
- Molecule 1: HIV-1 capsid protein

Chain AE:  89% 11%



- Molecule 1: HIV-1 capsid protein

Chain BE:  93% 6%

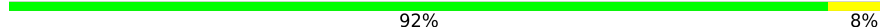


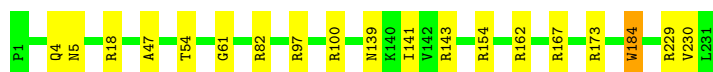
- Molecule 1: HIV-1 capsid protein

Chain CE:  91% 8%

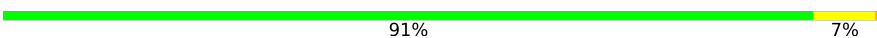


- Molecule 1: HIV-1 capsid protein

Chain DE:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain EE:  91% 7% .

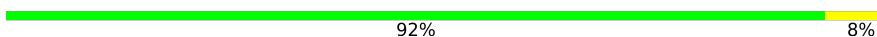


- Molecule 1: HIV-1 capsid protein

Chain FE:  91% 8% .

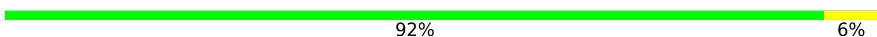


- Molecule 1: HIV-1 capsid protein

Chain GE:  92% 8% .

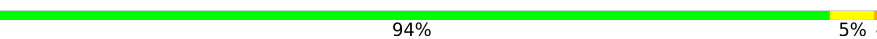


- Molecule 1: HIV-1 capsid protein

Chain HE:  92% 6% .



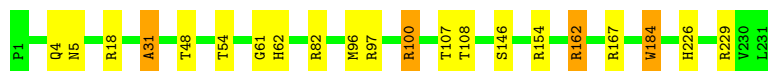
- Molecule 1: HIV-1 capsid protein

Chain IE:  94% 5% .



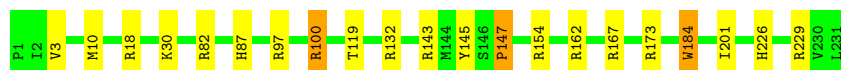
- Molecule 1: HIV-1 capsid protein

Chain JE:  91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain KE:  91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain LE:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain ME:  91% 9%

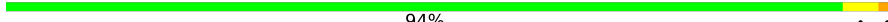


- Molecule 1: HIV-1 capsid protein

Chain NE:  94% 6%



- Molecule 1: HIV-1 capsid protein

Chain OE:  94% 6%



- Molecule 1: HIV-1 capsid protein

Chain PE:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain QE:  90% 9%



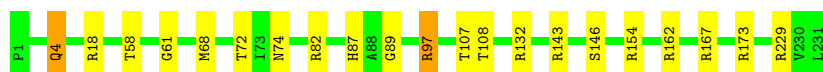
- Molecule 1: HIV-1 capsid protein

Chain RE:  91% 7%

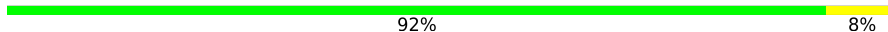


- Molecule 1: HIV-1 capsid protein

Chain SE:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain TE:  92% 8%

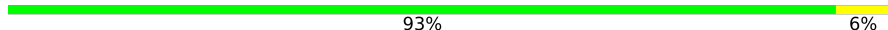


- Molecule 1: HIV-1 capsid protein

Chain UE:  93% 6%

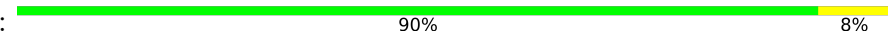


- Molecule 1: HIV-1 capsid protein

Chain VE:  93% 6%



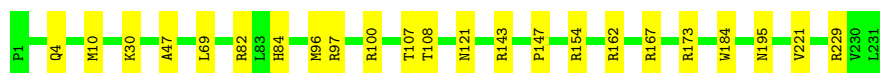
- Molecule 1: HIV-1 capsid protein

Chain WE:  90% 8%



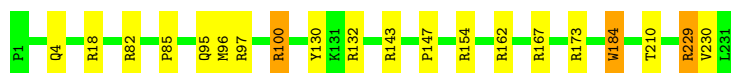
- Molecule 1: HIV-1 capsid protein

Chain XE:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain YE:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain ZE:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain aE: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain bE: 94% 6% .



- Molecule 1: HIV-1 capsid protein

Chain cE: 92% 6% .



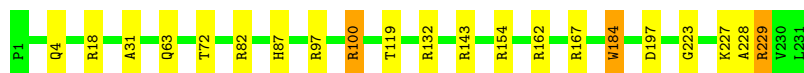
- Molecule 1: HIV-1 capsid protein

Chain dE: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain eE: 91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain fE: 92% 6% .

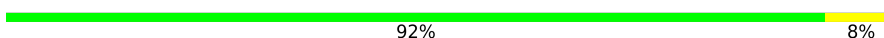


- Molecule 1: HIV-1 capsid protein

Chain gE: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain hE:  92% 8%

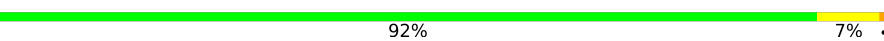


- Molecule 1: HIV-1 capsid protein

Chain iE:  91% 8%



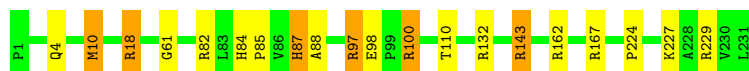
- Molecule 1: HIV-1 capsid protein

Chain jE:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain kE:  91% 6%

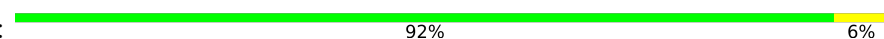


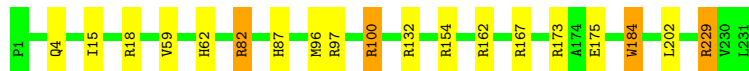
- Molecule 1: HIV-1 capsid protein

Chain lE:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain mE:  92% 6%

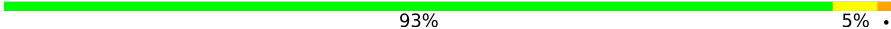


- Molecule 1: HIV-1 capsid protein

Chain nE:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain oE:  93% 5% .



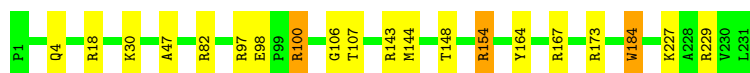
- Molecule 1: HIV-1 capsid protein

Chain pE:  89% 8% .



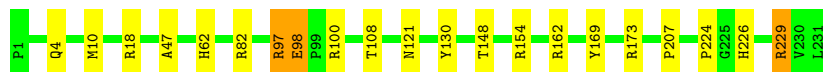
- Molecule 1: HIV-1 capsid protein

Chain qE:  91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain rE:  91% 8% .



- Molecule 1: HIV-1 capsid protein

Chain sE:  92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain tE:  92% 8% .



- Molecule 1: HIV-1 capsid protein

Chain uE:  91% 7% .



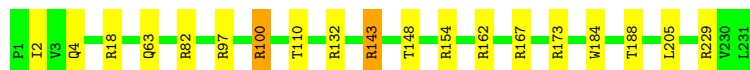
- Molecule 1: HIV-1 capsid protein

Chain vE:  92% 6% .



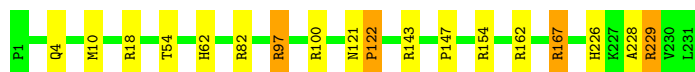
- Molecule 1: HIV-1 capsid protein

Chain wE: 92% 7% .



- Molecule 1: HIV-1 capsid protein

Chain xE: 92% 6% .



- Molecule 1: HIV-1 capsid protein

Chain yE: 93% 6% .



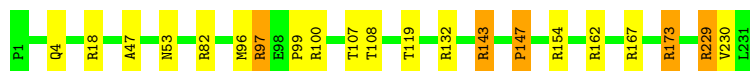
- Molecule 1: HIV-1 capsid protein

Chain zE: 90% 10% .



- Molecule 1: HIV-1 capsid protein

Chain 0E: 91% 7% .



- Molecule 1: HIV-1 capsid protein

Chain 1E: 90% 9% .

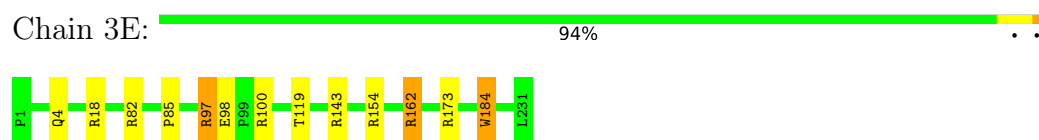


- Molecule 1: HIV-1 capsid protein

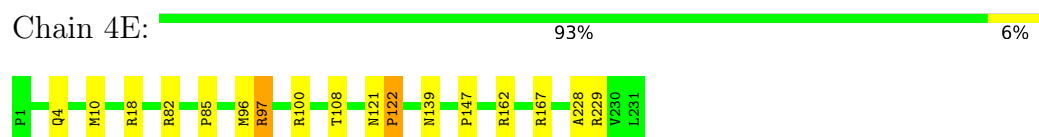
Chain 2E: 92% 8% .



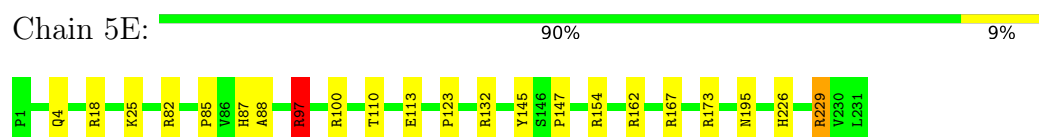
- Molecule 1: HIV-1 capsid protein



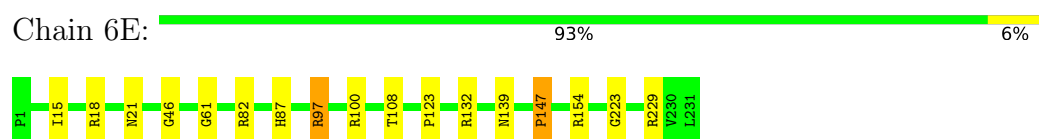
- Molecule 1: HIV-1 capsid protein



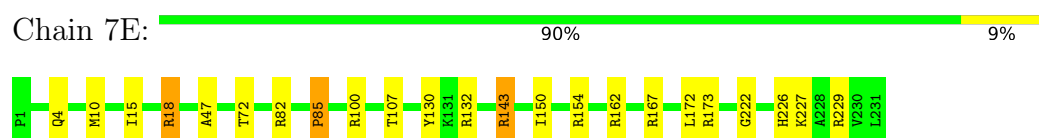
- Molecule 1: HIV-1 capsid protein



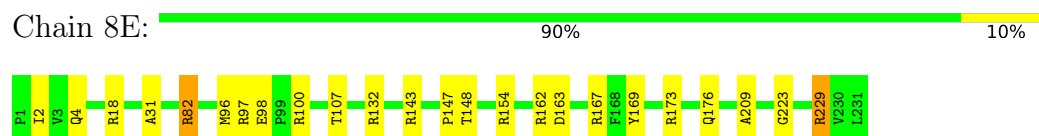
- Molecule 1: HIV-1 capsid protein



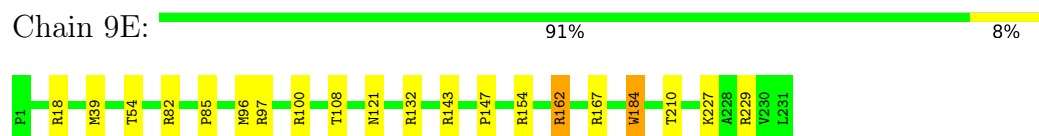
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain AF:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain BF:  91% 9%



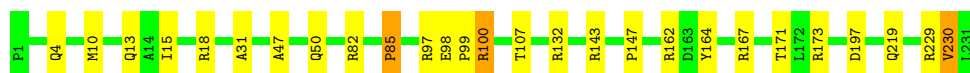
- Molecule 1: HIV-1 capsid protein

Chain CF:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain DF:  88% 10%



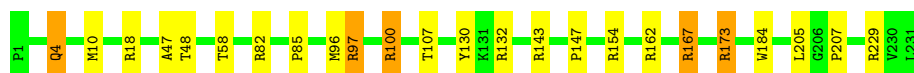
- Molecule 1: HIV-1 capsid protein

Chain EF:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain FF:  90% 8%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *data-guided molecular dynamics*.

Of the 87 calculated structures, 1 were deposited, based on the following criterion: *inner turns of helical assembly*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS	structure calculation	
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	
NAMD	structure calculation	2.13

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1126
Number of shifts mapped to atoms	1126
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality ⓘ

6.1 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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	0	0.87	0/1836 (0.0%)	1.61	9/2493 (0.4%)
1	0A	0.69	0/1836 (0.0%)	1.16	18/2493 (0.7%)
1	0B	0.68	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	0C	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	0D	0.69	0/1836 (0.0%)	1.09	10/2493 (0.4%)
1	0E	0.69	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	1	0.88	0/1836 (0.0%)	1.67	16/2493 (0.6%)
1	1A	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	1B	0.69	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	1C	0.70	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	1D	0.69	0/1836 (0.0%)	1.17	17/2493 (0.7%)
1	1E	0.68	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	2	0.87	0/1836 (0.0%)	1.65	20/2493 (0.8%)
1	2A	0.69	0/1836 (0.0%)	1.25	20/2493 (0.8%)
1	2B	0.68	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	2C	0.69	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	2D	0.69	0/1836 (0.0%)	1.18	17/2493 (0.7%)
1	2E	0.70	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	3	0.87	0/1836 (0.0%)	1.67	18/2493 (0.7%)
1	3A	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	3B	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	3C	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	3D	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	3E	0.69	0/1836 (0.0%)	1.19	12/2493 (0.5%)
1	4	0.86	0/1836 (0.0%)	1.63	9/2493 (0.4%)
1	4A	0.69	0/1836 (0.0%)	1.16	13/2493 (0.5%)
1	4B	0.68	0/1836 (0.0%)	1.18	16/2493 (0.6%)
1	4C	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	4D	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	4E	0.68	0/1836 (0.0%)	1.09	9/2493 (0.4%)
1	5	0.86	0/1836 (0.0%)	1.69	17/2493 (0.7%)
1	5A	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	5B	0.69	0/1836 (0.0%)	1.10	15/2493 (0.6%)
1	5C	0.69	0/1836 (0.0%)	1.17	15/2493 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	5D	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	5E	0.69	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	6	0.87	0/1836 (0.0%)	1.60	9/2493 (0.4%)
1	6A	0.69	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	6B	0.69	0/1836 (0.0%)	1.18	16/2493 (0.6%)
1	6C	0.69	0/1836 (0.0%)	1.11	10/2493 (0.4%)
1	6D	0.68	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	6E	0.69	0/1836 (0.0%)	1.11	10/2493 (0.4%)
1	7	0.88	0/1836 (0.0%)	1.66	18/2493 (0.7%)
1	7A	0.69	0/1836 (0.0%)	1.21	18/2493 (0.7%)
1	7B	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	7C	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	7D	0.69	0/1836 (0.0%)	1.18	14/2493 (0.6%)
1	7E	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	8	0.87	0/1836 (0.0%)	1.64	16/2493 (0.6%)
1	8A	0.68	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	8B	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	8C	0.70	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	8D	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	8E	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	9	0.87	0/1836 (0.0%)	1.64	10/2493 (0.4%)
1	9A	0.69	0/1836 (0.0%)	1.15	17/2493 (0.7%)
1	9B	0.69	0/1836 (0.0%)	1.18	17/2493 (0.7%)
1	9C	0.68	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	9D	0.68	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	9E	0.70	0/1836 (0.0%)	1.10	14/2493 (0.6%)
1	A	0.88	0/1836 (0.0%)	1.66	11/2493 (0.4%)
1	AA	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	AB	0.69	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	AC	0.68	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	AD	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	AE	0.69	0/1836 (0.0%)	1.17	18/2493 (0.7%)
1	AF	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	B	0.87	0/1836 (0.0%)	1.63	9/2493 (0.4%)
1	BA	0.69	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	BB	0.69	0/1836 (0.0%)	1.14	11/2493 (0.4%)
1	BC	0.69	0/1836 (0.0%)	1.10	10/2493 (0.4%)
1	BD	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	BE	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	BF	0.69	0/1836 (0.0%)	1.11	15/2493 (0.6%)
1	C	0.87	0/1836 (0.0%)	1.63	19/2493 (0.8%)
1	CA	0.68	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	CB	0.68	0/1836 (0.0%)	1.06	11/2493 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	CC	0.69	0/1836 (0.0%)	1.22	18/2493 (0.7%)
1	CD	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	CE	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	CF	0.69	0/1836 (0.0%)	1.19	18/2493 (0.7%)
1	D	0.87	0/1836 (0.0%)	1.65	9/2493 (0.4%)
1	DA	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	DB	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	DC	0.70	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	DD	0.69	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	DE	0.69	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	DF	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	E	0.87	0/1836 (0.0%)	1.62	10/2493 (0.4%)
1	EA	0.70	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	EB	0.69	0/1836 (0.0%)	1.17	14/2493 (0.6%)
1	EC	0.69	0/1836 (0.0%)	1.15	11/2493 (0.4%)
1	ED	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	EE	0.69	0/1836 (0.0%)	1.17	17/2493 (0.7%)
1	EF	0.69	0/1836 (0.0%)	1.14	12/2493 (0.5%)
1	F	0.88	0/1836 (0.0%)	1.64	16/2493 (0.6%)
1	FA	0.69	0/1836 (0.0%)	1.13	16/2493 (0.6%)
1	FB	0.69	0/1836 (0.0%)	1.19	18/2493 (0.7%)
1	FC	0.69	0/1836 (0.0%)	1.17	13/2493 (0.5%)
1	FD	0.69	0/1836 (0.0%)	1.10	12/2493 (0.5%)
1	FE	0.69	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	FF	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	G	0.87	0/1836 (0.0%)	1.65	12/2493 (0.5%)
1	GA	0.68	0/1836 (0.0%)	1.13	16/2493 (0.6%)
1	GB	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	GC	0.69	0/1836 (0.0%)	1.09	10/2493 (0.4%)
1	GD	0.69	0/1836 (0.0%)	1.18	19/2493 (0.8%)
1	GE	0.69	0/1836 (0.0%)	1.18	20/2493 (0.8%)
1	H	0.87	0/1836 (0.0%)	1.66	17/2493 (0.7%)
1	HA	0.69	0/1836 (0.0%)	1.14	11/2493 (0.4%)
1	HB	0.69	0/1836 (0.0%)	1.10	12/2493 (0.5%)
1	HC	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	HD	0.69	0/1836 (0.0%)	1.11	15/2493 (0.6%)
1	HE	0.70	0/1836 (0.0%)	1.11	16/2493 (0.6%)
1	I	0.87	0/1836 (0.0%)	1.62	15/2493 (0.6%)
1	IA	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	IB	0.69	0/1836 (0.0%)	1.14	17/2493 (0.7%)
1	IC	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	ID	0.69	0/1836 (0.0%)	1.12	10/2493 (0.4%)
1	IE	0.69	0/1836 (0.0%)	1.09	13/2493 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	J	0.87	0/1836 (0.0%)	1.65	13/2493 (0.5%)
1	JA	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	JB	0.70	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	JC	0.69	0/1836 (0.0%)	1.18	17/2493 (0.7%)
1	JD	0.68	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	JE	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	K	0.87	0/1836 (0.0%)	1.65	16/2493 (0.6%)
1	KA	0.69	0/1836 (0.0%)	1.13	15/2493 (0.6%)
1	KB	0.70	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	KC	0.69	0/1836 (0.0%)	1.09	12/2493 (0.5%)
1	KD	0.68	0/1836 (0.0%)	1.08	13/2493 (0.5%)
1	KE	0.69	0/1836 (0.0%)	1.19	18/2493 (0.7%)
1	L	0.88	0/1836 (0.0%)	1.68	15/2493 (0.6%)
1	LA	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	LB	0.69	0/1836 (0.0%)	1.16	13/2493 (0.5%)
1	LC	0.69	0/1836 (0.0%)	1.08	10/2493 (0.4%)
1	LD	0.69	0/1836 (0.0%)	1.15	10/2493 (0.4%)
1	LE	0.70	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	M	0.86	0/1836 (0.0%)	1.61	10/2493 (0.4%)
1	MA	0.69	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	MB	0.69	0/1836 (0.0%)	1.10	15/2493 (0.6%)
1	MC	0.69	0/1836 (0.0%)	1.10	11/2493 (0.4%)
1	MD	0.69	0/1836 (0.0%)	1.12	16/2493 (0.6%)
1	ME	0.68	0/1836 (0.0%)	1.11	15/2493 (0.6%)
1	N	0.88	0/1836 (0.0%)	1.62	13/2493 (0.5%)
1	NA	0.69	0/1836 (0.0%)	1.12	11/2493 (0.4%)
1	NB	0.69	0/1836 (0.0%)	1.12	11/2493 (0.4%)
1	NC	0.69	0/1836 (0.0%)	1.09	11/2493 (0.4%)
1	ND	0.68	0/1836 (0.0%)	1.15	12/2493 (0.5%)
1	NE	0.68	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	O	0.87	0/1836 (0.0%)	1.60	8/2493 (0.3%)
1	OA	0.69	0/1836 (0.0%)	1.11	14/2493 (0.6%)
1	OB	0.69	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	OC	0.69	0/1836 (0.0%)	1.11	14/2493 (0.6%)
1	OD	0.70	0/1836 (0.0%)	1.17	14/2493 (0.6%)
1	OE	0.69	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	P	0.87	0/1836 (0.0%)	1.63	9/2493 (0.4%)
1	PA	0.69	0/1836 (0.0%)	1.16	16/2493 (0.6%)
1	PB	0.68	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	PC	0.68	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	PD	0.69	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	PE	0.69	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	Q	0.86	0/1836 (0.0%)	1.63	16/2493 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	QA	0.68	0/1836 (0.0%)	1.13	9/2493 (0.4%)
1	QB	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	QC	0.69	0/1836 (0.0%)	1.14	17/2493 (0.7%)
1	QD	0.69	0/1836 (0.0%)	1.15	18/2493 (0.7%)
1	QE	0.68	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	R	0.88	0/1836 (0.0%)	1.70	22/2493 (0.9%)
1	RA	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	RB	0.68	0/1836 (0.0%)	1.12	16/2493 (0.6%)
1	RC	0.69	0/1836 (0.0%)	1.13	10/2493 (0.4%)
1	RD	0.70	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	RE	0.68	0/1836 (0.0%)	1.16	17/2493 (0.7%)
1	S	0.87	0/1836 (0.0%)	1.68	17/2493 (0.7%)
1	SA	0.70	0/1836 (0.0%)	1.22	21/2493 (0.8%)
1	SB	0.68	0/1836 (0.0%)	1.12	9/2493 (0.4%)
1	SC	0.68	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	SD	0.70	0/1836 (0.0%)	1.21	17/2493 (0.7%)
1	SE	0.70	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	T	0.88	0/1836 (0.0%)	1.64	8/2493 (0.3%)
1	TA	0.69	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	TB	0.69	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	TC	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	TD	0.68	0/1836 (0.0%)	1.15	12/2493 (0.5%)
1	TE	0.68	0/1836 (0.0%)	1.10	11/2493 (0.4%)
1	U	0.88	0/1836 (0.0%)	1.61	11/2493 (0.4%)
1	UA	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	UB	0.69	0/1836 (0.0%)	1.17	13/2493 (0.5%)
1	UC	0.69	0/1836 (0.0%)	1.17	15/2493 (0.6%)
1	UD	0.70	0/1836 (0.0%)	1.19	18/2493 (0.7%)
1	UE	0.68	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	V	0.87	0/1836 (0.0%)	1.68	26/2493 (1.0%)
1	VA	0.69	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	VB	0.69	0/1836 (0.0%)	1.11	11/2493 (0.4%)
1	VC	0.68	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	VD	0.70	0/1836 (0.0%)	1.15	12/2493 (0.5%)
1	VE	0.69	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	W	0.87	0/1836 (0.0%)	1.63	12/2493 (0.5%)
1	WA	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	WB	0.69	0/1836 (0.0%)	1.19	13/2493 (0.5%)
1	WC	0.69	0/1836 (0.0%)	1.12	12/2493 (0.5%)
1	WD	0.68	0/1836 (0.0%)	1.13	15/2493 (0.6%)
1	WE	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	X	0.88	0/1836 (0.0%)	1.62	15/2493 (0.6%)
1	XA	0.69	0/1836 (0.0%)	1.17	15/2493 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	XB	0.70	0/1836 (0.0%)	1.10	9/2493 (0.4%)
1	XC	0.69	0/1836 (0.0%)	1.10	9/2493 (0.4%)
1	XD	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	XE	0.69	0/1836 (0.0%)	1.14	12/2493 (0.5%)
1	Y	0.87	0/1836 (0.0%)	1.64	13/2493 (0.5%)
1	YA	0.69	0/1836 (0.0%)	1.13	15/2493 (0.6%)
1	YB	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	YC	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	YD	0.68	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	YE	0.69	0/1836 (0.0%)	1.20	22/2493 (0.9%)
1	Z	0.87	0/1836 (0.0%)	1.65	12/2493 (0.5%)
1	ZA	0.69	0/1836 (0.0%)	1.14	14/2493 (0.6%)
1	ZB	0.69	0/1836 (0.0%)	1.14	12/2493 (0.5%)
1	ZC	0.69	0/1836 (0.0%)	1.11	9/2493 (0.4%)
1	ZD	0.68	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	ZE	0.69	0/1836 (0.0%)	1.16	20/2493 (0.8%)
1	a	0.87	0/1836 (0.0%)	1.71	19/2493 (0.8%)
1	aA	0.69	0/1836 (0.0%)	1.13	10/2493 (0.4%)
1	aB	0.69	0/1836 (0.0%)	1.11	12/2493 (0.5%)
1	aC	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	aD	0.68	0/1836 (0.0%)	1.19	16/2493 (0.6%)
1	aE	0.69	0/1836 (0.0%)	1.10	15/2493 (0.6%)
1	b	0.87	0/1836 (0.0%)	1.70	18/2493 (0.7%)
1	bA	0.69	0/1836 (0.0%)	1.09	11/2493 (0.4%)
1	bB	0.69	0/1836 (0.0%)	1.15	19/2493 (0.8%)
1	bC	0.68	0/1836 (0.0%)	1.13	14/2493 (0.6%)
1	bD	0.69	0/1836 (0.0%)	1.15	12/2493 (0.5%)
1	bE	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	c	0.88	0/1836 (0.0%)	1.69	12/2493 (0.5%)
1	cA	0.68	0/1836 (0.0%)	1.17	17/2493 (0.7%)
1	cB	0.69	0/1836 (0.0%)	1.12	10/2493 (0.4%)
1	cC	0.70	0/1836 (0.0%)	1.17	13/2493 (0.5%)
1	cD	0.69	0/1836 (0.0%)	1.15	17/2493 (0.7%)
1	cE	0.68	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	d	0.88	0/1836 (0.0%)	1.63	16/2493 (0.6%)
1	dA	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	dB	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	dC	0.69	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	dD	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	dE	0.69	0/1836 (0.0%)	1.10	7/2493 (0.3%)
1	e	0.87	0/1836 (0.0%)	1.67	12/2493 (0.5%)
1	eA	0.69	0/1836 (0.0%)	1.08	10/2493 (0.4%)
1	eB	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	eC	0.69	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	eD	0.68	0/1836 (0.0%)	1.17	19/2493 (0.8%)
1	eE	0.70	0/1836 (0.0%)	1.13	12/2493 (0.5%)
1	f	0.88	0/1836 (0.0%)	1.63	11/2493 (0.4%)
1	fA	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	fB	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	fC	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	fD	0.68	0/1836 (0.0%)	1.19	18/2493 (0.7%)
1	fE	0.69	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	g	0.87	0/1836 (0.0%)	1.62	13/2493 (0.5%)
1	gA	0.69	0/1836 (0.0%)	1.10	14/2493 (0.6%)
1	gB	0.70	0/1836 (0.0%)	1.17	15/2493 (0.6%)
1	gC	0.69	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	gD	0.68	0/1836 (0.0%)	1.19	15/2493 (0.6%)
1	gE	0.69	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	h	0.89	0/1836 (0.0%)	1.67	22/2493 (0.9%)
1	hA	0.69	0/1836 (0.0%)	1.19	16/2493 (0.6%)
1	hB	0.69	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	hC	0.68	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	hD	0.69	0/1836 (0.0%)	1.11	16/2493 (0.6%)
1	hE	0.69	0/1836 (0.0%)	1.17	17/2493 (0.7%)
1	i	0.88	0/1836 (0.0%)	1.65	13/2493 (0.5%)
1	iA	0.69	0/1836 (0.0%)	1.17	15/2493 (0.6%)
1	iB	0.69	0/1836 (0.0%)	1.14	17/2493 (0.7%)
1	iC	0.69	0/1836 (0.0%)	1.13	11/2493 (0.4%)
1	iD	0.68	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	iE	0.69	0/1836 (0.0%)	1.18	17/2493 (0.7%)
1	j	0.88	0/1836 (0.0%)	1.67	19/2493 (0.8%)
1	jA	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	jB	0.69	0/1836 (0.0%)	1.15	12/2493 (0.5%)
1	jC	0.69	0/1836 (0.0%)	1.17	13/2493 (0.5%)
1	jD	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	jE	0.69	0/1836 (0.0%)	1.10	12/2493 (0.5%)
1	k	0.87	0/1836 (0.0%)	1.63	14/2493 (0.6%)
1	kA	0.70	0/1836 (0.0%)	1.18	18/2493 (0.7%)
1	kB	0.69	0/1836 (0.0%)	1.17	13/2493 (0.5%)
1	kC	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	kD	0.69	0/1836 (0.0%)	1.14	17/2493 (0.7%)
1	kE	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	l	0.87	0/1836 (0.0%)	1.65	10/2493 (0.4%)
1	lA	0.68	0/1836 (0.0%)	1.14	16/2493 (0.6%)
1	lB	0.69	0/1836 (0.0%)	1.20	19/2493 (0.8%)
1	lC	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	lD	0.69	0/1836 (0.0%)	1.12	10/2493 (0.4%)
1	lE	0.69	0/1836 (0.0%)	1.19	17/2493 (0.7%)
1	m	0.87	0/1836 (0.0%)	1.62	14/2493 (0.6%)
1	mA	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	mB	0.69	0/1836 (0.0%)	1.16	17/2493 (0.7%)
1	mC	0.69	0/1836 (0.0%)	1.16	16/2493 (0.6%)
1	mD	0.69	0/1836 (0.0%)	1.07	12/2493 (0.5%)
1	mE	0.69	0/1836 (0.0%)	1.15	17/2493 (0.7%)
1	n	0.86	0/1836 (0.0%)	1.61	6/2493 (0.2%)
1	nA	0.69	0/1836 (0.0%)	1.16	12/2493 (0.5%)
1	nB	0.68	0/1836 (0.0%)	1.09	10/2493 (0.4%)
1	nC	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	nD	0.69	0/1836 (0.0%)	1.08	13/2493 (0.5%)
1	nE	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	o	0.87	0/1836 (0.0%)	1.60	4/2493 (0.2%)
1	oA	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	oB	0.69	0/1836 (0.0%)	1.18	18/2493 (0.7%)
1	oC	0.69	0/1836 (0.0%)	1.14	12/2493 (0.5%)
1	oD	0.68	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	oE	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	p	0.88	0/1836 (0.0%)	1.63	12/2493 (0.5%)
1	pA	0.69	0/1836 (0.0%)	1.16	16/2493 (0.6%)
1	pB	0.69	0/1836 (0.0%)	1.16	13/2493 (0.5%)
1	pC	0.69	0/1836 (0.0%)	1.19	17/2493 (0.7%)
1	pD	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
1	pE	0.69	0/1836 (0.0%)	1.14	15/2493 (0.6%)
1	q	0.88	0/1836 (0.0%)	1.67	14/2493 (0.6%)
1	qA	0.68	0/1836 (0.0%)	1.16	18/2493 (0.7%)
1	qB	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	qC	0.69	0/1836 (0.0%)	1.10	14/2493 (0.6%)
1	qD	0.69	0/1836 (0.0%)	1.19	19/2493 (0.8%)
1	qE	0.69	0/1836 (0.0%)	1.17	15/2493 (0.6%)
1	r	0.86	0/1836 (0.0%)	1.67	18/2493 (0.7%)
1	rA	0.68	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	rB	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
1	rC	0.69	0/1836 (0.0%)	1.16	15/2493 (0.6%)
1	rD	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	rE	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	s	0.88	0/1836 (0.0%)	1.61	8/2493 (0.3%)
1	sA	0.68	0/1836 (0.0%)	1.10	11/2493 (0.4%)
1	sB	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	sC	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
1	sD	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	sE	0.68	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	t	0.86	0/1836 (0.0%)	1.65	16/2493 (0.6%)
1	tA	0.69	0/1836 (0.0%)	1.16	19/2493 (0.8%)
1	tB	0.70	0/1836 (0.0%)	1.14	12/2493 (0.5%)
1	tC	0.69	0/1836 (0.0%)	1.11	12/2493 (0.5%)
1	tD	0.69	0/1836 (0.0%)	1.17	14/2493 (0.6%)
1	tE	0.69	0/1836 (0.0%)	1.09	11/2493 (0.4%)
1	u	0.85	0/1836 (0.0%)	1.61	13/2493 (0.5%)
1	uA	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
1	uB	0.69	0/1836 (0.0%)	1.12	14/2493 (0.6%)
1	uC	0.69	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	uD	0.69	0/1836 (0.0%)	1.17	16/2493 (0.6%)
1	uE	0.69	0/1836 (0.0%)	1.16	16/2493 (0.6%)
1	v	0.87	0/1836 (0.0%)	1.60	12/2493 (0.5%)
1	vA	0.69	0/1836 (0.0%)	1.18	17/2493 (0.7%)
1	vB	0.69	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	vC	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	vD	0.69	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	vE	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
1	w	0.87	0/1836 (0.0%)	1.63	16/2493 (0.6%)
1	wA	0.69	0/1836 (0.0%)	1.14	13/2493 (0.5%)
1	wB	0.68	0/1836 (0.0%)	1.16	18/2493 (0.7%)
1	wC	0.69	0/1836 (0.0%)	1.10	13/2493 (0.5%)
1	wD	0.70	0/1836 (0.0%)	1.10	12/2493 (0.5%)
1	wE	0.69	0/1836 (0.0%)	1.19	15/2493 (0.6%)
1	x	0.87	0/1836 (0.0%)	1.66	10/2493 (0.4%)
1	xA	0.69	0/1836 (0.0%)	1.16	14/2493 (0.6%)
1	xB	0.68	0/1836 (0.0%)	1.15	13/2493 (0.5%)
1	xC	0.70	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	xD	0.69	0/1836 (0.0%)	1.12	16/2493 (0.6%)
1	xE	0.69	0/1836 (0.0%)	1.12	10/2493 (0.4%)
1	y	0.88	0/1836 (0.0%)	1.66	14/2493 (0.6%)
1	yA	0.69	0/1836 (0.0%)	1.18	16/2493 (0.6%)
1	yB	0.69	0/1836 (0.0%)	1.11	13/2493 (0.5%)
1	yC	0.69	0/1836 (0.0%)	1.11	12/2493 (0.5%)
1	yD	0.69	0/1836 (0.0%)	1.07	11/2493 (0.4%)
1	yE	0.68	0/1836 (0.0%)	1.16	17/2493 (0.7%)
1	z	0.87	0/1836 (0.0%)	1.62	11/2493 (0.4%)
1	zA	0.69	0/1836 (0.0%)	1.12	11/2493 (0.4%)
1	zB	0.69	0/1836 (0.0%)	1.16	20/2493 (0.8%)
1	zC	0.70	0/1836 (0.0%)	1.18	18/2493 (0.7%)
1	zD	0.69	0/1836 (0.0%)	1.15	14/2493 (0.6%)
1	zE	0.69	0/1836 (0.0%)	1.12	16/2493 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
All	All	0.72	0/694008 (0.0%)	1.24	5348/942354 (0.6%)

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	Planarity
1	0	0	4
1	0A	0	3
1	0B	0	2
1	0D	0	3
1	0E	0	4
1	1	0	3
1	1B	0	3
1	1C	0	2
1	1D	0	2
1	1E	0	2
1	2	0	5
1	2A	0	1
1	2B	0	2
1	2C	0	3
1	2D	0	3
1	2E	0	1
1	3	0	3
1	3A	0	3
1	3B	0	1
1	3D	0	2
1	3E	0	2
1	4	0	2
1	4A	0	3
1	4C	0	3
1	4D	0	1
1	5	0	2
1	5A	0	2
1	5B	0	1
1	5C	0	2
1	5D	0	1
1	5E	0	3
1	6	0	2
1	6A	0	3
1	6B	0	2

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Mol	Chain	Chirality	Planarity
1	6C	0	2
1	6D	0	2
1	6E	0	2
1	7C	0	2
1	7D	0	3
1	7E	0	3
1	8	0	3
1	8A	0	2
1	8B	0	2
1	8C	0	2
1	8D	0	1
1	8E	0	4
1	9	0	4
1	9A	0	3
1	9B	0	3
1	9C	0	1
1	9D	0	4
1	9E	0	2
1	A	0	3
1	AA	0	2
1	AC	0	3
1	AD	0	2
1	AF	0	1
1	B	0	2
1	BB	0	4
1	BC	0	2
1	BD	0	1
1	BE	0	2
1	BF	0	2
1	C	0	1
1	CA	0	2
1	CB	0	2
1	CC	0	3
1	CD	0	3
1	CE	0	1
1	CF	0	3
1	D	0	3
1	DA	0	5
1	DB	0	1
1	DC	0	2
1	DD	0	3
1	DE	0	1

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Mol	Chain	Chirality	Planarity
1	DF	0	3
1	EA	0	3
1	EB	0	1
1	EC	0	3
1	ED	0	5
1	EE	0	1
1	EF	0	3
1	F	0	1
1	FA	0	1
1	FB	0	3
1	FC	0	4
1	FD	0	2
1	FE	0	2
1	FF	0	5
1	G	0	2
1	GA	0	5
1	GC	0	2
1	GD	0	3
1	H	0	2
1	HA	0	1
1	HB	0	4
1	HC	0	2
1	HD	0	6
1	HE	0	4
1	I	0	1
1	IA	0	2
1	IB	0	3
1	IC	0	2
1	ID	0	4
1	IE	0	2
1	J	0	4
1	JA	0	2
1	JB	0	2
1	JD	0	2
1	JE	0	2
1	K	0	2
1	KA	0	4
1	KB	0	2
1	KC	0	1
1	KE	0	1
1	L	0	1
1	LA	0	1

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Mol	Chain	Chirality	Planarity
1	LC	0	1
1	LD	0	1
1	LE	0	1
1	M	0	3
1	MA	0	1
1	MB	0	1
1	MC	0	2
1	MD	0	2
1	ME	0	1
1	N	0	1
1	NA	0	1
1	NB	0	1
1	NC	0	3
1	O	0	4
1	OA	0	3
1	OB	0	1
1	OC	0	4
1	OD	0	2
1	OE	0	2
1	P	0	5
1	PA	0	1
1	PB	0	3
1	PC	0	3
1	PD	0	2
1	PE	0	1
1	Q	0	1
1	QB	0	2
1	QC	0	1
1	QD	0	1
1	QE	0	2
1	R	0	3
1	RA	0	1
1	RB	0	3
1	RC	0	1
1	RE	0	2
1	S	0	2
1	SA	0	4
1	SB	0	2
1	SD	0	4
1	SE	0	1
1	T	0	2
1	TA	0	1

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Mol	Chain	Chirality	Planarity
1	TB	0	3
1	TC	0	2
1	TD	0	2
1	TE	0	3
1	U	0	3
1	UA	0	1
1	UB	0	2
1	UC	0	5
1	UD	0	1
1	UE	0	2
1	VA	0	1
1	VB	0	3
1	VC	0	3
1	VD	0	2
1	VE	0	1
1	W	0	1
1	WA	0	1
1	WB	0	2
1	WC	0	2
1	WD	0	1
1	WE	0	2
1	X	0	3
1	XA	0	2
1	XB	0	3
1	XC	0	1
1	XD	0	2
1	XE	0	1
1	Y	0	2
1	YA	0	2
1	YB	0	1
1	YD	0	2
1	YE	0	2
1	ZA	0	1
1	ZB	0	5
1	ZC	0	4
1	ZD	0	1
1	a	0	3
1	aA	0	2
1	aB	0	3
1	aC	0	5
1	aD	0	1
1	aE	0	3

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Mol	Chain	Chirality	Planarity
1	b	0	3
1	bA	0	1
1	bB	0	2
1	bC	0	1
1	bD	0	3
1	bE	0	1
1	cA	0	3
1	cB	0	1
1	cC	0	3
1	cD	0	1
1	cE	0	2
1	d	0	1
1	dA	0	2
1	dB	0	1
1	dC	0	4
1	dD	0	2
1	dE	0	2
1	e	0	3
1	eA	0	1
1	eB	0	1
1	eD	0	1
1	eE	0	1
1	f	0	3
1	fA	0	2
1	fB	0	3
1	fC	0	3
1	fD	0	1
1	fE	0	2
1	g	0	2
1	gB	0	2
1	gC	0	3
1	gE	0	2
1	hA	0	3
1	hB	0	2
1	hC	0	1
1	hD	0	5
1	hE	0	2
1	i	0	1
1	iA	0	4
1	iB	0	4
1	iC	0	4
1	iD	0	3

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Mol	Chain	Chirality	Planarity
1	iE	0	4
1	j	0	3
1	jA	0	3
1	jB	0	3
1	jC	0	3
1	jD	0	1
1	jE	0	3
1	k	0	3
1	kA	0	3
1	kB	0	3
1	kC	0	3
1	kD	0	3
1	kE	0	2
1	l	0	3
1	lA	0	1
1	lB	0	2
1	lC	0	5
1	lE	0	4
1	m	0	2
1	mB	0	1
1	mE	0	3
1	n	0	3
1	nA	0	4
1	nB	0	1
1	nC	0	4
1	nD	0	2
1	o	0	1
1	oA	0	1
1	oB	0	2
1	oC	0	3
1	oD	0	1
1	oE	0	3
1	p	0	1
1	pA	0	2
1	pB	0	3
1	pC	0	1
1	pD	0	2
1	pE	0	6
1	q	0	3
1	qA	0	2
1	qC	0	1
1	qD	0	1

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Mol	Chain	Chirality	Planarity
1	qE	0	3
1	r	0	5
1	rA	0	4
1	rC	0	2
1	rD	0	3
1	rE	0	2
1	s	0	2
1	sA	0	2
1	sB	0	1
1	sC	0	1
1	sD	0	2
1	sE	0	4
1	t	0	1
1	tB	0	4
1	tC	0	2
1	tD	0	4
1	tE	0	1
1	u	0	1
1	uA	0	2
1	uB	0	6
1	uC	0	2
1	uD	0	1
1	uE	0	1
1	v	0	3
1	vA	0	2
1	vB	0	1
1	vC	0	2
1	vD	0	1
1	vE	0	2
1	w	0	1
1	wA	0	4
1	wB	0	2
1	wC	0	4
1	wD	0	2
1	wE	0	3
1	x	0	1
1	xA	0	1
1	xB	0	1
1	xC	0	1
1	xD	0	1
1	xE	0	1
1	y	0	1

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Mol	Chain	Chirality	Planarity
1	yA	0	2
1	yB	0	6
1	yC	0	3
1	yD	0	2
1	yE	0	1
1	z	0	2
1	zA	0	4
1	zB	0	3
1	zC	0	2
1	zD	0	2
All	All	0	775

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3E	184	TRP	CB-CG-CD2	-15.41	106.56	126.60
1	jC	173	ARG	NE-CZ-NH1	14.78	127.69	120.30
1	YE	184	TRP	CB-CG-CD2	-14.58	107.64	126.60
1	nA	184	TRP	CB-CG-CD2	-14.01	108.39	126.60
1	DC	162	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	eD	184	TRP	CB-CG-CD1	-13.19	109.85	127.00
1	CD	184	TRP	CB-CG-CD2	-12.97	109.73	126.60
1	PC	18	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	NE	173	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	dB	100	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	EC	173	ARG	NE-CZ-NH1	12.63	126.61	120.30
1	dC	167	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	qC	162	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	IC	162	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	7D	229	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	lE	82	ARG	NE-CZ-NH1	12.37	126.49	120.30
1	GE	184	TRP	CB-CG-CD2	-12.37	110.52	126.60
1	RC	162	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	UB	97	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	2D	100	ARG	NE-CZ-NH1	12.21	126.40	120.30
1	AA	97	ARG	NE-CZ-NH1	12.13	126.37	120.30
1	yC	97	ARG	NE-CZ-NH1	12.09	126.35	120.30
1	TC	82	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	kB	97	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	rC	162	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	BB	167	ARG	NE-CZ-NH1	11.88	126.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	LD	18	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	2A	229	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	OD	154	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	3E	143	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	AE	184	TRP	CB-CG-CD2	-11.79	111.27	126.60
1	KE	18	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	5E	97	ARG	NE-CZ-NH1	11.79	126.19	120.30
1	2C	18	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	SB	167	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	2A	18	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	qE	229	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	EB	97	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	xB	18	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	EB	162	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	RD	132	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	7A	173	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	WB	97	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	FC	143	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	tD	167	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	SA	154	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	UB	18	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	HA	97	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	gB	143	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	aA	154	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	4A	162	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	cC	229	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	yA	162	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	SA	229	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	5E	154	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	kA	132	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	wA	97	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	sC	184	TRP	CB-CG-CD1	-11.36	112.24	127.00
1	BB	100	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	ID	143	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	nA	167	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	SD	100	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	9E	167	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	NA	162	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	mA	184	TRP	CB-CG-CD2	-11.28	111.93	126.60
1	cC	18	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	PB	167	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	9C	173	ARG	NE-CZ-NH1	11.22	125.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vA	162	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	EE	100	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	pB	184	TRP	CB-CG-CD1	-11.19	112.45	127.00
1	OE	100	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	1C	100	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	sE	82	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	tB	100	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	hA	154	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	cE	162	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	nE	97	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	tD	184	TRP	CB-CG-CD2	-11.10	112.17	126.60
1	7D	162	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	SD	229	ARG	NE-CZ-NH2	11.08	125.84	120.30
1	AD	229	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	hE	184	TRP	CB-CG-CD1	-11.07	112.61	127.00
1	XA	173	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	pD	162	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	9A	154	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	6B	18	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	FF	167	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	hC	18	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	IA	18	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	ID	167	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	BC	97	ARG	NE-CZ-NH1	10.99	125.79	120.30
1	9C	162	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	2A	97	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	TD	132	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	pC	132	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	zD	100	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	BE	154	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	iE	162	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	CE	229	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	8E	18	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	JA	18	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	XD	82	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	CC	132	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	UC	132	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	iA	154	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	mA	82	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	lB	154	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	gD	162	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	PA	97	ARG	NE-CZ-NH1	10.81	125.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	MA	100	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	7D	100	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	bB	97	ARG	NE-CZ-NH1	10.77	125.68	120.30
1	xB	162	ARG	NE-CZ-NH1	10.77	125.68	120.30
1	gB	97	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	CF	229	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	zD	167	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	yE	100	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	3E	97	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	rE	162	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	CC	173	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	BF	18	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	8A	162	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	wE	173	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	XE	173	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	DA	173	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	JC	184	TRP	CB-CG-CD2	-10.66	112.74	126.60
1	hA	154	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	oB	184	TRP	CB-CG-CD1	-10.65	113.15	127.00
1	wA	132	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	2B	154	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	vA	167	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	aD	184	TRP	CB-CG-CD2	-10.60	112.83	126.60
1	jD	82	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	EB	167	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	bE	162	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	b	184	TRP	CB-CG-CD1	-10.57	111.04	126.90
1	jA	100	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	2A	229	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	oD	229	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	OB	167	ARG	NE-CZ-NH2	-10.55	115.02	120.30
1	XB	154	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	XA	100	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	dE	167	ARG	NE-CZ-NH1	10.55	125.57	120.30
1	AB	167	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	CC	97	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	QE	18	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	eD	184	TRP	CB-CG-CD2	-10.51	112.93	126.60
1	PE	154	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	DB	132	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	IC	18	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	FE	184	TRP	CB-CG-CD1	-10.50	113.35	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	lB	18	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	TB	97	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	DE	100	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	pA	132	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	7C	82	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	LB	143	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	sC	162	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	FF	18	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	4A	184	TRP	CB-CG-CD2	-10.43	113.05	126.60
1	UD	162	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	UA	82	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	jA	167	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	gE	100	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	rC	100	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	iE	18	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	fE	167	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	kB	18	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	pE	173	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	5C	154	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	YD	143	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	DD	173	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	LA	184	TRP	CB-CG-CD1	-10.36	113.54	127.00
1	jA	154	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	pD	173	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	VD	100	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	lD	97	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	ZE	82	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	FC	143	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	pC	18	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	6E	18	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	6B	162	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	lA	162	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	GB	82	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	PC	97	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	MB	167	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	DC	229	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	iD	162	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	EF	229	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	BA	97	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	QD	143	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	RD	229	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	qD	154	ARG	NE-CZ-NH1	10.28	125.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vC	173	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	aD	143	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	OD	132	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	AF	143	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	BD	82	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	pA	132	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	XA	167	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	7A	100	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	iD	100	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	pB	18	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	hC	100	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	UD	184	TRP	CB-CG-CD1	-10.24	113.69	127.00
1	QB	154	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	GC	154	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	7A	154	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	nC	18	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	9E	184	TRP	CB-CG-CD1	-10.22	113.72	127.00
1	WB	162	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	uD	132	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	QC	82	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	ZE	82	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	hA	184	TRP	CB-CG-CD1	-10.20	113.74	127.00
1	gC	97	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	rA	82	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	oC	18	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	TA	229	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	WD	184	TRP	CB-CG-CD1	-10.19	113.76	127.00
1	QD	229	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	hE	167	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	BE	82	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	lA	18	ARG	NE-CZ-NH1	10.17	125.38	120.30
1	CA	18	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	zD	143	ARG	NE-CZ-NH1	10.15	125.37	120.30
1	fA	132	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	yB	143	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	RB	167	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	zC	97	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	XA	82	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	4C	143	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	FB	162	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	TD	100	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	WD	229	ARG	NE-CZ-NH1	10.10	125.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EC	82	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	ED	184	TRP	CB-CG-CD1	-10.09	113.89	127.00
1	9B	154	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	BE	82	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	mE	154	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	FB	82	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	UA	97	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	ID	143	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	vD	162	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	WB	184	TRP	CB-CG-CD1	-10.06	113.92	127.00
1	jB	100	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	mB	167	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	YA	162	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	kD	143	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	XE	100	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	pB	132	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	JC	100	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	SD	162	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	gD	173	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	rA	97	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	3C	97	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	mC	100	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	iC	18	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	eC	18	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	IB	162	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	mC	173	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	vD	173	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	GE	18	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	3C	229	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	DC	82	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	PE	173	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	4A	143	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	KE	82	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	3E	162	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	vB	154	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	gB	100	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	4B	100	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	cA	173	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	ND	154	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	xA	97	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	3B	173	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	0E	132	ARG	NE-CZ-NH1	9.91	125.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	184	TRP	CB-CG-CD2	-9.91	112.92	126.80
1	hD	132	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	uD	154	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	AE	173	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	zE	100	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	gB	132	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	0D	184	TRP	CB-CG-CD1	-9.90	114.13	127.00
1	NB	229	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	CD	143	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	IB	18	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	cC	82	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	GA	167	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	1A	173	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	8C	229	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	ZD	173	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	vA	167	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	XD	132	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	cE	18	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	qB	162	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	cB	97	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	a	184	TRP	CB-CG-CD2	9.85	140.59	126.80
1	kA	143	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	fB	162	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	ZB	167	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	ID	97	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	EE	82	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	CC	162	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	2B	82	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	oC	167	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	BE	229	ARG	NE-CZ-NH2	9.80	125.20	120.30
1	ED	100	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	TD	167	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	uC	167	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	iD	167	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	GC	167	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	XD	82	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	gA	100	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	FD	167	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	TE	162	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	3B	154	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	PB	173	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	7A	184	TRP	CB-CG-CD1	-9.75	114.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	rC	173	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	gE	82	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	cD	100	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	2D	184	TRP	CB-CG-CD2	9.74	139.26	126.60
1	1E	162	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	EA	154	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	fD	100	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	eD	100	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	RA	229	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	iA	97	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	LB	167	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	IC	97	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	lA	162	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	aD	229	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	dE	162	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	tB	229	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	GA	167	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	CA	18	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	DD	162	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	FC	154	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	LE	167	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	JA	154	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	XD	167	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	aA	18	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	UC	18	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	dA	18	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	fC	18	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	WA	18	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	sB	154	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	AA	173	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	xA	162	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	tE	167	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	fB	82	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	bE	82	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	CC	132	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	jB	154	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	uA	97	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	cA	184	TRP	CB-CG-CD1	-9.63	114.48	127.00
1	RC	100	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	0B	154	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	KE	184	TRP	CB-CG-CD1	-9.62	114.49	127.00
1	4B	173	ARG	NE-CZ-NH1	9.62	125.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ND	154	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	JD	97	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	PE	82	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	9D	97	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	qE	173	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	DA	184	TRP	CB-CG-CD1	-9.61	114.50	127.00
1	gC	100	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	aD	82	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	7B	162	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	dA	100	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	YC	97	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	FE	167	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	sE	162	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	DD	229	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	ZD	167	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	lE	97	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	CC	229	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	HA	167	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	5A	184	TRP	CB-CG-CD1	-9.57	114.55	127.00
1	UA	173	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	UA	143	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	4D	173	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	KA	100	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	ZC	97	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	JC	184	TRP	CB-CG-CD1	-9.56	114.57	127.00
1	3A	18	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	5C	229	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	OD	154	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	sA	143	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	3D	173	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	9D	97	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	qB	97	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	oC	162	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	OA	100	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	KB	173	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	3E	100	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	BA	82	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	dA	100	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	OE	162	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	bD	18	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	OA	184	TRP	CB-CG-CD2	-9.51	114.24	126.60
1	5A	162	ARG	NE-CZ-NH1	9.51	125.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	OB	154	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	MA	82	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	AB	97	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	wD	154	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	rD	162	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	7D	173	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	2D	184	TRP	CB-CG-CD1	-9.49	114.66	127.00
1	CE	132	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	VE	132	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	IA	132	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	yA	18	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	4C	167	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	PD	97	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	zD	162	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	qE	97	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	1B	154	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	9D	173	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	eB	18	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	9D	82	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	vB	229	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	HC	82	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	nE	18	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	bA	82	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	JD	173	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	yC	154	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	ID	97	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	CE	100	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	9B	18	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	JC	132	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	dD	82	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	WA	97	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	xA	18	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	xC	82	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	RE	173	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	rB	184	TRP	CB-CG-CD1	-9.43	114.74	127.00
1	2E	162	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	QC	100	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	AE	154	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	xB	100	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	jB	100	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	5A	167	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	8D	173	ARG	NE-CZ-NH1	9.41	125.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	pA	162	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	wE	167	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	qE	82	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	zB	143	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	aE	184	TRP	CB-CG-CD1	-9.40	114.78	127.00
1	tE	143	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	fE	162	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	lB	82	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	aD	18	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	lA	132	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	YB	18	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	FE	162	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	nC	18	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	AE	100	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	2E	97	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	sA	18	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	BC	162	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	uC	162	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	pE	82	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	WD	154	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	sD	162	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	RA	154	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	4E	100	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	ME	18	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	kE	167	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	EA	229	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	YC	167	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	6A	154	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	JB	162	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	6B	184	TRP	CB-CG-CD1	-9.31	114.90	127.00
1	OE	229	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	PE	100	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	UC	97	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	BB	132	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	8D	132	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	QE	143	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	PA	100	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	2B	82	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	CD	18	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	LB	18	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	GC	173	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	qC	154	ARG	NE-CZ-NH1	9.28	124.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	xC	132	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	wA	100	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	4C	184	TRP	CB-CG-CD1	-9.27	114.95	127.00
1	PD	100	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	3E	82	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	QA	100	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	xE	154	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	LB	97	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	rB	18	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	9D	154	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	2A	100	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	YE	229	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	MD	154	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	eC	184	TRP	CB-CG-CD1	-9.25	114.98	127.00
1	bD	143	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	4C	154	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	lE	184	TRP	CB-CG-CD2	-9.24	114.59	126.60
1	LB	82	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	jD	100	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	xE	100	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	gD	132	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	jE	100	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	JD	154	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	AC	167	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	UD	100	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	7A	97	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	SA	184	TRP	CB-CG-CD1	-9.22	115.02	127.00
1	CA	132	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	rD	100	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	IB	154	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	lE	100	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	sB	173	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	kC	229	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	JE	100	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	ME	143	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	qD	167	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	WE	132	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	bC	18	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	CF	167	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	OB	132	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	WC	82	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	0C	97	ARG	NE-CZ-NH1	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	TD	100	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	aB	167	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	BD	167	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	cE	184	TRP	CB-CG-CD1	-9.18	115.06	127.00
1	AC	132	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	iC	229	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	DE	229	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	yA	97	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	HB	97	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	aC	167	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	QC	143	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	dA	229	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	qB	173	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	CE	132	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	HE	167	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	eB	229	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	UE	184	TRP	CB-CG-CD1	-9.17	115.08	127.00
1	pA	100	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	5C	100	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	1E	173	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	vB	167	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	SA	162	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	nE	184	TRP	CB-CG-CD1	-9.15	115.10	127.00
1	IB	229	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	nE	82	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	AC	184	TRP	CB-CG-CD1	-9.14	115.11	127.00
1	qE	184	TRP	CB-CG-CD1	-9.14	115.11	127.00
1	uE	154	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	BA	154	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	pC	143	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	xD	132	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	EF	97	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	HA	173	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	0C	18	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	UC	173	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	0E	18	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	WB	143	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	9C	97	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	5A	154	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	YA	18	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	WB	143	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	hC	167	ARG	NE-CZ-NH1	9.12	124.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	xE	229	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	GD	184	TRP	CB-CG-CD1	-9.11	115.15	127.00
1	gC	173	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	qD	167	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	NE	143	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	MD	229	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	uC	167	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	7	184	TRP	CB-CG-CD1	-9.10	113.25	126.90
1	NB	167	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	iA	184	TRP	CB-CG-CD2	-9.09	114.78	126.60
1	tA	154	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	kB	162	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	TA	143	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	SE	154	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	GD	184	TRP	CB-CG-CD2	9.08	138.40	126.60
1	wB	97	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	TD	162	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	KA	82	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	yB	162	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	oB	132	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	8C	184	TRP	CB-CG-CD1	-9.06	115.22	127.00
1	0A	132	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	gE	18	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	mA	167	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	CB	18	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	uE	173	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	vC	154	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	cC	97	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	EA	167	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	0A	184	TRP	CB-CG-CD1	-9.04	115.25	127.00
1	QE	173	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	ID	82	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	UB	167	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	yB	18	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	ID	154	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	nE	154	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	pC	100	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	uD	167	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	DE	154	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	rA	132	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	1D	229	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	cB	18	ARG	NE-CZ-NH1	9.02	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	pB	100	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	EF	82	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	DA	100	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	6B	229	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	5E	173	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	8E	167	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	iE	132	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	PA	167	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	pA	167	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	BF	18	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	fC	162	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	lB	229	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	2E	18	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	AD	229	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	lC	143	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	kE	132	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	mE	184	TRP	CB-CG-CD1	-8.99	115.31	127.00
1	xC	132	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	mE	167	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	2A	82	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	yE	154	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	IA	143	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	7B	167	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	gD	18	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	UB	82	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	GD	100	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	kB	229	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	7C	18	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	LD	173	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	8E	229	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	5B	154	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	sD	229	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	UC	82	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	5C	167	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	eC	18	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	tC	97	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	5D	229	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	8B	100	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	TC	229	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	WC	162	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	OE	154	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	xA	82	ARG	NE-CZ-NH1	8.95	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BB	167	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	iC	132	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	0E	143	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	8C	154	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	BC	167	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	pC	100	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	OB	82	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	7B	229	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	SD	143	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	zA	229	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	YD	173	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	jB	132	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	vC	162	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	7D	154	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	ZA	100	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	vC	173	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	qE	143	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	5D	97	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	5D	173	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	aB	154	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	rD	154	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	AF	154	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	1D	132	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	LC	82	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	8A	100	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	mB	100	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	OE	184	TRP	CB-CG-CD1	-8.91	115.42	127.00
1	JA	162	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	SA	143	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	YA	100	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	3A	184	TRP	CB-CG-CD1	-8.90	115.43	127.00
1	xC	143	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	cD	82	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	iA	162	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	ZA	229	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	5C	82	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	bC	82	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	8A	167	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	ZB	82	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	TB	229	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	gD	184	TRP	CB-CG-CD1	-8.88	115.46	127.00
1	LE	100	ARG	NE-CZ-NH2	-8.88	115.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	gD	100	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	DB	97	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	CA	97	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	IA	167	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	EA	132	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	qB	82	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	IB	229	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	cE	97	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	zC	154	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	pB	167	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	nC	162	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	5A	132	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	8B	82	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	8C	184	TRP	CB-CG-CD2	8.85	138.10	126.60
1	eE	154	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	pE	18	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	mC	143	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	fD	82	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	KB	143	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	uD	229	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	SA	162	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	6A	132	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	7A	229	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	LB	100	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	wE	132	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	FC	82	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	eC	132	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	cA	97	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	5A	100	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	BA	132	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	nB	229	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	tA	229	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	gC	184	TRP	CB-CG-CD1	-8.82	115.53	127.00
1	1D	154	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	3D	18	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	GB	18	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	UB	184	TRP	CB-CG-CD1	-8.81	115.55	127.00
1	FA	229	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	OB	167	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	GB	173	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	EB	173	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	CC	154	ARG	NE-CZ-NH1	8.80	124.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2D	167	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	jB	82	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	1A	162	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	IC	167	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	ED	18	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	r	184	TRP	CB-CG-CD1	-8.79	113.72	126.90
1	mB	18	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	ED	82	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	PD	100	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	7D	18	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	TE	82	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	tD	18	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	fB	130	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	wB	82	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	HB	100	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	VB	173	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	SC	167	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	k	230	VAL	N-CA-C	8.78	119.57	110.62
1	CF	173	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	MA	184	TRP	CB-CG-CD1	-8.77	115.59	127.00
1	qA	162	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	mB	18	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	uE	100	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	cC	143	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	NB	18	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	hB	167	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	9B	162	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	XC	100	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	6E	82	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	CF	154	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	CC	18	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	IA	154	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	yC	162	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	XC	97	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	fD	162	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	VC	154	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	pC	229	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	sC	97	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	WC	143	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	fA	132	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	jB	132	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	5D	154	ARG	NE-CZ-NH1	8.74	124.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	rB	229	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	kD	18	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	6A	97	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	8C	162	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	xD	132	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	qB	18	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	7C	167	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	hD	100	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	kD	229	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	qD	132	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	UE	143	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	eE	18	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	a	184	TRP	CB-CG-CD1	-8.72	113.81	126.90
1	dA	167	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	PC	100	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	dC	154	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	rC	100	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	wD	173	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	PE	184	TRP	CB-CG-CD1	-8.72	115.66	127.00
1	VA	154	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	zC	184	TRP	CB-CG-CD1	-8.72	115.67	127.00
1	VA	229	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	nA	97	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	JE	82	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	aA	132	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	oE	184	TRP	CB-CG-CD1	-8.71	115.67	127.00
1	2A	100	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	0B	82	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	kE	97	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	YE	132	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	CA	167	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	jA	173	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	2	184	TRP	CB-CG-CD1	-8.70	113.86	126.90
1	VC	82	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	uD	18	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	yE	18	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	eD	229	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	xC	184	TRP	CB-CG-CD1	-8.68	115.71	127.00
1	iD	82	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	W	86	VAL	N-CA-C	8.68	119.47	110.62
1	gC	173	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	eC	154	ARG	NE-CZ-NH1	8.68	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	rE	97	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	2A	184	TRP	CB-CG-CD1	-8.68	115.72	127.00
1	lA	167	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	nD	173	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	iE	154	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	NA	229	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	JB	167	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	5C	162	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	fA	100	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	PC	162	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	tB	167	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	FE	173	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	FD	97	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	hB	167	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	AC	173	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	qD	173	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	SE	18	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	0E	100	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	HA	82	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	oA	132	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	mA	173	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	xE	18	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	oB	143	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	vE	82	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	fB	100	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	aB	184	TRP	CB-CG-CD1	-8.63	115.78	127.00
1	kB	130	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	yD	132	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	iE	154	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	4D	162	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	BE	143	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	VB	154	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	AC	132	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	qA	18	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	jC	154	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	3D	154	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	xC	162	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	3C	143	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	EB	162	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	vB	100	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	CF	143	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	iA	100	ARG	NE-CZ-NH1	8.61	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bB	154	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	RC	82	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	pD	143	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	TA	154	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	7E	100	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	0A	82	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	zB	162	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	JC	97	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	mE	18	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	zC	173	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	GE	132	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	RC	97	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	hA	18	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	5C	229	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	TD	173	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	XD	132	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	yE	18	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	S	184	TRP	CB-CG-CD1	-8.59	114.02	126.90
1	KA	173	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	NB	229	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	2E	82	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	CD	229	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	nD	18	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	SE	173	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	IB	82	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	eC	173	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	FB	143	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	SA	143	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	HC	162	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	sE	143	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	jB	154	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	zA	173	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	RE	154	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	iA	167	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	8D	167	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	FE	229	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	6A	100	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	XC	167	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	kA	162	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	hC	82	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	bD	18	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	pE	100	ARG	NE-CZ-NH1	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	130	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	3B	154	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	YE	82	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	lB	82	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	iA	18	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	nD	154	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	DF	18	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	kE	143	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	5E	18	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	2A	162	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	1E	97	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	EF	167	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	lC	132	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	xD	143	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	CB	229	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	JB	82	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	TB	162	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	ND	82	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	lB	97	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	9A	132	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	WB	173	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	SC	97	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	RD	154	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	UE	82	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	kC	100	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	2E	100	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	XA	97	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	WC	100	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	lA	154	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	0A	229	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	TE	100	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	sA	132	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	zA	18	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	eC	100	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	7C	184	TRP	CB-CG-CD2	-8.48	115.58	126.60
1	OD	132	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	6A	162	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	DB	167	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	9B	97	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	QD	184	TRP	CB-CG-CD1	-8.47	115.98	127.00
1	2E	154	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	RE	132	ARG	NE-CZ-NH2	-8.47	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	mE	18	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	6D	97	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	iB	82	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	uE	143	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	UD	143	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	yA	184	TRP	CB-CG-CD1	-8.46	116.01	127.00
1	ZB	162	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	IC	100	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	DC	167	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	DD	229	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	hE	162	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	VD	18	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	nD	97	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	rE	18	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	0E	18	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	XD	143	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	2D	82	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	IE	100	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	NE	132	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	1A	167	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	ZA	18	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	WB	100	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	rD	97	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	hB	184	TRP	CB-CG-CD1	-8.43	116.04	127.00
1	oA	97	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	GB	97	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	VB	97	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	wB	132	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	192	GLN	N-CA-C	8.42	120.46	111.28
1	EA	162	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	FA	162	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	aA	132	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	wC	167	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	VD	229	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	hB	154	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	LC	18	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	ZB	132	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	SD	173	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	oE	154	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	wE	97	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	kD	82	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	PB	162	ARG	NE-CZ-NH1	8.41	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CF	100	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	DE	184	TRP	CB-CG-CD1	-8.41	116.07	127.00
1	xE	162	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	YA	97	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	1A	132	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	PB	97	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	RA	229	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	0C	97	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	OB	82	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	8B	132	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	fC	173	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	gB	100	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	6B	82	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	QC	18	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	1E	132	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	TA	18	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	mB	184	TRP	CB-CG-CD1	-8.39	116.09	127.00
1	CE	229	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	fC	97	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	8C	100	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	vA	82	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	HC	167	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	2E	154	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	OC	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	dD	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	tA	229	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	FD	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	5D	100	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	JB	132	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	xE	143	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	DF	162	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	vA	100	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	YB	130	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	aC	167	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	8D	18	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	SE	82	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	hE	162	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	TB	154	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	jC	18	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	7A	82	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	dC	167	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	YD	18	ARG	NE-CZ-NH1	8.36	124.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FF	184	TRP	CB-CG-CD2	-8.36	115.73	126.60
1	KE	154	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	8E	167	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	QA	154	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	oA	229	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	2A	184	TRP	CB-CG-CD2	8.35	137.45	126.60
1	wB	18	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	tC	154	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	wD	18	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	MC	154	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	ND	100	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	qD	82	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	lB	167	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	JE	82	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	t	184	TRP	CB-CG-CD1	-8.34	114.40	126.90
1	lB	130	TYR	CB-CG-CD2	8.34	126.00	121.00
1	OC	82	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	BC	167	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	hC	154	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	EF	154	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	LD	167	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	fA	143	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	KB	97	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	oC	143	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	mA	132	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	7D	167	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	lA	82	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	GB	184	TRP	CB-CG-CD1	-8.32	116.19	127.00
1	kC	18	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	WA	167	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	JC	82	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	4D	154	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	lA	100	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	KC	82	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	NB	173	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	TA	100	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	pB	229	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	sD	229	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	WC	154	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	lD	100	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	oD	184	TRP	CB-CG-CD1	-8.30	116.21	127.00
1	0A	130	TYR	CB-CG-CD2	-8.29	116.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5B	18	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	FC	132	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	0C	229	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	wB	100	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	fD	173	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	wE	154	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	qA	97	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	eC	143	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	N	189	LEU	N-CA-C	8.28	119.93	111.07
1	KA	97	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	8B	143	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	NC	132	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	JD	173	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	cB	143	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	eC	143	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	uC	143	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	TD	154	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	OB	18	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	GC	132	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	6D	184	TRP	CB-CG-CD1	-8.26	116.26	127.00
1	jA	97	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	FB	97	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	FB	173	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	AD	154	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	sC	154	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	uD	173	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	9B	184	TRP	CB-CG-CD1	-8.25	116.27	127.00
1	gE	184	TRP	CB-CG-CD1	-8.25	116.28	127.00
1	PA	162	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	8A	100	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	oD	167	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	bB	162	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	bC	167	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	gE	100	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	lC	154	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	CD	143	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	YB	184	TRP	CB-CG-CD1	-8.24	116.29	127.00
1	YD	184	TRP	CB-CG-CD1	-8.24	116.29	127.00
1	bD	132	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	vE	154	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	gE	132	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	PA	130	TYR	CB-CG-CD2	-8.23	116.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bB	173	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	pD	100	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	HA	143	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	OB	162	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	YB	162	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	xA	100	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	EE	18	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	3B	82	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	oE	162	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	qE	100	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	MA	97	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	RC	154	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	RD	162	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	oE	132	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	cA	100	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	AA	184	TRP	CB-CG-CD1	-8.21	116.32	127.00
1	KA	184	TRP	CB-CG-CD1	-8.21	116.32	127.00
1	pC	162	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	cD	132	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	5E	229	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	YE	154	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	ZA	162	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	sA	167	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	OD	229	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	SD	154	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	JC	162	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	kD	97	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	YC	229	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	rD	82	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	eE	167	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	pE	167	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	oB	229	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	nC	143	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	GD	82	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	OC	132	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	ID	100	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	PC	82	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	bD	100	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	KE	18	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	3A	82	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	xB	132	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	EB	154	ARG	NE-CZ-NH1	8.18	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	111	LEU	N-CA-C	8.18	119.82	111.07
1	oC	18	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	bA	154	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	OB	100	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	MC	173	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	iC	97	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	iD	97	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	yE	82	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	qC	82	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	tC	167	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	XB	100	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	7E	229	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	fB	100	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	yD	143	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	rC	82	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	yE	167	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	2E	132	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	MB	82	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	2C	132	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	RE	97	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	aE	229	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	0A	82	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	mD	167	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	xB	82	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	zC	82	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	yB	167	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	jD	162	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	GE	229	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	FA	82	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	dA	167	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	8A	82	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	lC	154	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	FD	82	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	oE	154	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	JA	82	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	uC	18	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	iA	154	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	DA	18	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	nD	162	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	LE	184	TRP	CB-CG-CD1	-8.13	116.43	127.00
1	OE	167	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	XE	82	ARG	NE-CZ-NH2	-8.13	116.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	154	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	QD	18	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	1C	97	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	bD	229	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	PA	143	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	hE	167	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	LB	82	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	9B	173	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	0C	132	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	wD	143	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	h	184	TRP	CB-CG-CD1	-8.11	114.73	126.90
1	vA	229	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	jD	82	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	fE	154	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	qA	162	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	FA	97	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	aA	82	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	KB	132	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	YB	100	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	uD	100	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	yD	18	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	IE	167	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	QE	82	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	gE	132	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	JD	167	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	5E	97	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	KA	162	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	RA	154	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	JD	162	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	UE	97	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	lE	162	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	zE	162	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	xC	184	TRP	CB-CG-CD2	8.10	137.13	126.60
1	9C	82	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	BF	132	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	tA	167	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	NA	100	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	VA	184	TRP	CB-CG-CD1	-8.09	116.48	127.00
1	XB	82	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	KC	184	TRP	CB-CG-CD1	-8.09	116.48	127.00
1	dE	97	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	kB	173	ARG	NE-CZ-NH1	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	oB	100	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	SD	184	TRP	CB-CG-CD1	-8.09	116.48	127.00
1	BD	184	TRP	CB-CG-CD2	8.09	137.12	126.60
1	DB	100	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	vD	97	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	FB	100	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	ND	184	TRP	CB-CG-CD1	-8.08	116.49	127.00
1	6E	229	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	IC	18	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	DE	18	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	TB	100	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	9B	82	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	VD	184	TRP	CB-CG-CD1	-8.08	116.50	127.00
1	eA	154	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	YC	132	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	8D	167	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	lE	82	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	WE	143	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	YA	82	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	fE	82	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	PD	229	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	rD	167	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	FB	82	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	VC	18	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	YE	154	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	QA	229	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	JA	167	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	AC	18	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	iA	18	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	XD	154	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	cD	18	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	UE	100	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	VE	100	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	ZC	154	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	FE	97	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	kA	154	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	uD	97	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	NB	154	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	fE	100	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	rA	167	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	JE	97	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	PA	130	TYR	CB-CG-CD1	8.04	125.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9A	18	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	YB	132	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	MC	154	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	tD	162	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	TE	18	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	UA	154	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	yE	132	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	WA	162	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	oB	18	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	VC	229	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	5D	18	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	xA	229	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	lB	130	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	wE	82	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	OD	100	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	KE	162	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	CA	100	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	IB	167	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	HD	97	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	cA	184	TRP	N-CA-CB	-8.02	96.16	110.60
1	iD	132	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	dD	173	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	7	195	ASN	CA-CB-CG	8.02	120.62	112.60
1	VA	132	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	8A	154	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	oD	132	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	t	121	ASN	CA-CB-CG	8.01	120.61	112.60
1	BA	154	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	FA	132	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	kA	100	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	3A	130	TYR	CB-CG-CD1	8.01	125.81	121.00
1	UB	154	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	xD	173	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	GE	162	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	XC	132	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	dC	143	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	7C	162	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	cD	162	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	NA	82	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	fB	97	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	mC	97	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	qC	97	ARG	NE-CZ-NH1	8.01	124.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	lE	229	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	ZB	100	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	XC	154	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	fC	132	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	9A	173	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	NA	132	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	BD	100	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	fD	229	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	XE	82	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	rA	154	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	4B	97	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	KC	97	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	zA	154	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	ID	82	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	vD	97	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	wB	82	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	6B	132	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	lE	82	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	lA	154	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	oC	162	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	DF	173	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	kB	132	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	kC	132	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	rC	18	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	LD	100	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	9B	100	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	qE	97	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	HA	229	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	uE	143	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	9C	229	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	pD	162	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	AE	167	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	zE	162	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	AF	229	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	ZD	167	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	oA	167	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	tB	82	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	hD	132	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	JE	167	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	BA	100	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	bB	97	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	2C	132	ARG	NE-CZ-NH1	7.96	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	VE	143	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	ED	167	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	5A	143	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	FD	100	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	DE	82	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	a	184	TRP	N-CA-CB	-7.95	97.44	110.40
1	qD	18	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	rE	82	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	ND	132	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	IE	18	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	hA	143	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	CD	154	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	WE	100	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	bD	162	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	KA	97	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	yA	167	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	4D	132	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	2E	82	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	JB	154	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	wB	167	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	RE	82	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	uD	167	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	4D	132	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	NB	100	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	6B	132	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	SB	162	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	zB	100	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	tC	229	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	5D	18	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	qA	229	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	pB	97	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	UC	184	TRP	CB-CG-CD1	-7.93	116.69	127.00
1	nC	167	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	xD	229	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	TC	132	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	cC	167	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	LD	97	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	OE	229	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	4E	18	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	LA	132	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	nA	18	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	KA	132	ARG	NE-CZ-NH1	7.92	124.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2C	167	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	0B	184	TRP	CB-CG-CD1	-7.92	116.70	127.00
1	XD	97	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	cD	18	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	tD	154	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	qB	97	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	qE	143	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	lB	100	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	mA	167	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	TB	18	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	zC	100	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	4C	97	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	xE	143	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	DF	82	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	ZB	130	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	OA	229	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	SB	18	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	zB	184	TRP	CB-CG-CD1	-7.90	116.73	127.00
1	HC	154	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	rD	97	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	FB	18	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	fB	184	TRP	CB-CG-CD1	-7.90	116.73	127.00
1	LD	18	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	vE	132	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	bC	162	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	gE	173	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	gA	154	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	wE	143	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	lB	97	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	sD	130	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	qD	82	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	cA	229	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	JB	173	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	FB	184	TRP	CB-CG-CD1	-7.87	116.77	127.00
1	2D	18	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	7D	229	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	l	184	TRP	CB-CG-CD1	-7.87	115.09	126.90
1	fD	97	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	MA	132	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	0E	154	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	gD	143	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	u	184	TRP	CB-CG-CD1	-7.87	115.10	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	fB	18	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	1D	18	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	YE	167	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	VD	154	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	WD	100	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	XE	154	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	LE	100	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	UA	97	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	wA	229	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	yC	100	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	vE	167	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	xA	154	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	FB	229	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	0A	100	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	jE	100	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	vD	82	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	zA	167	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	1A	143	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	FB	97	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	bB	18	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	wC	229	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	WE	82	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	9A	229	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	rA	154	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	QB	184	TRP	CB-CG-CD1	-7.84	116.81	127.00
1	IC	82	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	cD	162	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	RE	154	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	2B	184	TRP	CB-CG-CD2	-7.84	116.41	126.60
1	0C	229	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	7C	154	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	tA	154	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	QD	97	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	zE	167	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	dA	132	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	AA	154	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	gB	162	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	AF	184	TRP	CB-CG-CD1	-7.83	116.82	127.00
1	rB	97	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	YC	82	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	jA	184	TRP	CB-CG-CD1	-7.83	116.83	127.00
1	kC	167	ARG	NE-CZ-NH1	7.83	124.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SA	82	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	DD	82	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	a	184	TRP	CA-CB-CG	7.82	128.46	113.60
1	VD	162	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	dA	173	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	oC	167	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	3D	18	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	VE	173	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	uA	132	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	3D	173	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	uC	100	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	tB	154	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	tB	162	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	gD	18	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	qE	229	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	EB	100	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	3B	100	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	4D	18	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	GE	143	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	ZE	18	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	CC	82	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	kC	82	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	fA	18	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	mC	132	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	IE	173	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	bA	100	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	yA	143	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	8A	18	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	dA	162	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	zB	82	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	qC	154	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	RE	229	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	J	195	ASN	CA-CB-CG	7.79	120.39	112.60
1	fD	167	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	6C	97	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	YD	100	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	PB	229	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	CD	173	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	wA	82	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	MD	154	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	aE	167	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	XA	82	ARG	NE-CZ-NH2	-7.78	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	jD	132	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	fB	130	TYR	CB-CG-CD1	7.78	125.67	121.00
1	4B	162	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	3A	82	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	7B	154	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	BE	100	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	FE	132	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	AA	162	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	eA	229	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	qA	229	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	xB	229	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	YC	162	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	QD	143	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	bE	82	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	eE	100	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	8A	145	TYR	CB-CG-CD2	-7.77	116.34	121.00
1	iD	154	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	pD	154	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	TE	162	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	iD	162	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	1A	97	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	rB	229	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	sA	173	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	iB	184	TRP	CB-CG-CD1	-7.76	116.92	127.00
1	mC	162	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	qC	82	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	eD	143	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	jE	154	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	lB	97	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	CC	97	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	3C	100	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	qD	100	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	sD	100	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	zD	132	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	SE	167	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	uB	132	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	oB	154	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	uE	132	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	DA	162	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	6A	18	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	GD	132	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	0E	100	ARG	NE-CZ-NH2	-7.74	116.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ND	229	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	HA	143	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	EC	132	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	wE	100	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	1C	18	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	7C	97	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	HC	82	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	iC	100	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	kD	173	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	tD	97	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	RE	18	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	ZB	97	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	UD	154	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	kB	130	TYR	CB-CG-CD1	7.73	125.64	121.00
1	JE	184	TRP	CB-CG-CD1	-7.73	116.95	127.00
1	hB	162	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	HC	143	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	QA	173	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	pA	18	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	uB	143	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	AD	143	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	BB	18	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	VC	100	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	2C	82	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	2A	167	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	BD	167	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	IE	162	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	KD	132	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	0B	154	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	FA	97	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	UA	100	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	4B	82	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	QA	18	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	cA	184	TRP	CA-CB-CG	7.71	128.34	113.70
1	QB	167	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	dA	154	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	uA	82	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	1B	132	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	EC	132	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	aC	229	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	K	184	TRP	CB-CG-CD1	-7.70	115.34	126.90
1	vA	162	ARG	NE-CZ-NH2	-7.70	116.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bD	154	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	dA	18	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	nA	100	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	4A	18	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	eB	173	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	FD	97	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	7A	18	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	JC	18	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	lC	167	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	wC	132	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	dE	184	TRP	CB-CG-CD1	-7.70	116.99	127.00
1	KD	229	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	iA	173	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	JB	100	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	lB	132	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	KB	132	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	fD	132	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	DF	97	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	rE	82	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	fD	143	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	fD	173	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	uE	82	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	4D	167	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	wE	132	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	sC	82	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	DB	162	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	JC	154	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	0A	100	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	qB	100	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	xB	97	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	jE	173	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	FA	132	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	gC	82	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	5D	162	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	l	36	VAL	CA-C-N	7.67	125.07	120.24
1	l	36	VAL	C-N-CA	7.67	125.07	120.24
1	4A	229	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	WB	162	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	VA	229	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	dA	143	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	SE	229	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	mE	100	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vC	143	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	ZD	162	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	LD	162	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	XA	143	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	xC	162	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	4D	82	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	dC	173	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	JB	132	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	WB	154	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	cA	167	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	uB	184	TRP	CB-CG-CD2	-7.64	116.67	126.60
1	8A	97	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	0A	130	TYR	CB-CG-CD1	7.64	125.58	121.00
1	7A	167	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	jC	132	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	sC	167	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	lC	97	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	VD	97	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	yC	97	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	EF	82	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	7E	162	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	yA	143	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	9A	132	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	SE	167	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	xE	97	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	cD	97	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	j	81	ASP	CA-CB-CG	7.62	120.22	112.60
1	ZD	97	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	qA	132	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	eE	132	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	tD	173	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	EE	162	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	7E	132	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	CC	143	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	vB	154	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	RE	132	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	VB	229	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	vD	100	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	vB	82	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	xC	229	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	fD	162	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	bB	100	ARG	NE-CZ-NH1	7.61	124.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	mA	132	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	pE	173	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	hE	173	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	hA	167	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	6C	100	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	iD	154	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	wE	154	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	mE	229	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	tA	173	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	UB	143	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	oB	82	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	NE	162	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	lE	130	TYR	CB-CG-CD2	-7.59	116.44	121.00
1	6B	154	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	TC	167	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	4C	132	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	VD	82	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	WB	82	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	fE	154	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	DA	162	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	FA	18	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	WA	154	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	yB	132	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	EC	97	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	dC	229	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	wC	162	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	8E	18	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	bB	132	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	EB	154	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	3C	162	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	CF	82	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	RD	100	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	5	184	TRP	CB-CG-CD1	-7.57	115.54	126.90
1	zB	82	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	iB	82	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	zD	82	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	RA	173	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	3D	229	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	MC	143	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	5C	18	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	wB	154	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	bA	100	ARG	NE-CZ-NH2	-7.56	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	nB	154	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	2C	162	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	nD	100	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	vC	229	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	iC	82	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	vD	154	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	1D	132	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	kE	229	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	fA	167	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	ZD	82	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	SA	154	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	YA	18	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	OE	167	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	ZE	229	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	PD	132	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	LC	162	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	uC	18	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	aD	184	TRP	N-CA-CB	-7.54	97.03	110.60
1	sC	18	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	jD	162	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	kD	100	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	tE	18	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	MB	18	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	DC	97	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	SE	97	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	cA	162	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	uD	184	TRP	CB-CG-CD1	-7.54	117.20	127.00
1	4A	184	TRP	CB-CG-CD1	-7.53	117.21	127.00
1	iE	229	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	MD	184	TRP	CB-CG-CD1	-7.53	117.21	127.00
1	0D	18	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	KD	143	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	ZD	154	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	xD	173	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	TD	132	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	eD	132	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	XC	82	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	2C	82	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	zD	154	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	jD	132	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	CE	167	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	NE	18	ARG	NE-CZ-NH1	7.52	124.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	167	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	ND	143	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	bD	167	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	LD	132	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	vC	154	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	HD	97	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	PE	162	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	pE	132	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	jD	18	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	DC	18	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	FF	173	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	4B	132	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	oD	100	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	bE	97	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	1A	100	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	4A	97	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	FB	173	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	189	LEU	N-CA-C	7.50	119.45	111.28
1	cA	143	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	CC	143	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	dC	100	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	nC	82	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	cE	167	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	iA	229	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	fC	97	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	GE	143	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	fB	173	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	7A	162	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	hC	173	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	WE	154	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	pE	154	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	RB	132	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	ZB	130	TYR	CB-CG-CD1	7.48	125.49	121.00
1	aB	18	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	vC	132	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	nE	100	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	sE	173	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	CA	143	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	PD	154	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	eD	97	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	wD	97	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	WA	100	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	gE	167	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	fA	229	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	1E	229	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	UD	130	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	PA	82	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	mB	97	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	ND	143	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	IC	132	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	xA	167	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	SC	100	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	jC	162	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	0C	82	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	zE	97	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	7E	173	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	GE	154	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	BD	184	TRP	CB-CG-CD1	-7.46	117.31	127.00
1	1D	162	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	tA	132	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	IB	173	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	UD	97	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	sD	18	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	gE	154	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	2E	132	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	GB	173	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	RB	162	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	OD	18	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	OD	167	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	0C	162	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	iE	97	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	3C	162	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	IE	154	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	hE	82	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	gA	229	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	zB	97	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	1B	132	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	qC	229	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	jC	132	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	eB	132	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	aE	97	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	9B	97	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	cC	100	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	4C	143	ARG	NE-CZ-NH2	-7.43	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HB	143	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	aC	100	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	9D	154	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	KE	132	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	BA	167	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	LD	82	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	gD	167	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	VA	162	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	gA	184	TRP	CB-CG-CD1	-7.42	117.35	127.00
1	oD	173	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	GA	82	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	uA	229	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	1D	173	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	EE	173	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	RA	143	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	0B	162	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	KE	143	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	LD	167	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	uE	18	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	FB	18	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	RC	167	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	JD	82	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	oD	82	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	cA	18	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	1B	18	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	3B	97	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	TC	97	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	lC	82	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	6D	18	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	SB	100	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	4E	82	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	sE	184	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	cC	97	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	cC	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	lC	132	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	dE	132	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	6D	97	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	kE	82	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	9E	162	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	pC	154	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	HC	132	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	QE	162	ARG	NE-CZ-NH1	7.39	124.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	sB	97	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	IA	100	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	FD	167	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	bD	162	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	tD	132	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	OB	18	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	mB	229	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	gD	97	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	NA	154	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	SA	132	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	JB	143	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	YB	82	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	4B	154	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	XA	18	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	5	192	GLN	N-CA-C	7.37	118.96	111.07
1	VC	167	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	lC	173	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	9C	167	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	ME	82	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	rB	100	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	vC	82	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	6C	154	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	8D	184	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	4E	97	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	HB	162	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	uC	162	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	lB	162	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	sD	130	TYR	CB-CG-CD1	7.36	125.42	121.00
1	ME	167	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	gB	184	TRP	CB-CG-CD1	-7.36	117.44	127.00
1	EA	173	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	jC	97	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	sE	132	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	bE	167	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	uA	100	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	BB	143	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	eB	132	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	DC	132	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	uC	97	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	KD	167	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	oA	18	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	2B	18	ARG	NE-CZ-NH1	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	nA	97	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	KE	154	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	uB	229	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	0B	173	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	hE	18	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	EF	132	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	fD	184	TRP	CB-CG-CD1	-7.33	117.46	127.00
1	8C	132	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	oC	132	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	hE	143	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	lA	154	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	YB	82	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	QC	143	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	TE	173	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	aA	97	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	kA	132	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	GB	100	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	5D	100	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	vA	173	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	9D	100	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	cB	82	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	mC	18	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	yE	162	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	AA	18	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	dB	173	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	lE	154	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	QE	97	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	4A	100	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	eC	229	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	HE	82	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	VA	18	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	aA	162	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	bC	82	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	FA	173	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	ZB	97	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	bB	143	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	eD	18	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	7D	132	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	AC	154	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	BC	100	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	uA	132	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	NB	167	ARG	NE-CZ-NH2	-7.30	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	uB	132	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	UD	97	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	pC	167	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	nC	162	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	0E	173	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	MA	167	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	iA	132	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	7B	100	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	GD	100	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	GD	173	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	z	175	GLU	N-CA-C	7.29	119.23	111.28
1	KE	167	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	KE	162	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	y	184	TRP	CB-CG-CD1	-7.29	115.96	126.90
1	YB	130	TYR	CB-CG-CD1	7.29	125.37	121.00
1	TC	132	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	CD	82	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	RE	100	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	3A	97	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	CD	154	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	GE	162	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	jB	18	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	PD	132	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	WA	184	TRP	CB-CG-CD1	-7.28	117.54	127.00
1	AF	167	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	XA	143	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	8D	145	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	FE	82	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	NA	173	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	1D	82	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	NE	229	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	3B	82	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	LE	18	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	aB	162	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	aC	82	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	NE	97	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	JD	143	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	GA	184	TRP	CB-CG-CD1	-7.26	117.56	127.00
1	2B	100	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	9B	82	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	S	195	ASN	CA-CB-CG	7.26	119.86	112.60
1	PE	100	ARG	NE-CZ-NH1	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	OC	100	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	mB	82	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	3C	167	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	2B	167	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	HC	154	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	x	221	VAL	N-CA-C	7.25	118.01	110.62
1	iE	82	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	tA	97	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	JC	132	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	iD	184	TRP	CB-CG-CD1	-7.24	117.58	127.00
1	jA	143	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	4B	130	TYR	CB-CG-CD2	-7.24	116.66	121.00
1	5	10	MET	N-CA-C	7.24	120.49	110.35
1	ME	162	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	ZE	167	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	1C	162	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	2D	154	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	fD	97	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	VE	18	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	mC	154	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	nC	97	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	RB	100	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	MA	162	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	WA	18	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	kA	82	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	BD	97	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	w	122	PRO	N-CA-C	7.22	119.51	110.70
1	ED	229	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	kE	100	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	TB	82	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	yB	97	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	LC	173	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	QE	143	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	hE	132	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	tA	82	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	4A	97	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	vA	18	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	vB	173	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	aE	173	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	3B	132	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	IE	82	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	FF	229	ARG	NE-CZ-NH1	7.21	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	TA	82	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	mE	162	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	oA	173	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	eE	184	TRP	CB-CG-CD1	-7.21	117.63	127.00
1	nA	143	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	2A	132	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	eC	167	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	HD	82	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	oD	82	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	dD	184	TRP	CB-CG-CD1	-7.21	117.63	127.00
1	AB	18	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	NB	143	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	eB	97	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	OA	154	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	9C	167	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	vD	173	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	CE	162	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	AC	162	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	lE	130	TYR	CB-CG-CD1	7.20	125.32	121.00
1	eC	97	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	BF	97	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	wB	184	TRP	CB-CG-CD2	-7.19	117.25	126.60
1	5B	18	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	lE	97	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	6B	143	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	YC	143	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	EF	18	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	cB	18	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	VC	167	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	FE	162	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	lE	100	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	ZA	100	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	ID	18	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	cB	132	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	CD	82	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	wA	154	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	ED	132	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	ZE	154	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	yA	154	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	3C	18	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	7D	100	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	IA	97	ARG	NE-CZ-NH1	7.17	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	167	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	YB	167	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	iE	173	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	SC	184	TRP	CB-CG-CD1	-7.16	117.69	127.00
1	HB	229	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	8E	162	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	2A	167	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	9E	18	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	LA	184	TRP	N-CA-CB	-7.16	97.72	110.60
1	hD	229	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	mC	97	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	YA	154	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	wC	100	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	PD	82	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	S	122	PRO	N-CA-C	7.15	119.42	110.70
1	qD	143	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	kE	100	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	zE	132	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	pA	143	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	kE	18	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	tA	18	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	rA	173	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	pA	97	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	iB	162	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	qA	173	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	wA	143	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	AB	132	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	fD	154	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	hD	167	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	ND	97	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	ZC	100	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	ZA	82	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	VC	162	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	xD	100	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	2	183	ASN	CA-CB-CG	7.13	119.73	112.60
1	uD	82	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	pE	229	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	zE	82	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	YA	229	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	MD	132	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	OD	100	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	6E	97	ARG	NE-CZ-NH2	-7.13	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	hE	82	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	uC	82	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	SD	18	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	QE	100	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	rD	143	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	BE	100	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	HE	173	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	sB	229	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	EB	82	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	aC	18	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	VB	162	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	RC	82	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	PD	18	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	EF	167	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	zC	162	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	aA	167	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	9A	18	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	4C	145	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	OA	132	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	5A	229	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	5C	184	TRP	CB-CG-CD1	-7.11	117.76	127.00
1	EE	145	TYR	CB-CG-CD2	-7.11	116.74	121.00
1	Z	184	TRP	CB-CG-CD1	-7.11	116.24	126.90
1	JA	143	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	zA	82	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	MB	132	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	VB	97	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	AD	162	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	BD	154	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	ID	162	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	9	192	GLN	N-CA-C	7.10	119.02	111.28
1	1A	143	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	R	86	VAL	N-CA-C	7.10	117.86	110.62
1	yB	18	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	zB	167	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	hC	132	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	GD	154	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	pE	154	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	BF	154	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	N	139	ASN	CA-CB-CG	7.10	119.70	112.60
1	DC	18	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	VE	18	ARG	NE-CZ-NH2	-7.10	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	173	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	qD	154	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	AD	82	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	bC	229	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	8E	82	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	gB	18	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	DC	132	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	ZE	132	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	jA	18	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	TC	229	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	xC	97	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	UB	100	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	VD	162	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	JA	229	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	JB	82	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	GD	18	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	1D	18	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	qE	18	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	O	192	GLN	N-CA-C	7.08	119.00	111.28
1	BA	100	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	bA	132	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	FA	18	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	tE	162	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	cA	143	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	qA	167	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	3C	100	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	EF	173	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	4D	167	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	4A	167	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	dB	229	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	3B	229	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	SE	132	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	v	189	LEU	N-CA-C	7.07	118.63	111.07
1	kA	184	TRP	CB-CG-CD1	-7.07	117.81	127.00
1	KA	132	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	IA	173	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	iC	143	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	lE	132	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	bB	143	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	ME	18	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	dC	82	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	ME	229	ARG	NE-CZ-NH1	7.06	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	yE	229	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	wC	173	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	gD	162	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	aB	162	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	tE	154	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	GD	82	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	YA	97	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	eB	82	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	aD	167	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	Y	36	VAL	CA-C-N	7.05	124.68	120.24
1	Y	36	VAL	C-N-CA	7.05	124.68	120.24
1	XA	154	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	PD	173	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	9A	162	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	TD	229	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	W	175	GLU	N-CA-C	7.04	118.96	111.28
1	xB	82	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	lC	229	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	7A	143	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	EB	18	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	dD	173	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	BB	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	3B	132	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	RD	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	XD	18	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	QC	229	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	UD	143	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	FE	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	9C	143	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	HD	173	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	EA	173	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	QC	162	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	ZD	100	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	sB	229	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	5D	167	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	VD	154	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	bE	229	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	JB	162	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	qB	229	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	9B	132	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	HD	100	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	KE	100	ARG	NE-CZ-NH1	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	uC	173	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	tD	82	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	f	230	VAL	N-CA-C	7.02	117.16	110.42
1	lB	167	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	l	183	ASN	CA-CB-CG	7.01	119.61	112.60
1	TA	229	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	PB	132	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	RE	162	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	jA	97	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	qB	132	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	WA	173	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	ZA	154	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	ED	173	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	9C	18	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	fD	154	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	yE	154	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	bE	143	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	2B	97	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	eA	173	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	5B	132	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	jA	18	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	mC	132	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	AD	167	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	pA	82	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	OA	167	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	ZA	82	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	vB	132	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	tA	132	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	6D	185	MET	CG-SD-CE	-7.00	89.01	100.20
1	JA	100	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	oB	82	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	RD	82	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	SD	97	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	SD	162	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	FE	132	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	RE	167	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	RB	18	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	qC	167	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	cE	143	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	5B	143	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	XD	162	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	2C	184	TRP	CB-CG-CD2	6.98	135.68	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6A	154	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	PE	132	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	YB	143	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	vB	82	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	DC	162	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	VC	132	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	LA	167	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	gB	82	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	HC	18	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	HC	167	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	AE	18	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	6	36	VAL	CA-C-N	6.97	124.63	120.24
1	6	36	VAL	C-N-CA	6.97	124.63	120.24
1	9A	100	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	DE	162	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	nA	82	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	UB	143	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	0D	132	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	h	184	TRP	N-CA-CB	-6.96	99.85	110.16
1	rA	97	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	iB	100	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	AD	18	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	yE	229	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	DA	154	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	jC	143	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	iD	143	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	rE	130	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	vE	173	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	aE	82	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	1E	18	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	DD	154	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	OD	167	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	0E	82	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	I	195	ASN	CA-CB-CG	6.96	119.56	112.60
1	GE	97	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	OA	97	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	yC	18	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	6C	82	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	2E	162	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	LA	173	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	vA	173	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	ED	97	ARG	NE-CZ-NH1	6.95	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GD	132	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	qE	154	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	wA	18	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	xA	132	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	XE	97	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	sB	167	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	tB	154	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	VB	132	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	WB	173	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	bC	18	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	4D	143	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	XD	229	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	RD	173	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	VA	82	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	GD	154	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	sD	18	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	bB	18	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	dD	143	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	XA	132	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	4C	154	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	uB	167	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	hD	100	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	PD	173	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	CF	97	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	YC	173	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	zC	82	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	nE	132	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	QD	132	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	YE	130	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	kE	18	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	c	184	TRP	N-CA-CB	-6.92	99.92	110.16
1	DA	97	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	rC	97	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	CF	167	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	EC	154	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	zE	143	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	ZA	143	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	lB	162	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	nC	229	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	oA	162	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	1A	167	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	KE	229	ARG	NE-CZ-NH1	6.91	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vA	132	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	lD	132	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	BF	154	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	1B	100	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	7E	154	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	tC	143	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	BF	173	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	r	99	PRO	N-CA-C	6.90	122.05	111.15
1	yC	167	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	LE	154	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	UD	130	TYR	CB-CG-CD1	6.90	125.14	121.00
1	tD	143	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	XD	167	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	hB	18	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	qD	162	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	YE	229	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	4A	162	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	qB	167	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	rB	162	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	RA	97	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	5A	130	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	ZE	130	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	ZE	132	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	V	184	TRP	CB-CG-CD1	-6.88	116.57	126.90
1	lC	97	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	cD	132	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	EE	143	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	gD	82	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	gE	97	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	BB	82	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	SC	82	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	rE	162	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	nB	100	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	3B	229	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	7B	143	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	AC	97	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	JC	97	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	hD	154	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	EC	97	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	pC	97	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	3	189	LEU	N-CA-C	6.87	118.85	111.36
1	9B	184	TRP	CA-CB-CG	6.87	126.75	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8A	145	TYR	CB-CG-CD1	6.87	125.12	121.00
1	ZE	173	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	PB	167	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	5A	132	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	ZD	229	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	uE	97	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	T	184	TRP	CB-CG-CD1	-6.86	116.60	126.90
1	TA	173	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	BF	82	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	9E	97	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	QA	132	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	LB	229	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	rD	82	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	RA	82	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	LA	154	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	PE	97	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	8A	143	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	4B	132	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	JA	97	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	kC	132	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	1C	154	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	6C	97	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	FE	184	TRP	CA-CB-CG	6.84	126.71	113.70
1	CC	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	9	229	ARG	N-CA-C	6.84	119.13	110.24
1	0A	18	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	eB	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	4B	143	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	3A	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	mB	143	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	CE	162	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	QA	82	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	CA	82	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	iE	100	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	rE	173	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	6E	132	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	uA	97	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	tE	82	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	v	192	GLN	N-CA-C	6.83	118.72	111.28
1	bE	167	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	9E	18	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	iA	82	ARG	NE-CZ-NH1	6.83	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	wB	143	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	3D	167	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	XB	132	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	4B	130	TYR	CB-CG-CD1	6.82	125.09	121.00
1	QE	167	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	zC	132	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	zE	18	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	7E	82	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	iC	97	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	x	86	VAL	N-CA-C	6.81	117.57	110.62
1	rA	100	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	AB	154	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	SC	132	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	E	120	HIS	N-CA-C	6.81	118.35	111.07
1	6E	18	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	aC	143	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	nE	229	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	6D	132	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	LA	132	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	oB	143	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	kC	162	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	DD	167	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	3E	154	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	NA	173	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	xD	154	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	w	195	ASN	CA-CB-CG	6.79	119.39	112.60
1	R	195	ASN	CA-CB-CG	6.79	119.39	112.60
1	BB	143	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	0D	97	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	wE	184	TRP	CB-CG-CD2	-6.79	117.78	126.60
1	0E	162	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	QC	18	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	uD	162	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	W	63	GLN	N-CA-C	6.78	119.51	111.71
1	5B	132	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	AA	82	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	fC	82	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	jE	162	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	t	111	LEU	N-CA-C	6.78	118.32	111.07
1	pA	97	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	tA	100	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	nA	162	ARG	NE-CZ-NH1	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0B	18	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	fC	154	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	YA	132	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	RB	154	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	4B	167	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	tE	229	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	mD	229	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	dB	97	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	2B	173	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	WC	173	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	ZE	143	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	GE	132	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	DC	82	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	vD	162	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	w	192	GLN	N-CA-C	6.76	118.30	111.07
1	fA	82	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	3C	132	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	BE	97	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	LA	184	TRP	CA-CB-CG	6.76	126.54	113.70
1	aC	143	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	1E	132	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	X	192	GLN	N-CA-C	6.75	118.44	111.14
1	aC	162	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	OE	173	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	gA	82	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	6A	167	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	rB	154	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	1D	173	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	JE	154	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	rE	130	TYR	CB-CG-CD1	6.75	125.05	121.00
1	A	84	HIS	CA-CB-CG	-6.75	107.05	113.80
1	cA	184	TRP	CB-CG-CD2	6.75	135.37	126.60
1	8B	18	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	qD	145	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	MA	167	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	qA	100	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	rA	162	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	IC	100	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	pC	184	TRP	CB-CG-CD2	-6.74	117.84	126.60
1	D	36	VAL	CA-C-N	6.74	124.49	120.24
1	D	36	VAL	C-N-CA	6.74	124.49	120.24
1	gC	154	ARG	NE-CZ-NH1	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	kD	167	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	eC	162	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	hA	173	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	WE	173	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	DB	82	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	FC	132	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	LC	143	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	NC	162	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	189	LEU	N-CA-C	6.72	118.27	111.07
1	5	82	ARG	CA-C-N	6.72	129.29	120.28
1	5	82	ARG	C-N-CA	6.72	129.29	120.28
1	YB	173	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	7C	132	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	aD	184	TRP	CA-CB-CG	6.72	126.48	113.70
1	7	86	VAL	N-CA-C	6.72	117.47	110.62
1	sA	173	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	iA	229	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	zB	143	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	MC	82	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	ZC	162	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	1C	132	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	3C	18	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	sA	82	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	rC	162	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	kA	173	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	oB	97	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	nD	173	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	UD	18	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	sA	100	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	aB	82	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	lC	18	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	HE	154	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	BC	18	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	NC	82	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	HE	143	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	rC	132	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	sE	167	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	9A	82	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	3B	167	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	KB	162	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	PD	162	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	q	195	ASN	CA-CB-CG	6.70	119.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	iE	97	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	jE	82	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	TE	97	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	fC	100	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	yE	100	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	EE	229	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	AF	184	TRP	CA-CB-CG	6.69	126.42	113.70
1	IB	162	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	8E	97	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	ZA	18	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	IC	154	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	lB	143	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	sB	184	TRP	CB-CG-CD1	-6.68	118.31	127.00
1	tD	132	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	CD	97	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	3D	82	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	2	184	TRP	N-CA-CB	-6.68	100.30	110.12
1	rB	154	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	JD	100	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	EE	97	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	DE	143	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	cA	82	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	XE	167	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	CB	184	TRP	CB-CG-CD1	-6.67	118.33	127.00
1	CF	82	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	y	29	GLU	N-CA-C	6.67	118.34	111.14
1	yB	143	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	X	195	ASN	CA-CB-CG	6.67	119.27	112.60
1	OB	132	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	wB	18	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	SD	167	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	YD	162	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	lD	229	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	oD	132	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	nB	143	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	Y	195	ASN	CA-CB-CG	6.65	119.25	112.60
1	TA	173	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	hA	132	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	5C	132	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	9E	100	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	gB	18	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	LE	97	ARG	NE-CZ-NH1	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	zC	167	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	EE	173	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	h	222	GLY	CA-C-N	6.64	132.29	121.87
1	h	222	GLY	C-N-CA	6.64	132.29	121.87
1	0B	132	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	NC	154	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	HD	229	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	iE	143	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	xB	162	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	8B	132	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	2D	154	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	SC	18	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	rD	18	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	kA	184	TRP	CB-CG-CD2	6.63	135.22	126.60
1	lC	162	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	rD	173	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	CF	229	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	ED	229	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	HE	18	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	CB	167	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	jC	100	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	k	122	PRO	N-CA-C	6.62	118.78	110.70
1	gB	97	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	ZD	184	TRP	CB-CG-CD1	-6.62	118.39	127.00
1	iE	167	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	3C	154	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	j	60	GLY	CA-C-N	6.62	127.33	119.98
1	j	60	GLY	C-N-CA	6.62	127.33	119.98
1	GA	162	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	uA	162	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	rB	132	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	FC	100	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	hC	229	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	fD	18	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	DF	82	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	H	10	MET	N-CA-C	6.61	119.61	110.35
1	NA	18	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	IC	162	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	6C	167	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	VE	173	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	SC	154	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	0C	132	ARG	NE-CZ-NH2	-6.61	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	lA	229	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	SB	97	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	xB	18	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	7B	18	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	dB	154	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	LC	132	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	mD	97	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	kA	145	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	LB	229	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	OB	143	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	gE	229	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	BA	143	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	DA	154	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	dD	132	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	dC	100	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	dD	100	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	J	36	VAL	CA-C-N	6.60	125.61	120.33
1	J	36	VAL	C-N-CA	6.60	125.61	120.33
1	hB	82	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	HC	97	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	ID	167	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	sC	132	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	aD	100	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	GC	229	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	ND	97	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	CF	162	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	QB	184	TRP	CB-CG-CD2	6.59	135.17	126.60
1	rC	229	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	yE	97	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	UB	18	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	XB	173	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	7E	18	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	EE	145	TYR	CB-CG-CD1	6.59	124.95	121.00
1	BF	167	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	MD	143	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	RD	229	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	kE	97	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	mB	132	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	2C	184	TRP	CB-CG-CD1	-6.58	118.44	127.00
1	BD	162	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	MA	82	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	M	195	ASN	CA-CB-CG	6.58	119.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	mB	173	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	HE	173	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	wE	167	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	hB	18	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	jD	97	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	fB	154	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	HE	18	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	7	122	PRO	CA-C-O	-6.57	116.17	120.90
1	rC	143	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	oD	154	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	nD	167	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	7E	143	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	eB	162	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	CD	97	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	SD	143	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	l	184	TRP	N-CA-CB	-6.56	100.49	110.33
1	bB	82	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	XC	173	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	0C	100	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	GE	167	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	GE	18	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	6	175	GLU	N-CA-C	6.56	118.43	111.28
1	GB	167	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	yD	154	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	c	183	ASN	CA-C-N	6.55	129.60	120.29
1	c	183	ASN	C-N-CA	6.55	129.60	120.29
1	PB	162	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	RC	173	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	QE	154	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	E	36	VAL	CA-C-N	6.55	124.37	120.24
1	E	36	VAL	C-N-CA	6.55	124.37	120.24
1	kA	229	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	rB	173	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	HC	97	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	VC	229	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	PC	143	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	qD	100	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	ZA	184	TRP	CB-CG-CD1	-6.55	118.49	127.00
1	dA	143	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	gA	143	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	1C	82	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	eD	82	ARG	NE-CZ-NH1	6.55	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	mE	100	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	eC	132	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	2D	162	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	ZE	184	TRP	CB-CG-CD2	-6.54	118.09	126.60
1	aB	100	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	oB	162	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	3B	173	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	2C	143	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	OD	82	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	4E	167	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	mD	97	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	gC	82	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	jC	18	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	OD	162	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	1	192	GLN	N-CA-C	6.54	118.41	111.28
1	zD	18	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	EA	143	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	iC	132	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	tC	132	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	UC	167	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	eD	100	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	oA	132	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	uA	100	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	r	159	GLU	N-CA-C	6.53	117.88	109.65
1	OC	229	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	TC	162	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	9D	82	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	XE	167	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	KA	154	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	PA	82	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	EC	82	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	hE	100	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	WA	132	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	GB	229	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	2	195	ASN	CA-CB-CG	6.52	119.12	112.60
1	oA	100	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	yA	167	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	gB	173	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	KC	162	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	wA	97	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	9D	143	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	DF	132	ARG	NE-CZ-NH2	-6.52	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	dD	132	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	mD	173	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	tE	132	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	vE	154	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	aD	162	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	8D	154	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	5E	82	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	FA	100	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	AB	162	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	qD	229	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	hE	154	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	kC	97	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	LB	154	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	yE	167	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	BB	229	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	IA	167	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	KD	173	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	6E	132	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	pC	184	TRP	CA-CB-CG	6.50	126.05	113.70
1	AE	132	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	yA	100	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	zA	18	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	WD	132	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	jA	143	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	RC	143	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	DD	143	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	DE	173	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	WE	229	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	VB	82	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	mB	100	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	wC	18	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	FC	18	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	YC	100	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	WE	154	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	zA	132	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	L	195	ASN	CA-CB-CG	6.49	119.09	112.60
1	qC	132	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	QD	167	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	tE	143	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	zE	173	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	zB	154	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	dC	18	ARG	NE-CZ-NH1	6.49	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	iD	229	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	VE	229	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	V	31	ALA	N-CA-C	6.48	119.17	111.33
1	bE	154	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	O	159	GLU	N-CA-C	6.48	119.03	109.50
1	gA	162	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	YD	143	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	AA	100	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	sB	18	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	lA	143	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	yB	154	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	4D	100	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	IA	162	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	WB	82	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	HC	132	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	GA	143	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	KA	167	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	ZC	167	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	rC	167	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	ID	184	TRP	CB-CG-CD1	-6.47	118.59	127.00
1	SE	162	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	nD	162	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	DF	167	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	lB	167	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	VA	82	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	NC	173	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	bA	97	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	XA	167	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	cA	184	TRP	CB-CA-C	6.46	123.32	110.40
1	fA	18	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	zC	143	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	VD	167	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	nE	100	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	LA	18	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	OA	18	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	dB	100	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	7B	82	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	kD	145	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	2D	145	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	fE	184	TRP	CB-CG-CD1	-6.46	118.61	127.00
1	SC	229	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	2	120	HIS	N-CA-C	6.45	117.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4C	184	TRP	N-CA-CB	-6.45	98.99	110.60
1	5C	100	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	WC	132	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	9A	97	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	lE	162	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	0E	132	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	hB	154	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	xB	132	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	mE	132	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	FF	154	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	uE	184	TRP	CB-CG-CD1	-6.44	118.63	127.00
1	jB	184	TRP	CB-CG-CD2	6.44	134.97	126.60
1	RB	162	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	yB	173	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	TD	82	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	RA	132	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	jA	184	TRP	CB-CG-CD2	6.44	134.97	126.60
1	2D	132	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	HD	18	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	ZE	143	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	FB	184	TRP	CA-CB-CG	6.43	125.92	113.70
1	1C	184	TRP	CB-CG-CD1	-6.43	118.64	127.00
1	SD	132	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	6E	229	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	iB	173	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	1C	167	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	cB	229	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	YA	162	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	RB	18	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	mC	82	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	MD	173	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	KB	154	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	4C	145	TYR	CB-CG-CD1	6.42	124.85	121.00
1	VE	167	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	tA	130	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	9E	143	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	LA	229	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	0A	18	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	xD	154	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	8D	82	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	AE	143	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	y	122	PRO	N-CA-C	6.41	118.52	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aB	97	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	jE	143	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	oD	162	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	kA	82	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	0A	167	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	BD	143	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	jD	154	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	cB	82	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	UC	18	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	LE	229	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	pE	18	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	3B	162	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	5B	82	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	LE	82	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	OB	173	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	EE	143	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	kE	229	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	vB	167	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	VA	100	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	hC	132	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	GA	18	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	XB	143	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	ZE	154	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	mE	82	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	AD	154	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	RB	132	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	ME	132	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	3B	97	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	HC	18	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	KD	100	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	PE	132	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	kC	143	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	DD	132	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	IB	100	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	2B	229	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	PD	167	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	V	53	ASN	CA-CB-CG	6.38	118.97	112.60
1	MD	184	TRP	CB-CG-CD2	6.38	134.89	126.60
1	bE	97	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	eB	167	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	WD	154	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	7A	162	ARG	NE-CZ-NH1	6.37	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6C	162	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	KD	82	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	0A	162	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	5B	97	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	vE	97	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	wB	162	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	JA	132	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	DE	229	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	yE	143	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	o	120	HIS	N-CA-C	6.36	117.88	111.07
1	4B	154	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	9E	162	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	pB	143	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	YE	97	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	eA	100	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	SC	82	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	mD	82	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	c	189	LEU	N-CA-C	6.35	118.20	111.28
1	GE	167	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	3E	18	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	hA	162	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	mB	154	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	eC	82	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	DB	169	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	TC	167	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	KA	82	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	DA	132	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	GC	18	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	cD	143	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	1E	229	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	mB	184	TRP	CA-CB-CG	6.33	125.73	113.70
1	QC	167	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	TC	143	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	w	9	GLN	N-CA-C	6.33	118.96	110.35
1	YC	229	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	AD	145	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	9D	132	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	oA	162	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	6B	82	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	F	195	ASN	CA-CB-CG	6.33	118.93	112.60
1	SA	229	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	NC	82	ARG	NE-CZ-NH1	6.33	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	wC	143	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	3C	97	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	G	122	PRO	N-CA-C	6.33	118.42	110.70
1	QD	100	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	1	195	ASN	CA-CB-CG	6.33	118.93	112.60
1	AC	97	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	CC	167	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	QD	162	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	YE	143	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	XE	143	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	GB	162	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	IE	100	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	sE	18	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	RB	100	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	bC	100	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	OB	100	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	SD	229	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	VB	18	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	ZC	143	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	OC	18	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	LE	132	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	v	195	ASN	CA-CB-CG	6.31	118.91	112.60
1	7B	143	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	VA	97	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	PC	143	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	BB	162	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	zE	229	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	3	115	ILE	CA-C-N	6.30	127.11	119.99
1	3	115	ILE	C-N-CA	6.30	127.11	119.99
1	PA	18	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	CB	100	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	SC	100	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	zE	173	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	AF	82	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	G	36	VAL	CA-C-N	6.30	125.37	120.33
1	G	36	VAL	C-N-CA	6.30	125.37	120.33
1	OD	143	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	0E	97	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	OE	100	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	lC	18	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	eE	82	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	uE	229	ARG	NE-CZ-NH1	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5E	173	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	0B	100	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	iE	167	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	Z	184	TRP	N-CA-CB	-6.29	100.81	110.44
1	lB	229	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	BC	229	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	lB	167	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	OC	173	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	UD	167	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	2D	18	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	tA	18	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	FC	229	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	YD	229	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	hD	97	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	lD	143	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	fE	132	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	5	195	ASN	CA-CB-CG	6.28	118.88	112.60
1	lB	18	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	aB	154	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	HD	18	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	KD	82	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	gA	167	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	HB	82	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	YE	162	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	lE	82	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	jA	184	TRP	CA-CB-CG	6.28	125.62	113.70
1	KC	167	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	gC	145	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	GB	132	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	yD	97	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	YD	82	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	qE	154	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	lB	132	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	UC	229	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	5C	82	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	EA	97	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	9C	100	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	ND	82	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	GA	82	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	0	195	ASN	CA-CB-CG	6.26	118.86	112.60
1	xA	132	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	7E	167	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IA	100	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	UD	162	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	TA	162	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	hA	100	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	3	195	ASN	CA-CB-CG	6.25	118.86	112.60
1	DA	173	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	vA	132	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	xC	167	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	5E	167	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	cC	82	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	WD	167	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	0D	82	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	0B	97	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	NC	18	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	fA	229	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	pB	82	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	3	188	THR	N-CA-C	6.24	118.16	111.36
1	MA	143	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	SA	173	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	zB	132	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	YE	130	TYR	CB-CG-CD1	6.24	124.74	121.00
1	vE	173	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	TA	154	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	cD	154	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	eA	145	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	ID	100	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	fE	132	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	pA	162	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	dC	82	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	8D	145	TYR	CB-CG-CD1	6.24	124.74	121.00
1	2E	167	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	RB	173	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	AE	130	TYR	CB-CG-CD1	6.23	124.74	121.00
1	sD	173	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	9E	154	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	189	LEU	N-CA-C	6.23	118.07	111.28
1	eD	173	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	y	189	LEU	N-CA-C	6.23	118.07	111.28
1	5C	18	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	OA	162	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	zA	162	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	zB	97	ARG	NE-CZ-NH2	-6.22	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	fC	143	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	CE	154	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	cB	132	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	sC	100	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	xD	100	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	HE	100	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	sC	82	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	AE	82	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	J	179	GLN	N-CA-C	6.22	118.06	111.28
1	uA	18	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	XB	154	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	2B	132	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	wE	229	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	UC	100	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	sE	82	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	i	175	GLU	N-CA-C	6.21	117.72	111.07
1	zD	167	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	rC	82	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	bE	100	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	IB	154	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	MC	162	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	4A	132	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	eB	154	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	nC	229	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	pC	184	TRP	N-CA-CB	-6.21	99.43	110.60
1	jA	154	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	aA	229	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	vE	229	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	u	189	LEU	N-CA-C	6.20	117.70	111.07
1	3D	97	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	QE	97	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	4D	143	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	sE	100	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	iB	154	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	BC	18	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	3C	173	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	RD	132	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	1E	18	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	EF	162	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	KB	82	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	i	195	ASN	CA-CB-CG	6.19	118.79	112.60
1	WD	143	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4E	162	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	2B	162	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	AC	143	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	LC	229	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	NC	229	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	nE	173	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	jE	229	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	kB	143	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	GC	82	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	QC	82	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	ZA	229	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	oC	173	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	HA	154	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	0D	154	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	oB	167	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	FC	100	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	VE	97	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	6	85	PRO	CA-C-N	6.17	128.92	120.46
1	6	85	PRO	C-N-CA	6.17	128.92	120.46
1	fC	229	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	mC	154	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	q	172	LEU	N-CA-C	6.17	118.52	111.11
1	AA	97	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	7A	82	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	0A	162	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	wD	167	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	DE	82	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	cE	229	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	M	36	VAL	CA-C-N	6.17	124.12	120.24
1	M	36	VAL	C-N-CA	6.17	124.12	120.24
1	AE	229	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	DF	143	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	kA	167	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	rA	184	TRP	CB-CG-CD1	-6.16	118.99	127.00
1	lA	18	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	uA	184	TRP	CB-CG-CD1	-6.16	118.99	127.00
1	5B	82	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	AD	100	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	GD	143	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	ZB	173	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	6B	184	TRP	CA-CB-CG	6.16	125.41	113.70
1	9C	162	ARG	NE-CZ-NH2	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	nB	82	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	G	192	GLN	N-CA-C	6.16	117.99	111.28
1	ID	173	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	mD	229	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	8	122	PRO	N-CA-C	6.15	118.21	110.70
1	jA	184	TRP	N-CA-CB	-6.15	99.53	110.60
1	aC	145	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	UD	82	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	QD	229	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	MC	184	TRP	CB-CG-CD1	-6.15	119.01	127.00
1	xA	173	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	DB	167	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	jD	154	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	Z	195	ASN	CA-CB-CG	6.14	118.75	112.60
1	eE	162	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	M	230	VAL	N-CA-C	6.14	116.88	110.62
1	N	120	HIS	N-CA-C	6.14	117.97	111.28
1	m	195	ASN	CA-CB-CG	6.14	118.74	112.60
1	wB	154	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	2E	143	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	XA	229	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	c	192	GLN	N-CA-C	6.14	117.97	111.28
1	k	60	GLY	CA-C-N	6.14	126.91	120.03
1	k	60	GLY	C-N-CA	6.14	126.91	120.03
1	ED	100	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	UA	162	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	kB	132	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	uE	167	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	zD	97	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	b	192	GLN	N-CA-C	6.13	117.97	111.28
1	zA	229	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	FD	18	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	c	229	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	9B	229	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	bC	154	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	r	195	ASN	CA-CB-CG	6.13	118.73	112.60
1	bB	229	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	LC	154	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	q	189	LEU	N-CA-C	6.13	118.46	111.11
1	cD	97	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	zD	173	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	115	ILE	CA-C-N	6.12	126.78	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ILE	C-N-CA	6.12	126.78	119.98
1	B	120	HIS	N-CA-C	6.12	117.95	111.28
1	M	189	LEU	N-CA-C	6.12	117.95	111.28
1	6B	97	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	aD	97	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	fB	229	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	MC	184	TRP	CB-CG-CD2	6.12	134.55	126.60
1	C	175	GLU	N-CA-C	6.12	117.61	111.07
1	p	195	ASN	CA-CB-CG	6.12	118.72	112.60
1	EC	162	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	DF	100	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	DC	97	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	N	53	ASN	CA-CB-CG	6.11	118.71	112.60
1	M	29	GLU	N-CA-C	6.11	118.02	111.36
1	j	122	PRO	N-CA-C	6.11	118.15	110.70
1	gE	162	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	FA	143	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	VA	143	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	JB	18	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	QB	143	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	jA	167	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	VB	18	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	sB	154	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	PC	154	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	F	3	VAL	CA-C-N	6.10	133.20	121.54
1	F	3	VAL	C-N-CA	6.10	133.20	121.54
1	UA	167	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	CE	143	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	MD	167	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	bD	97	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	pD	132	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	eE	143	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	R	60	GLY	CA-C-N	6.10	126.86	120.03
1	R	60	GLY	C-N-CA	6.10	126.86	120.03
1	tD	100	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	oE	229	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	GC	162	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	P	192	GLN	N-CA-C	6.09	118.00	111.36
1	yC	173	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	oD	18	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	eD	184	TRP	N-CA-CB	-6.09	99.63	110.60
1	N	29	GLU	N-CA-C	6.09	118.00	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	mE	184	TRP	CA-CB-CG	6.09	125.27	113.70
1	a	171	THR	CA-C-N	6.09	129.05	120.28
1	a	171	THR	C-N-CA	6.09	129.05	120.28
1	MC	229	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	JE	18	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	SE	132	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	T	29	GLU	N-CA-C	6.09	118.00	111.36
1	l	184	TRP	CA-CB-CG	6.09	125.16	113.60
1	GB	97	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	NC	167	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	SD	145	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	7D	154	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	0B	167	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	8B	97	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	UC	132	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	fC	143	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	eE	184	TRP	CA-CB-CG	6.08	125.26	113.70
1	4	185	MET	N-CA-C	6.08	117.71	111.14
1	OC	154	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	8C	143	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	WD	162	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	ZB	229	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	EC	143	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	BD	229	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	2B	100	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	gD	152	ASP	CB-CG-OD1	6.08	123.77	118.30
1	AE	130	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	QC	184	TRP	CB-CG-CD2	-6.07	118.71	126.60
1	2C	143	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	PE	167	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	5A	173	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	iB	145	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	qB	100	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	gC	145	TYR	CB-CG-CD1	6.07	124.64	121.00
1	cA	173	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	zB	229	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	cE	154	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	6B	184	TRP	CB-CG-CD2	6.07	134.49	126.60
1	PA	132	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	WA	97	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	UB	173	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	3D	143	ARG	NE-CZ-NH1	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	UE	162	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	jA	132	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	YE	162	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	BF	132	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	Y	206	GLY	CA-C-N	6.06	126.08	119.90
1	Y	206	GLY	C-N-CA	6.06	126.08	119.90
1	rE	18	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	TB	18	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	aC	154	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	DA	130	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	hE	18	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	N	187	GLU	N-CA-C	6.06	117.88	111.28
1	e	195	ASN	CA-CB-CG	6.06	118.66	112.60
1	MA	18	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	hA	132	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	SC	167	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	iC	167	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	xD	97	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	1D	82	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	y	147	PRO	CA-N-CD	-6.06	103.52	112.00
1	TE	132	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	hB	162	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	jE	97	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	fC	162	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	QE	229	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	S	60	GLY	CA-C-N	6.05	126.83	119.99
1	S	60	GLY	C-N-CA	6.05	126.83	119.99
1	p	175	GLU	N-CA-C	6.05	117.88	111.28
1	4B	82	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	pD	167	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	vE	100	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	6A	184	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	t	219	GLN	N-CA-C	6.04	117.87	111.28
1	gA	97	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	iB	162	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	tC	162	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	uE	132	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	j	192	GLN	N-CA-C	6.04	117.86	111.28
1	dB	229	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	IE	97	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	U	192	GLN	N-CA-C	6.04	117.86	111.28
1	2A	18	ARG	NE-CZ-NH2	-6.04	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8B	130	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	DC	143	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	qC	167	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	1	120	HIS	CA-CB-CG	6.03	119.83	113.80
1	CB	154	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	jE	18	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	2	36	VAL	CA-C-N	6.03	124.04	120.24
1	2	36	VAL	C-N-CA	6.03	124.04	120.24
1	UE	18	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	WA	82	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	xA	97	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	FF	100	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	3A	132	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	cC	162	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	jC	229	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	Q	62	HIS	CA-C-N	6.03	128.96	120.28
1	Q	62	HIS	C-N-CA	6.03	128.96	120.28
1	lA	97	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	hD	143	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	tD	97	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	O	146	SER	N-CA-C	6.02	116.98	109.57
1	iA	132	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	pE	143	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	60	GLY	CA-C-N	6.02	126.77	120.03
1	C	60	GLY	C-N-CA	6.02	126.77	120.03
1	JA	130	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	QB	145	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	zD	132	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	2D	143	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	2	183	ASN	CA-C-N	6.02	128.35	120.28
1	2	183	ASN	C-N-CA	6.02	128.35	120.28
1	kD	145	TYR	CB-CG-CD1	6.02	124.61	121.00
1	ZE	130	TYR	CB-CG-CD1	6.02	124.61	121.00
1	2E	173	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	IC	145	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	b	85	PRO	CA-C-N	6.01	128.71	120.35
1	b	85	PRO	C-N-CA	6.01	128.71	120.35
1	jD	173	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	CA	82	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	XB	18	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	uB	184	TRP	CB-CG-CD1	6.01	134.82	127.00
1	sC	184	TRP	CB-CA-C	6.01	122.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KC	184	TRP	CA-CB-CG	6.01	125.12	113.70
1	YE	18	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	J	29	GLU	N-CA-C	6.01	117.83	111.28
1	IC	132	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	9A	162	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	QC	173	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	bC	144	MET	CG-SD-CE	-6.00	90.59	100.20
1	AF	82	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	uB	173	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	z	192	GLN	N-CA-C	6.00	117.49	111.07
1	JB	154	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	uC	173	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	WD	163	ASP	CB-CG-OD2	6.00	123.70	118.30
1	FE	143	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	c	184	TRP	CA-CB-CG	6.00	124.99	113.60
1	qA	143	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	7A	18	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	CD	132	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	hD	173	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	BF	82	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	vA	97	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	oC	184	TRP	CB-CG-CD1	-6.00	119.21	127.00
1	kA	145	TYR	CB-CG-CD1	5.99	124.60	121.00
1	OC	97	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	uC	184	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	7C	143	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	nD	82	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	64	ALA	N-CA-C	5.99	118.30	111.11
1	H	120	HIS	N-CA-C	5.99	117.81	111.28
1	7	60	GLY	CA-C-N	5.99	126.74	120.03
1	7	60	GLY	C-N-CA	5.99	126.74	120.03
1	OB	229	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	GE	97	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	q	60	GLY	CA-C-N	5.99	126.76	119.99
1	q	60	GLY	C-N-CA	5.99	126.76	119.99
1	sA	184	TRP	CB-CG-CD2	-5.99	118.82	126.60
1	uB	82	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	uB	82	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	5B	97	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	XB	100	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	YB	229	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	kD	173	ARG	NE-CZ-NH2	-5.99	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ME	154	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	MB	173	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	UC	100	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	L	175	GLU	N-CA-C	5.98	117.80	111.28
1	h	184	TRP	CB-CA-C	5.98	121.02	110.85
1	y	184	TRP	N-CA-CB	-5.98	101.09	110.30
1	qC	162	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	wD	145	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	lE	167	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	8B	162	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	BD	132	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	gA	97	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	JC	143	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	qA	154	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	AB	132	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	rB	167	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	MD	132	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	uD	143	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	9E	229	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	SA	132	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	kA	147	PRO	CA-N-CD	-5.97	103.14	111.50
1	fA	173	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	PB	18	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	1B	143	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	vC	97	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	NE	82	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	fE	82	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	85	PRO	CA-C-N	5.96	128.49	120.50
1	A	85	PRO	C-N-CA	5.96	128.49	120.50
1	nB	82	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	8C	167	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	f	63	GLN	N-CA-C	5.96	117.78	111.28
1	1D	167	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	9D	143	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	KD	167	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	KE	173	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	S	184	TRP	N-CA-CB	-5.96	101.35	110.16
1	1C	173	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	YD	97	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	PA	167	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	192	GLN	N-CA-C	5.95	117.77	111.28
1	eA	184	TRP	CB-CG-CD1	-5.95	119.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	PC	132	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	vC	97	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	aD	173	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	lA	184	TRP	CB-CG-CD2	-5.95	118.86	126.60
1	q	183	ASN	CA-CB-CG	5.95	118.55	112.60
1	HA	18	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	BE	97	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	bC	162	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	o	111	LEU	N-CA-C	5.95	117.43	111.07
1	BA	18	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	MB	130	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	eA	18	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	8B	130	TYR	CB-CG-CD1	5.94	124.57	121.00
1	vB	132	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	i	31	ALA	N-CA-C	5.94	117.75	111.28
1	FC	173	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	d	4	GLN	N-CA-C	5.94	123.44	110.80
1	GA	229	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	3E	184	TRP	N-CA-CB	-5.93	99.92	110.60
1	FF	162	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	l	199	LYS	N-CA-C	5.93	118.51	111.33
1	0A	229	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	CE	18	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	t	122	PRO	N-CA-C	5.93	117.93	110.70
1	wB	173	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	R	189	LEU	N-CA-C	5.92	117.74	111.28
1	9A	167	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	UB	132	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	ZB	154	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	FD	132	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	qD	145	TYR	CB-CG-CD1	5.92	124.55	121.00
1	w	84	HIS	CA-CB-CG	-5.92	107.88	113.80
1	OA	100	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	pA	18	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	MB	167	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	gB	154	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	iB	143	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	1E	143	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	FA	100	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	yD	82	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	zB	184	TRP	N-CA-CB	-5.92	99.95	110.60
1	yD	173	ARG	NE-CZ-NH1	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HB	154	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	dB	162	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	wC	132	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	9	187	GLU	N-CA-C	5.91	117.40	111.07
1	FE	167	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	tD	162	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	H	3	VAL	CA-C-N	5.91	132.82	121.54
1	H	3	VAL	C-N-CA	5.91	132.82	121.54
1	p	122	PRO	N-CA-C	5.91	117.91	110.70
1	3	206	GLY	CA-C-N	5.91	125.92	119.89
1	3	206	GLY	C-N-CA	5.91	125.92	119.89
1	AB	100	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	X	48	THR	CA-C-N	5.91	125.38	119.24
1	X	48	THR	C-N-CA	5.91	125.38	119.24
1	jA	169	TYR	CB-CG-CD1	-5.91	117.46	121.00
1	DB	169	TYR	CB-CG-CD2	5.91	124.54	121.00
1	H	192	GLN	N-CA-C	5.91	117.72	111.28
1	FB	154	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	wB	97	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	oC	100	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	qC	132	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	l	195	ASN	CA-CB-CG	5.90	118.50	112.60
1	EA	18	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	zA	173	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	RE	100	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	EA	82	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	NC	97	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	FF	82	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	H	111	LEU	N-CA-C	5.90	118.19	111.11
1	ZC	154	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	vD	167	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	X	227	LYS	N-CA-C	5.90	117.71	111.28
1	8E	143	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	EA	100	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	VD	132	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	sD	132	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	MC	100	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	fC	173	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	gD	184	TRP	CA-CB-CG	5.89	124.89	113.70
1	U	195	ASN	CA-CB-CG	5.89	118.49	112.60
1	tA	162	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	zC	143	ARG	NE-CZ-NH2	-5.89	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	107	THR	N-CA-C	5.89	117.70	111.28
1	SB	97	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	PC	167	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	HD	100	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	UD	184	TRP	N-CA-CB	-5.89	100.00	110.60
1	6D	18	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	K	175	GLU	N-CA-C	5.88	120.07	113.01
1	cB	100	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	5D	82	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	WE	97	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	CF	18	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	T	184	TRP	N-CA-CB	-5.88	101.45	110.16
1	1	3	VAL	CA-C-N	5.88	132.78	121.54
1	1	3	VAL	C-N-CA	5.88	132.78	121.54
1	UC	147	PRO	CA-N-CD	-5.88	103.27	111.50
1	SB	173	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	HD	229	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	iB	154	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	iB	229	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	jB	184	TRP	CB-CG-CD1	-5.87	119.36	127.00
1	fD	144	MET	CG-SD-CE	-5.87	90.80	100.20
1	QE	82	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	5E	18	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	6E	154	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	BF	162	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	LC	100	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	XC	162	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	gD	229	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	JB	229	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	eD	162	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	YB	143	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	yC	145	TYR	CB-CG-CD1	5.87	124.52	121.00
1	I	175	GLU	N-CA-C	5.87	117.35	111.07
1	8A	173	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	aE	154	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	E	192	GLN	N-CA-C	5.86	117.67	111.28
1	HB	132	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	WB	97	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	6C	132	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	6D	173	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	pC	97	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	TE	143	ARG	NE-CZ-NH1	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8C	132	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	QE	132	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	NB	132	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	mC	167	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	RD	143	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	ME	132	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	V	192	GLN	N-CA-C	5.85	117.33	111.07
1	i	228	ALA	N-CA-C	5.85	117.66	111.28
1	z	36	VAL	CA-C-N	5.85	123.93	120.24
1	z	36	VAL	C-N-CA	5.85	123.93	120.24
1	QB	184	TRP	N-CA-CB	-5.85	100.07	110.60
1	aE	167	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	yE	173	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	i	16	SER	N-CA-C	5.85	117.07	109.64
1	KC	143	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	5E	162	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	aC	97	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	e	226	HIS	CA-CB-CG	5.84	119.64	113.80
1	BE	18	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	uA	167	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	yA	162	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	zB	18	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	QD	97	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	226	HIS	CA-CB-CG	5.84	119.64	113.80
1	u	36	VAL	CA-C-N	5.84	123.92	120.24
1	u	36	VAL	C-N-CA	5.84	123.92	120.24
1	cD	167	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	yD	154	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	hB	97	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	R	115	ILE	CA-C-N	5.84	126.59	119.99
1	R	115	ILE	C-N-CA	5.84	126.59	119.99
1	tB	100	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	pD	132	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	mE	173	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	vE	18	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	4D	184	TRP	CB-CG-CD2	-5.83	119.01	126.60
1	KA	18	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	YD	145	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	dD	82	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	aE	162	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	8E	154	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	pC	162	ARG	NE-CZ-NH2	-5.83	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	tA	130	TYR	CB-CG-CD1	5.83	124.50	121.00
1	LB	18	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	dD	229	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	YC	154	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	IB	143	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	Z	101	GLY	CA-C-N	5.82	128.08	120.28
1	Z	101	GLY	C-N-CA	5.82	128.08	120.28
1	JA	229	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	hB	229	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	xA	18	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	AB	82	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	hD	143	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	r	122	PRO	N-CA-C	5.81	117.79	110.70
1	CE	173	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	X	111	LEU	N-CA-C	5.81	117.61	111.28
1	aE	132	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	184	TRP	CB-CG-CD1	-5.81	118.18	126.90
1	nC	97	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	4C	229	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	MB	154	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	mC	82	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	wE	82	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	fB	154	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	NE	82	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	mE	162	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	JC	143	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	WD	18	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	CF	18	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	Z	60	GLY	CA-C-N	5.80	126.53	120.03
1	Z	60	GLY	C-N-CA	5.80	126.53	120.03
1	VA	167	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	TC	97	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	pD	18	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	ZE	100	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	0A	154	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	BC	173	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	ZE	184	TRP	CB-CG-CD1	5.80	134.53	127.00
1	1E	154	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	LE	173	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	d	3	VAL	CA-C-N	5.79	132.60	121.54
1	d	3	VAL	C-N-CA	5.79	132.60	121.54
1	RB	82	ARG	NE-CZ-NH1	5.79	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	OE	132	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	pE	162	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	qA	97	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	8B	229	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	1A	173	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	tB	143	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	7C	100	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	JE	184	TRP	N-CA-CB	-5.79	100.18	110.60
1	VE	82	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	fA	97	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	KD	97	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	AE	162	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	KD	173	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	pD	173	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	5A	130	TYR	CB-CG-CD1	5.78	124.47	121.00
1	LB	173	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	PC	167	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	9B	18	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	KE	184	TRP	N-CA-CB	-5.78	100.20	110.60
1	5	184	TRP	CB-CG-CD2	5.78	134.89	126.80
1	QB	97	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	7B	154	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	EE	97	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	MB	229	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	yC	145	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	dD	97	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	zE	97	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	hC	229	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	k	36	VAL	CA-C-N	5.77	123.88	120.24
1	k	36	VAL	C-N-CA	5.77	123.88	120.24
1	FC	81	ASP	CB-CG-OD1	5.77	123.49	118.30
1	NE	173	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	4	195	ASN	CA-CB-CG	5.77	118.37	112.60
1	nE	162	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	lB	154	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	tC	162	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	u	230	VAL	N-CA-C	5.77	116.54	110.72
1	GB	132	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	FA	229	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	9B	100	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	HD	154	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	IE	143	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KB	147	PRO	CA-N-CD	-5.76	103.43	111.50
1	YD	145	TYR	CB-CG-CD1	5.76	124.46	121.00
1	zD	143	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	118	MET	N-CA-C	5.76	117.56	111.28
1	e	111	LEU	N-CA-C	5.76	117.23	111.07
1	H	195	ASN	CA-CB-CG	5.76	118.36	112.60
1	b	175	GLU	N-CA-C	5.76	118.02	111.11
1	oA	97	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	yB	100	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	a	36	VAL	CA-C-N	5.76	124.94	120.33
1	a	36	VAL	C-N-CA	5.76	124.94	120.33
1	lA	97	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	mD	154	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	lD	97	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	2A	184	TRP	CA-CB-CG	5.75	124.64	113.70
1	4A	154	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	7A	132	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	PB	173	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	7	192	GLN	N-CA-C	5.75	117.55	111.28
1	AB	173	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	iB	147	PRO	CA-N-CD	-5.75	103.45	111.50
1	I	206	GLY	CA-C-N	5.75	125.75	119.89
1	I	206	GLY	C-N-CA	5.75	125.75	119.89
1	CA	173	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	2E	97	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	H	60	GLY	CA-C-N	5.75	126.48	119.99
1	H	60	GLY	C-N-CA	5.75	126.48	119.99
1	bB	100	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	xB	143	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	2	31	ALA	N-CA-C	5.75	118.28	111.33
1	IC	167	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	CD	184	TRP	N-CA-CB	-5.75	100.26	110.60
1	wB	100	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	H	63	GLN	N-CA-C	5.74	117.54	111.28
1	qA	143	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	UB	173	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	xC	154	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	CF	154	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	V	107	THR	N-CA-C	5.74	117.54	111.28
1	d	192	GLN	N-CA-C	5.74	117.53	111.28
1	OD	100	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	HE	184	TRP	CB-CG-CD2	-5.74	119.14	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	29	GLU	N-CA-C	5.74	117.33	111.14
1	RB	229	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	ZC	229	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	9D	18	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	hB	184	TRP	CB-CG-CD2	5.73	134.05	126.60
1	CD	229	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	aD	132	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	RE	229	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	h	192	GLN	N-CA-C	5.73	117.53	111.28
1	cC	143	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	q	192	GLN	N-CA-C	5.73	117.53	111.28
1	A	10	MET	N-CA-C	5.73	118.37	110.35
1	Y	111	LEU	N-CA-C	5.73	117.20	111.07
1	l	184	TRP	CB-CG-CD2	5.73	134.82	126.80
1	vD	229	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	AE	184	TRP	N-CA-CB	-5.73	100.29	110.60
1	KD	162	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	b	184	TRP	N-CA-CB	-5.72	101.69	110.16
1	3	230	VAL	N-CA-C	5.72	117.67	112.29
1	hD	82	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	fE	97	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	UA	18	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	UA	162	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	4E	82	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	OA	82	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	7B	173	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	zC	184	TRP	N-CA-CB	-5.72	100.30	110.60
1	AD	145	TYR	CB-CG-CD1	5.72	124.43	121.00
1	4D	184	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	2	111	LEU	N-CA-C	5.72	117.19	111.07
1	UD	229	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	UE	154	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	R	175	GLU	N-CA-C	5.72	117.19	111.07
1	3D	162	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	AF	162	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	F	36	VAL	CA-C-N	5.71	124.90	120.33
1	F	36	VAL	C-N-CA	5.71	124.90	120.33
1	YE	100	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	zE	100	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	zC	162	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	K	195	ASN	CA-CB-CG	5.71	118.31	112.60
1	4	60	GLY	CA-C-N	5.71	126.32	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	60	GLY	C-N-CA	5.71	126.32	119.98
1	YA	143	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	AC	167	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	OC	143	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	OC	145	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	xD	229	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	DA	97	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	YA	173	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	lB	18	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	oE	173	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	MB	97	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	pC	143	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	dD	100	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	BA	173	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	sB	167	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	hA	97	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	hA	162	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	4C	184	TRP	CB-CA-C	5.70	121.81	110.40
1	TD	143	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	3D	229	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	2D	145	TYR	CB-CG-CD1	5.70	124.42	121.00
1	wA	100	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	2D	100	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	Y	189	LEU	N-CA-C	5.70	117.49	111.28
1	iB	145	TYR	CB-CG-CD1	5.70	124.42	121.00
1	KE	145	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	N	184	TRP	CB-CG-CD1	-5.70	118.36	126.90
1	zB	132	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	IC	145	TYR	CB-CG-CD1	5.70	124.42	121.00
1	TD	18	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	5B	144	MET	CG-SD-CE	-5.69	91.09	100.20
1	B	121	ASN	CA-C-O	-5.69	115.19	120.94
1	8	62	HIS	CA-C-N	5.69	127.91	120.28
1	8	62	HIS	C-N-CA	5.69	127.91	120.28
1	iB	143	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	u	63	GLN	N-CA-C	5.69	117.48	111.28
1	hB	100	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	gC	143	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	KC	18	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	ID	97	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	ME	173	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	DF	100	ARG	NE-CZ-NH1	5.69	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	189	LEU	N-CA-C	5.69	117.48	111.28
1	VA	143	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	qA	82	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	0A	154	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	MB	100	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	oE	167	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	hC	162	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	wC	100	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	LE	173	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	J	175	GLU	N-CA-C	5.68	117.47	111.28
1	DD	100	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	2D	173	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	N	195	ASN	CA-CB-CG	5.68	118.28	112.60
1	l	189	LEU	N-CA-C	5.68	117.47	111.28
1	ME	173	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	mB	184	TRP	N-CA-CB	-5.68	100.38	110.60
1	KA	18	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	hE	229	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	I	86	VAL	N-CA-C	5.67	115.87	110.42
1	n	36	VAL	CA-C-N	5.67	123.81	120.24
1	n	36	VAL	C-N-CA	5.67	123.81	120.24
1	r	184	TRP	N-CA-CB	-5.67	101.76	110.16
1	CD	100	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	wD	82	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	W	31	ALA	N-CA-C	5.67	117.14	111.07
1	xD	162	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	qB	167	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	199	LYS	N-CA-C	5.67	118.19	111.33
1	Q	31	ALA	N-CA-C	5.67	117.14	111.07
1	7	107	THR	N-CA-C	5.67	117.46	111.28
1	i	192	GLN	N-CA-C	5.67	117.46	111.28
1	oA	82	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	IC	184	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	ED	162	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	YD	173	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	FF	132	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	eA	143	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	kB	154	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	sB	97	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	cD	154	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	aE	100	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	uC	229	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	115	ILE	CA-C-N	5.66	126.39	119.99
1	8	115	ILE	C-N-CA	5.66	126.39	119.99
1	WE	147	PRO	CA-N-CD	-5.66	103.57	111.50
1	A	184	TRP	N-CA-CB	-5.66	101.78	110.16
1	A	200	THR	N-CA-C	5.66	118.18	111.33
1	qB	130	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	DE	167	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	LC	173	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	mD	184	TRP	CA-CB-CG	5.66	124.45	113.70
1	EE	184	TRP	CB-CG-CD1	-5.66	119.65	127.00
1	CC	173	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	XC	18	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	29	GLU	N-CA-C	5.65	117.44	111.28
1	1	189	LEU	N-CA-C	5.65	117.44	111.28
1	OA	154	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	nA	184	TRP	CA-CB-CG	5.65	124.44	113.70
1	mE	154	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	VE	154	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	d	120	HIS	N-CA-C	5.65	117.44	111.28
1	MA	97	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	mA	154	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	hD	229	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	PA	173	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	E	84	HIS	CA-C-O	-5.64	115.52	120.60
1	L	206	GLY	CA-C-N	5.64	126.89	119.84
1	L	206	GLY	C-N-CA	5.64	126.89	119.84
1	U	175	GLU	N-CA-C	5.64	117.11	111.07
1	f	195	ASN	CA-CB-CG	5.64	118.24	112.60
1	MD	162	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	8D	162	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	AE	229	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	GE	184	TRP	N-CA-CB	-5.64	100.44	110.60
1	h	36	VAL	CA-C-N	5.64	123.80	120.24
1	h	36	VAL	C-N-CA	5.64	123.80	120.24
1	QB	162	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	8D	100	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	d	195	ASN	CA-CB-CG	5.64	118.24	112.60
1	r	184	TRP	CA-CB-CG	5.64	124.31	113.60
1	IA	229	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	GE	154	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	AF	184	TRP	N-CA-CB	-5.64	100.45	110.60
1	8A	229	ARG	NE-CZ-NH1	5.64	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	PC	173	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	mA	18	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	mA	229	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	KD	18	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	fE	229	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	HA	97	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	4B	100	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	2C	18	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	9A	184	TRP	N-CA-CB	-5.63	100.46	110.60
1	4C	82	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	6D	143	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	jE	18	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	6C	173	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	s	121	ASN	CA-C-O	-5.63	116.07	121.08
1	uA	154	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	WC	143	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	kD	154	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	2B	132	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	gC	132	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	WE	145	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	r	162	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	WC	229	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	sE	18	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	oB	184	TRP	N-CA-CB	-5.62	100.49	110.60
1	D	189	LEU	N-CA-C	5.62	117.40	111.28
1	x	195	ASN	CA-CB-CG	5.62	118.22	112.60
1	FD	143	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	3A	229	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	QD	82	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	5E	154	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	pC	173	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	rC	173	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	tC	82	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	XE	184	TRP	CB-CG-CD2	-5.61	119.30	126.60
1	kD	162	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	8E	173	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	SA	18	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	fE	18	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	oE	100	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	ED	162	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	FD	154	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	iB	132	ARG	NE-CZ-NH1	5.60	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DF	143	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	CA	100	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	gB	229	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	tB	97	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	WC	173	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	8C	39	MET	CG-SD-CE	-5.60	91.24	100.20
1	bA	173	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	bB	154	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	bB	167	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	RE	143	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	JA	143	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	OA	18	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	LE	154	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	kE	162	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	h	223	GLY	N-CA-C	5.60	123.76	112.34
1	GA	100	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	c	111	LEU	N-CA-C	5.59	117.05	111.07
1	TB	173	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	2A	145	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	kB	100	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	ED	143	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	cE	173	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	lD	167	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	UE	82	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	DB	162	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	2B	154	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	UE	229	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	K	192	GLN	N-CA-C	5.58	117.37	111.28
1	bB	229	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	GC	132	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	V	206	GLY	CA-C-N	5.58	125.58	119.89
1	V	206	GLY	C-N-CA	5.58	125.58	119.89
1	YB	167	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	rB	143	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	gE	162	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	kC	18	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	122	PRO	N-CA-C	5.58	117.51	110.70
1	9D	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	ZA	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	UD	184	TRP	CB-CA-C	5.58	121.55	110.40
1	0E	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	sB	162	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vB	173	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	0C	154	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	MB	130	TYR	CB-CG-CD1	5.57	124.34	121.00
1	zE	167	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	mB	143	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	6D	154	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	HE	132	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	6	184	TRP	CB-CG-CD1	-5.57	118.55	126.90
1	1B	229	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	vD	18	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	3	190	LEU	N-CA-C	5.57	117.81	111.02
1	8	36	VAL	CA-C-N	5.57	123.75	120.24
1	8	36	VAL	C-N-CA	5.57	123.75	120.24
1	cA	82	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	KB	229	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	TB	184	TRP	CB-CG-CD1	-5.57	119.77	127.00
1	rB	184	TRP	CB-CG-CD2	5.57	133.84	126.60
1	dE	82	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	f	126	VAL	N-CA-C	5.56	116.30	110.62
1	r	159	GLU	CA-C-N	5.56	125.56	119.89
1	r	159	GLU	C-N-CA	5.56	125.56	119.89
1	jB	173	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	oB	184	TRP	CA-CB-CG	5.56	124.27	113.70
1	2E	130	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	d	89	GLY	CA-C-N	5.56	125.56	119.89
1	d	89	GLY	C-N-CA	5.56	125.56	119.89
1	x	179	GLN	N-CA-C	5.56	118.06	111.33
1	5A	100	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	163	ASP	CA-CB-CG	5.56	118.16	112.60
1	8	183	ASN	CB-CA-C	-5.56	102.15	110.88
1	HB	167	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	zB	173	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	mE	167	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	L	115	ILE	CA-C-N	5.56	126.11	119.94
1	L	115	ILE	C-N-CA	5.56	126.11	119.94
1	nD	143	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	RA	18	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	7D	82	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	u	60	GLY	CA-C-N	5.55	126.27	119.99
1	u	60	GLY	C-N-CA	5.55	126.27	119.99
1	kD	143	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	b	31	ALA	N-CA-C	5.55	118.05	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	167	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	m	147	PRO	CA-N-CD	-5.55	104.23	112.00
1	aD	162	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	KC	173	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	QD	173	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	3	163	ASP	CA-CB-CG	5.54	118.14	112.60
1	vC	167	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	xC	100	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	vE	143	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	3	36	VAL	CA-C-N	5.54	124.76	120.33
1	3	36	VAL	C-N-CA	5.54	124.76	120.33
1	7A	143	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	kD	132	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	I	147	PRO	CA-N-CD	-5.54	104.24	112.00
1	i	229	ARG	N-CA-C	5.54	118.83	111.30
1	sC	97	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	vE	162	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	cE	167	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	CD	132	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	9B	167	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	7C	132	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	YB	97	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	hD	162	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	UE	97	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	qD	147	PRO	CA-N-CD	-5.53	103.75	111.50
1	3D	100	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	XE	229	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	j	175	GLU	N-CA-C	5.53	118.07	111.71
1	6A	143	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	JC	184	TRP	N-CA-CB	-5.53	100.64	110.60
1	gC	229	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	U	106	GLY	CA-C-N	5.53	127.69	120.28
1	U	106	GLY	C-N-CA	5.53	127.69	120.28
1	j	92	ALA	N-CA-C	5.53	117.52	109.84
1	4	147	PRO	CA-N-CD	-5.53	104.26	112.00
1	YC	167	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	N	221	VAL	N-CA-C	5.53	116.26	110.62
1	FB	184	TRP	N-CA-CB	-5.53	100.66	110.60
1	TB	132	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	0C	18	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	JE	167	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	9	122	PRO	N-CA-C	5.52	117.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bA	18	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	yB	82	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	QC	152	ASP	CB-CG-OD1	5.52	123.27	118.30
1	NE	167	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	PE	173	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	HE	100	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	GC	97	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	7E	143	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	cC	167	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	X	3	VAL	CA-C-N	5.51	132.07	121.54
1	X	3	VAL	C-N-CA	5.51	132.07	121.54
1	RA	100	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	nA	184	TRP	N-CA-CB	-5.51	100.67	110.60
1	PC	173	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	W	85	PRO	CA-C-N	5.51	128.01	120.46
1	W	85	PRO	C-N-CA	5.51	128.01	120.46
1	4B	18	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	R	171	THR	CA-C-N	5.51	127.67	120.28
1	R	171	THR	C-N-CA	5.51	127.67	120.28
1	e	175	GLU	N-CA-C	5.51	117.29	111.28
1	xA	100	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	9E	82	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	CF	145	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	UE	167	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	mC	162	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	BC	82	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	jC	229	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	uD	173	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	jE	167	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Q	184	TRP	CA-CB-CG	5.50	124.05	113.60
1	SA	184	TRP	CB-CG-CD2	5.50	133.75	126.60
1	qA	147	PRO	CA-N-CD	-5.50	103.80	111.50
1	MB	143	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	7C	100	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	CD	173	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	oD	143	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	pE	143	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	J	60	GLY	CA-C-N	5.50	127.06	120.13
1	J	60	GLY	C-N-CA	5.50	127.06	120.13
1	m	192	GLN	N-CA-C	5.50	117.27	111.28
1	0B	147	PRO	CA-N-CD	-5.50	103.80	111.50
1	Q	36	VAL	CA-C-N	5.50	124.73	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	36	VAL	C-N-CA	5.50	124.73	120.33
1	7A	184	TRP	N-CA-CB	-5.50	100.70	110.60
1	ZD	143	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	bE	18	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	O	147	PRO	CA-N-CD	-5.50	104.31	112.00
1	Q	195	ASN	CA-CB-CG	5.50	118.09	112.60
1	b	183	ASN	CA-C-N	5.50	128.09	120.29
1	b	183	ASN	C-N-CA	5.50	128.09	120.29
1	PA	143	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	RB	82	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	wC	97	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	TE	100	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	vE	18	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	S	121	ASN	CA-C-N	5.49	126.04	120.38
1	S	121	ASN	C-N-CA	5.49	126.04	120.38
1	V	184	TRP	CA-CB-CG	5.49	124.04	113.60
1	d	86	VAL	N-CA-C	5.49	115.69	110.42
1	8C	173	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	6D	167	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	OE	132	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	h	106	GLY	CA-C-N	5.49	127.64	120.28
1	h	106	GLY	C-N-CA	5.49	127.64	120.28
1	GA	173	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	CB	154	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	7D	166	ASP	CB-CG-OD1	5.49	123.24	118.30
1	P	106	GLY	CA-C-N	5.49	127.63	120.28
1	P	106	GLY	C-N-CA	5.49	127.63	120.28
1	1B	97	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	lE	143	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	9B	154	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	CC	145	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	WC	97	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	mD	100	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	p	184	TRP	CB-CG-CD1	-5.48	118.67	126.90
1	SC	162	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	YD	97	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	cE	154	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	Y	62	HIS	CA-C-N	5.48	127.62	120.28
1	Y	62	HIS	C-N-CA	5.48	127.62	120.28
1	hA	82	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	3A	154	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	yC	82	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	kD	167	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	NA	97	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	DB	229	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	QE	229	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	M	192	GLN	N-CA-C	5.48	117.25	111.28
1	ZA	85	PRO	CA-N-CD	-5.48	103.83	111.50
1	W	192	GLN	N-CA-C	5.47	117.25	111.28
1	a	195	ASN	CA-CB-CG	5.47	118.08	112.60
1	mA	97	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	dB	167	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	IC	97	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	8D	97	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	aE	184	TRP	N-CA-CB	-5.47	100.75	110.60
1	cE	184	TRP	CA-CB-CG	5.47	124.10	113.70
1	FF	18	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	gA	184	TRP	CB-CG-CD2	5.47	133.72	126.60
1	uB	162	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	sC	184	TRP	CA-CB-CG	5.47	124.10	113.70
1	xD	167	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	6D	154	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	a	206	GLY	CA-C-N	5.47	126.68	119.84
1	a	206	GLY	C-N-CA	5.47	126.68	119.84
1	e	29	GLU	N-CA-C	5.47	117.05	111.14
1	EB	169	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	TB	167	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	wE	143	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	WC	197	ASP	CB-CG-OD1	5.47	123.22	118.30
1	K	36	VAL	CA-C-N	5.47	123.68	120.24
1	K	36	VAL	C-N-CA	5.47	123.68	120.24
1	JA	130	TYR	CB-CG-CD1	5.47	124.28	121.00
1	qB	162	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	lC	162	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	9C	97	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	WD	18	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	wD	162	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	V	178	SER	CA-C-N	5.46	127.60	120.28
1	V	178	SER	C-N-CA	5.46	127.60	120.28
1	X	89	GLY	CA-C-N	5.46	126.67	119.84
1	X	89	GLY	C-N-CA	5.46	126.67	119.84
1	aB	167	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	hB	100	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	rB	100	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GD	184	TRP	CA-CB-CG	5.46	124.08	113.70
1	eD	132	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	ME	100	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	nE	97	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	NA	144	MET	CG-SD-CE	-5.46	91.46	100.20
1	yA	130	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	OB	97	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	AD	147	PRO	CA-N-CD	-5.46	103.85	111.50
1	fA	154	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	I	92	ALA	CA-C-N	5.46	125.46	119.89
1	I	92	ALA	C-N-CA	5.46	125.46	119.89
1	LE	162	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	gE	143	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	i	187	GLU	N-CA-C	5.46	116.91	111.07
1	OA	184	TRP	CA-CB-CG	5.46	124.07	113.70
1	uB	97	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	zE	154	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	8A	97	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	HB	143	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	iB	97	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	aC	145	TYR	CB-CG-CD1	5.46	124.27	121.00
1	O	31	ALA	N-CA-C	5.45	117.22	111.28
1	q	198	CYS	CA-C-N	5.45	127.59	120.28
1	q	198	CYS	C-N-CA	5.45	127.59	120.28
1	w	118	MET	N-CA-C	5.45	117.22	111.28
1	iC	162	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	GD	143	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	EE	147	PRO	CA-N-CD	-5.45	103.86	111.50
1	SB	167	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	v	3	VAL	CA-C-N	5.45	131.95	121.54
1	v	3	VAL	C-N-CA	5.45	131.95	121.54
1	MD	97	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	6E	97	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	EF	144	MET	CG-SD-CE	-5.45	91.48	100.20
1	H	202	LEU	CA-C-N	5.45	127.52	120.44
1	H	202	LEU	C-N-CA	5.45	127.52	120.44
1	L	187	GLU	N-CA-C	5.45	117.22	111.28
1	pE	100	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	qE	144	MET	CG-SD-CE	-5.45	91.48	100.20
1	h	228	ALA	CA-C-N	5.45	131.94	121.54
1	h	228	ALA	C-N-CA	5.45	131.94	121.54
1	p	189	LEU	N-CA-C	5.45	117.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JE	162	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	rB	82	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	JD	143	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	1C	162	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	SA	82	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	wA	143	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	CB	184	TRP	N-CA-CB	-5.44	100.81	110.60
1	hD	18	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	36	VAL	CA-C-N	5.44	124.68	120.33
1	B	36	VAL	C-N-CA	5.44	124.68	120.33
1	U	147	PRO	CA-N-CD	-5.44	104.38	112.00
1	h	85	PRO	CA-C-N	5.44	127.91	120.35
1	h	85	PRO	C-N-CA	5.44	127.91	120.35
1	LA	167	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	rA	184	TRP	CB-CG-CD2	-5.44	119.53	126.60
1	F	60	GLY	CA-C-N	5.44	126.14	119.99
1	F	60	GLY	C-N-CA	5.44	126.14	119.99
1	3	224	PRO	N-CA-C	-5.44	107.04	114.98
1	QD	184	TRP	N-CA-CB	-5.44	100.81	110.60
1	7D	162	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	nE	167	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	e	206	GLY	CA-C-N	5.44	125.44	119.89
1	e	206	GLY	C-N-CA	5.44	125.44	119.89
1	RA	18	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	5B	100	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	X	189	LEU	N-CA-C	5.43	117.20	111.28
1	w	121	ASN	CA-C-N	5.43	125.98	120.38
1	w	121	ASN	C-N-CA	5.43	125.98	120.38
1	JE	97	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	ZE	184	TRP	N-CA-CB	-5.43	100.82	110.60
1	1	89	GLY	CA-C-N	5.43	126.63	119.84
1	1	89	GLY	C-N-CA	5.43	126.63	119.84
1	5E	132	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	h	221	VAL	N-CA-C	5.43	116.16	110.62
1	SA	167	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	T	122	PRO	N-CA-C	5.43	117.32	110.70
1	V	189	LEU	N-CA-C	5.43	117.20	111.28
1	f	146	SER	N-CA-C	5.43	116.25	109.57
1	HE	97	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	CA	132	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	vD	132	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	oC	132	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZD	97	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	g	147	PRO	CA-N-CD	-5.42	104.41	112.00
1	AA	143	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	yB	229	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	3	82	ARG	N-CA-C	5.42	118.36	111.69
1	GD	97	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	aE	173	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	TA	97	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	IC	173	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	1C	184	TRP	CA-CB-CG	5.42	123.99	113.70
1	TE	18	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	nE	132	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	7	92	ALA	CA-C-N	5.42	125.42	119.90
1	7	92	ALA	C-N-CA	5.42	125.42	119.90
1	zD	97	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	R	219	GLN	CA-C-N	5.41	125.99	119.98
1	R	219	GLN	C-N-CA	5.41	125.99	119.98
1	YA	147	PRO	CA-N-CD	-5.41	103.92	111.50
1	FA	143	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	nA	166	ASP	CB-CG-OD1	5.41	123.17	118.30
1	3E	97	ARG	C-N-CA	5.41	135.23	121.70
1	g	196	PRO	CA-C-N	5.41	127.53	120.28
1	g	196	PRO	C-N-CA	5.41	127.53	120.28
1	8A	162	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	FB	167	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	bC	143	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	fE	18	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	fA	143	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	gA	132	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	bC	132	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	xE	167	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	b	184	TRP	CA-C-N	5.41	127.52	120.28
1	b	184	TRP	C-N-CA	5.41	127.52	120.28
1	rA	82	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	bA	143	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	uE	145	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	C	195	ASN	CA-CB-CG	5.40	118.00	112.60
1	g	63	GLN	N-CA-C	5.40	117.17	111.28
1	8	159	GLU	N-CA-C	5.40	117.44	109.50
1	uE	145	TYR	CB-CG-CD1	5.40	124.24	121.00
1	yE	143	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	kA	97	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	229	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	JC	173	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	WA	132	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	UE	173	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	FB	162	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	iE	132	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	tA	97	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	b	111	LEU	N-CA-C	5.39	116.84	111.07
1	n	10	MET	N-CA-C	5.39	117.85	110.24
1	8	195	ASN	CA-CB-CG	5.39	117.99	112.60
1	VA	173	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	nD	132	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	CE	18	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	V	184	TRP	N-CA-CB	-5.39	101.92	110.28
1	NE	97	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	YE	167	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	nB	18	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	dC	132	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	bA	229	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	eA	145	TYR	CB-CG-CD1	5.39	124.23	121.00
1	4C	97	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	rD	162	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	FE	100	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	KE	97	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	XD	184	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	mD	162	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	7E	132	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	m	96	MET	N-CA-C	5.39	117.91	111.71
1	t	185	MET	N-CA-C	5.39	117.15	111.28
1	7	219	GLN	N-CA-C	5.39	117.15	111.28
1	pA	100	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	AB	184	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	pB	184	TRP	N-CA-CB	-5.38	100.91	110.60
1	dC	162	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	k	145	TYR	N-CA-C	5.38	117.15	111.28
1	YB	184	TRP	CB-CG-CD2	-5.38	119.60	126.60
1	O	60	GLY	CA-C-N	5.38	126.91	120.13
1	O	60	GLY	C-N-CA	5.38	126.91	120.13
1	b	10	MET	N-CA-C	5.38	122.26	110.80
1	g	192	GLN	N-CA-C	5.38	117.14	111.28
1	AA	173	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	2A	143	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IB	100	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	QD	100	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	aD	103	ASP	CB-CG-OD2	5.38	123.14	118.30
1	rE	100	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	kB	97	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	FC	130	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	PA	96	MET	CG-SD-CE	-5.38	91.60	100.20
1	MD	147	PRO	CA-N-CD	-5.38	103.97	111.50
1	F	206	GLY	CA-C-N	5.38	126.56	119.84
1	F	206	GLY	C-N-CA	5.38	126.56	119.84
1	h	195	ASN	CA-CB-CG	5.38	117.98	112.60
1	kC	162	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	U	189	LEU	N-CA-C	5.38	117.14	111.28
1	6C	229	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	vA	169	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	nC	154	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	BD	82	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	S	61	GLY	N-CA-C	5.37	119.14	112.64
1	s	31	ALA	N-CA-C	5.37	117.83	111.33
1	z	121	ASN	N-CA-C	-5.37	103.29	108.07
1	OC	100	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	YC	18	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	7	6	LEU	N-CA-C	5.37	117.13	111.28
1	M	206	GLY	CA-C-N	5.37	126.55	119.84
1	M	206	GLY	C-N-CA	5.37	126.55	119.84
1	QB	143	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	nB	154	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	0B	184	TRP	CB-CG-CD2	5.37	133.58	126.60
1	w	221	VAL	N-CA-C	5.37	116.09	110.62
1	lB	39	MET	CG-SD-CE	-5.37	91.61	100.20
1	aC	100	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	0E	229	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	147	PRO	CA-N-CD	-5.37	104.49	112.00
1	b	81	ASP	N-CA-CB	-5.37	102.69	110.47
1	5	121	ASN	CA-CB-CG	5.37	117.97	112.60
1	PA	154	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	KC	229	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	tE	229	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	sA	229	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	mD	18	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	V	36	VAL	CA-C-N	5.36	124.62	120.33
1	V	36	VAL	C-N-CA	5.36	124.62	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	14	ALA	N-CA-C	5.36	117.64	110.35
1	q	4	GLN	N-CA-CB	5.36	119.55	110.49
1	1C	173	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	EA	82	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	5D	132	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	JE	229	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	UA	18	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	ZC	82	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	GD	163	ASP	CB-CG-OD1	5.36	123.12	118.30
1	6	206	GLY	CA-C-N	5.36	126.53	119.84
1	6	206	GLY	C-N-CA	5.36	126.53	119.84
1	oE	18	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	s	10	MET	N-CA-C	5.35	117.99	110.23
1	P	10	MET	N-CA-C	5.35	117.79	110.24
1	Q	195	ASN	CA-C-N	5.35	124.81	119.24
1	Q	195	ASN	C-N-CA	5.35	124.81	119.24
1	CA	154	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	DB	132	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	8B	18	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	jD	143	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	R	178	SER	N-CA-C	5.35	118.23	110.42
1	R	230	VAL	N-CA-C	5.35	117.78	111.09
1	GE	184	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	wA	147	PRO	CA-N-CD	-5.35	104.01	111.50
1	jB	144	MET	CG-SD-CE	-5.35	91.64	100.20
1	pB	100	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	r	206	GLY	CA-C-N	5.35	125.34	119.89
1	r	206	GLY	C-N-CA	5.35	125.34	119.89
1	eA	147	PRO	CA-N-CD	-5.35	104.02	111.50
1	AB	143	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	bB	132	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	fB	167	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	8B	167	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	PE	154	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	VC	97	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	tC	229	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	jD	143	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	JE	184	TRP	CB-CG-CD2	-5.34	119.65	126.60
1	Y	115	ILE	CA-C-N	5.34	125.91	119.98
1	Y	115	ILE	C-N-CA	5.34	125.91	119.98
1	WD	82	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	CF	147	PRO	CA-N-CD	-5.34	104.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	111	LEU	N-CA-C	5.34	116.79	111.07
1	0	115	ILE	CA-C-N	5.34	126.01	120.03
1	0	115	ILE	C-N-CA	5.34	126.01	120.03
1	oA	154	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	5A	18	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	NB	162	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	ED	154	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	MD	18	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	cD	144	MET	CG-SD-CE	-5.34	91.65	100.20
1	Q	120	HIS	N-CA-C	5.34	117.10	111.28
1	i	189	LEU	N-CA-C	5.34	117.18	111.36
1	aA	173	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	N	86	VAL	N-CA-C	5.34	116.06	110.62
1	lA	184	TRP	CB-CG-CD1	5.34	133.94	127.00
1	3A	184	TRP	N-CA-CB	-5.33	101.00	110.60
1	pD	229	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	mE	184	TRP	N-CA-CB	-5.33	101.00	110.60
1	wA	162	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	eB	162	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	uB	100	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	p	206	GLY	CA-C-N	5.33	126.50	119.84
1	p	206	GLY	C-N-CA	5.33	126.50	119.84
1	v	111	LEU	N-CA-C	5.33	117.09	111.28
1	rA	132	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	2A	154	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	nE	167	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	G	184	TRP	CB-CG-CD1	-5.33	118.91	126.90
1	e	192	GLN	N-CA-C	5.33	117.09	111.28
1	mA	97	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	HE	132	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	i	228	ALA	CA-C-N	5.33	129.97	122.46
1	i	228	ALA	C-N-CA	5.33	129.97	122.46
1	QB	184	TRP	CA-CB-CG	5.33	123.82	113.70
1	vB	144	MET	CG-SD-CE	-5.33	91.68	100.20
1	9D	18	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	0	53	ASN	CA-CB-CG	5.33	117.93	112.60
1	TA	18	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	xB	167	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	AC	184	TRP	CB-CG-CD2	5.33	133.52	126.60
1	tC	97	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	pD	82	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	226	HIS	N-CA-C	5.32	122.14	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	195	ASN	CA-C-N	5.32	124.78	119.24
1	j	195	ASN	C-N-CA	5.32	124.78	119.24
1	BF	143	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	r	115	ILE	CA-C-N	5.32	126.00	119.99
1	r	115	ILE	C-N-CA	5.32	126.00	119.99
1	3A	162	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	CB	184	TRP	CA-CB-CG	5.32	123.81	113.70
1	KC	184	TRP	N-CA-CB	-5.32	101.02	110.60
1	zC	97	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	7E	167	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	NC	18	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	BF	143	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	UC	184	TRP	CA-CB-CG	5.32	123.80	113.70
1	qD	229	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	IE	162	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	YE	143	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	L	107	THR	N-CA-C	5.32	117.76	111.33
1	S	184	TRP	CB-CA-C	5.32	119.89	110.85
1	5	206	GLY	CA-C-N	5.32	125.31	119.89
1	5	206	GLY	C-N-CA	5.32	125.31	119.89
1	DC	143	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	s	147	PRO	CA-N-CD	-5.31	104.56	112.00
1	gA	173	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	5B	163	ASP	CB-CG-OD1	5.31	123.08	118.30
1	ME	97	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	vE	100	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	DA	144	MET	CG-SD-CE	-5.31	91.70	100.20
1	MD	100	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	e	36	VAL	CA-C-N	5.31	123.59	120.24
1	e	36	VAL	C-N-CA	5.31	123.59	120.24
1	MA	147	PRO	CA-N-CD	-5.31	104.06	111.50
1	1A	18	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	7B	82	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	yD	162	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	UA	173	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	eE	97	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	V	62	HIS	CA-C-N	5.31	127.39	120.28
1	V	62	HIS	C-N-CA	5.31	127.39	120.28
1	a	18	ARG	CA-C-N	5.31	127.39	120.28
1	a	18	ARG	C-N-CA	5.31	127.39	120.28
1	z	198	CYS	CA-C-N	5.31	127.39	120.28
1	z	198	CYS	C-N-CA	5.31	127.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8D	173	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	9E	184	TRP	CB-CA-C	5.31	121.01	110.40
1	c	120	HIS	N-CA-C	5.30	117.06	111.28
1	9	228	ALA	CA-C-N	5.30	128.62	120.82
1	9	228	ALA	C-N-CA	5.30	128.62	120.82
1	7C	154	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	iD	4	GLN	N-CA-CB	5.30	120.15	110.60
1	rD	132	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	vA	97	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	aB	184	TRP	N-CA-CB	-5.30	101.06	110.60
1	uB	154	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	xC	143	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	kD	147	PRO	CA-N-CD	-5.30	104.08	111.50
1	sE	132	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	G	195	ASN	CA-CB-CG	5.30	117.90	112.60
1	r	185	MET	N-CA-C	5.30	117.14	111.36
1	nB	143	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	Y	192	GLN	N-CA-C	5.30	117.05	111.28
1	AA	162	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	0B	229	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	UC	143	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	GA	162	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	tB	162	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	HD	167	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	t	84	HIS	O-C-N	-5.29	115.23	121.32
1	YE	173	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	4E	162	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	b	178	SER	N-CA-C	5.29	117.75	110.35
1	oE	18	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	3E	184	TRP	CA-CB-CG	5.29	123.75	113.70
1	8E	163	ASP	CB-CG-OD2	5.29	123.06	118.30
1	7B	229	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	uE	147	PRO	CA-N-CD	-5.29	104.10	111.50
1	gB	229	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	R	112	GLN	CA-C-N	5.28	127.36	120.28
1	R	112	GLN	C-N-CA	5.28	127.36	120.28
1	MB	100	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	RB	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	gC	100	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	uD	184	TRP	CB-CG-CD2	-5.28	119.73	126.60
1	cE	229	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	5	85	PRO	CA-C-N	5.28	127.58	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	85	PRO	C-N-CA	5.28	127.58	120.50
1	YE	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	I	36	VAL	CA-C-N	5.28	124.56	120.33
1	I	36	VAL	C-N-CA	5.28	124.56	120.33
1	2	184	TRP	CA-CB-CG	5.28	123.63	113.60
1	GA	229	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	DD	143	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	QD	184	TRP	CA-CB-CG	5.28	123.73	113.70
1	G	178	SER	N-CA-C	5.28	118.12	110.42
1	4C	184	TRP	CB-CG-CD2	5.28	133.46	126.60
1	i	87	HIS	CA-CB-CG	5.28	119.08	113.80
1	3	228	ALA	N-CA-C	5.28	117.63	110.35
1	tA	143	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	qB	130	TYR	CB-CG-CD1	5.28	124.17	121.00
1	DD	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	JD	229	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	150	ILE	N-CA-C	5.27	116.00	110.62
1	2A	97	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	BE	144	MET	CG-SD-CE	-5.27	91.77	100.20
1	L	163	ASP	CA-CB-CG	5.27	117.87	112.60
1	a	184	TRP	CB-CA-C	5.27	121.00	109.99
1	T	195	ASN	CA-CB-CG	5.27	117.87	112.60
1	3E	184	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	Q	192	GLN	N-CA-C	5.27	117.02	111.28
1	GA	100	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	8A	147	PRO	CA-N-CD	-5.27	104.13	111.50
1	9A	184	TRP	CB-CG-CD2	-5.27	119.75	126.60
1	lB	143	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	e	86	VAL	N-CA-C	5.26	116.33	108.54
1	5	36	VAL	CA-C-N	5.26	124.54	120.33
1	5	36	VAL	C-N-CA	5.26	124.54	120.33
1	SC	18	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	eD	162	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	BE	167	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	GE	100	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	lE	173	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	0	192	GLN	N-CA-C	5.26	117.02	111.28
1	E	121	ASN	CA-C-N	5.26	125.80	120.38
1	E	121	ASN	C-N-CA	5.26	125.80	120.38
1	LA	100	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	tA	144	MET	CG-SD-CE	-5.26	91.78	100.20
1	EB	229	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SB	162	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	CF	100	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	j	179	GLN	N-CA-C	5.26	116.70	111.07
1	m	99	PRO	N-CA-C	5.26	119.47	111.11
1	y	36	VAL	CA-C-N	5.26	123.55	120.24
1	y	36	VAL	C-N-CA	5.26	123.55	120.24
1	qD	97	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	LE	85	PRO	CA-N-CD	-5.26	104.14	111.50
1	RE	143	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	9	14	ALA	N-CA-C	5.26	117.50	110.35
1	KC	132	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	4C	100	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	QC	154	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	qC	173	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	tC	173	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	HD	143	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	206	GLY	CA-C-N	5.25	126.41	119.84
1	C	206	GLY	C-N-CA	5.25	126.41	119.84
1	h	176	GLN	N-CA-C	5.25	118.68	111.54
1	z	3	VAL	CA-C-N	5.25	131.57	121.54
1	z	3	VAL	C-N-CA	5.25	131.57	121.54
1	3A	97	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	FD	154	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	rE	154	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	195	ASN	CA-CB-CG	5.25	117.85	112.60
1	0D	162	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	IC	154	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	nC	82	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	K	206	GLY	CA-C-N	5.25	126.40	119.84
1	K	206	GLY	C-N-CA	5.25	126.40	119.84
1	HA	162	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	YA	154	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	2C	154	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	AD	143	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	ZE	97	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	a	169	TYR	N-CA-C	5.25	117.00	111.28
1	CA	154	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	UA	100	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	IB	167	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	SD	145	TYR	CB-CG-CD1	5.25	124.15	121.00
1	q	185	MET	CA-C-N	5.25	127.31	120.28
1	q	185	MET	C-N-CA	5.25	127.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	206	GLY	CA-C-N	5.25	126.40	119.84
1	1	206	GLY	C-N-CA	5.25	126.40	119.84
1	SA	147	PRO	CA-N-CD	-5.25	104.16	111.50
1	wB	229	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	MD	97	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	CE	82	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	zB	100	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	wD	145	TYR	CB-CG-CD1	5.24	124.15	121.00
1	0E	143	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	QB	132	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	AE	162	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	w	9	GLN	CA-C-N	5.24	131.55	121.54
1	w	9	GLN	C-N-CA	5.24	131.55	121.54
1	4	199	LYS	N-CA-C	5.24	117.67	111.33
1	WA	162	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	WE	147	PRO	N-CA-C	5.24	125.72	112.10
1	m	98	GLU	CA-C-N	5.24	125.23	119.89
1	m	98	GLU	C-N-CA	5.24	125.23	119.89
1	p	3	VAL	CA-C-N	5.24	131.54	121.54
1	p	3	VAL	C-N-CA	5.24	131.54	121.54
1	p	122	PRO	CA-C-N	5.24	126.39	119.84
1	p	122	PRO	C-N-CA	5.24	126.39	119.84
1	3A	184	TRP	CA-CB-CG	5.23	123.64	113.70
1	sD	167	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	0D	173	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	oD	173	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	V	207	PRO	N-CA-C	5.23	119.43	111.11
1	tB	143	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	hC	97	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	EE	215	MET	CG-SD-CE	-5.23	91.83	100.20
1	U	206	GLY	CA-C-N	5.23	126.38	119.84
1	U	206	GLY	C-N-CA	5.23	126.38	119.84
1	w	150	ILE	N-CA-C	5.23	116.58	110.62
1	5E	229	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	DF	132	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	EA	162	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	OC	82	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	L	3	VAL	CA-C-N	5.22	131.52	121.54
1	L	3	VAL	C-N-CA	5.22	131.52	121.54
1	yA	130	TYR	CB-CG-CD1	5.22	124.13	121.00
1	EB	167	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	fB	143	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9C	18	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	JD	97	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	OE	82	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	V	50	GLN	N-CA-C	5.22	116.65	111.07
1	3	226	HIS	CA-C-N	5.22	128.12	120.71
1	3	226	HIS	C-N-CA	5.22	128.12	120.71
1	pA	154	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	AD	132	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	PD	97	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	AF	132	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	OD	18	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	d	105	ALA	CA-C-N	5.22	125.87	120.03
1	d	105	ALA	C-N-CA	5.22	125.87	120.03
1	7	206	GLY	CA-C-N	5.22	126.36	119.84
1	7	206	GLY	C-N-CA	5.22	126.36	119.84
1	AA	145	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	lE	184	TRP	N-CA-CB	-5.22	101.21	110.60
1	K	195	ASN	CA-C-N	5.21	124.66	119.24
1	K	195	ASN	C-N-CA	5.21	124.66	119.24
1	O	99	PRO	N-CA-C	5.21	119.39	111.15
1	0A	184	TRP	CA-CB-CG	5.21	123.60	113.70
1	KB	100	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	xE	82	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	R	14	ALA	N-CA-C	5.21	117.01	110.24
1	6	150	ILE	N-CA-C	5.21	115.93	110.62
1	sB	184	TRP	N-CA-CB	-5.21	101.22	110.60
1	ID	97	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	sE	145	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	H	9	GLN	N-CA-C	5.21	117.22	109.25
1	pB	154	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	fD	18	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	FF	130	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	sB	173	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	hC	97	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	zC	100	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	SD	97	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	sD	167	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	1D	154	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	2C	229	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	8	184	TRP	N-CA-CB	-5.20	102.46	110.16
1	QC	229	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	yD	167	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZE	184	TRP	CA-CB-CG	5.20	123.59	113.70
1	8E	100	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	G	121	ASN	CA-C-N	5.20	125.74	120.38
1	G	121	ASN	C-N-CA	5.20	125.74	120.38
1	V	52	LEU	CA-C-N	5.20	127.25	120.28
1	V	52	LEU	C-N-CA	5.20	127.25	120.28
1	Z	86	VAL	N-CA-C	5.20	115.93	110.62
1	6B	145	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	MC	132	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	j	89	GLY	CA-C-N	5.20	125.19	119.89
1	j	89	GLY	C-N-CA	5.20	125.19	119.89
1	ME	154	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	iE	173	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	122	PRO	CA-C-N	5.20	126.34	119.84
1	F	122	PRO	C-N-CA	5.20	126.34	119.84
1	Z	121	ASN	CA-C-O	-5.20	115.49	120.64
1	6B	162	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	DA	130	TYR	CB-CG-CD1	5.20	124.12	121.00
1	cD	100	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	5D	82	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	m	63	GLN	N-CA-C	5.20	117.69	111.71
1	y	60	GLY	CA-C-N	5.20	125.75	119.98
1	y	60	GLY	C-N-CA	5.20	125.75	119.98
1	9	195	ASN	CA-CB-CG	5.20	117.80	112.60
1	ZD	18	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	wD	100	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	sB	82	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	5C	173	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	u	183	ASN	CA-C-N	5.19	127.24	120.28
1	u	183	ASN	C-N-CA	5.19	127.24	120.28
1	8C	184	TRP	CA-CB-CG	5.19	123.56	113.70
1	NE	184	TRP	CB-CG-CD2	-5.19	119.85	126.60
1	WA	229	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	jC	167	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	ZD	173	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	KE	184	TRP	CA-CB-CG	5.19	123.56	113.70
1	Z	187	GLU	N-CA-C	5.19	117.34	111.11
1	0	175	GLU	N-CA-C	5.19	116.62	111.07
1	m	62	HIS	CA-C-N	5.18	127.75	120.28
1	m	62	HIS	C-N-CA	5.18	127.75	120.28
1	YE	18	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	156	GLY	CA-C-N	5.18	125.23	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	156	GLY	C-N-CA	5.18	125.23	119.32
1	sC	184	TRP	N-CA-CB	-5.18	101.27	110.60
1	Z	122	PRO	N-CA-C	5.18	117.02	110.70
1	MB	162	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	wD	229	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	U	122	PRO	N-CA-C	5.18	117.02	110.70
1	t	89	GLY	CA-C-N	5.18	125.17	119.89
1	t	89	GLY	C-N-CA	5.18	125.17	119.89
1	9	36	VAL	CA-C-N	5.18	124.47	120.33
1	9	36	VAL	C-N-CA	5.18	124.47	120.33
1	mC	147	PRO	CA-N-CD	-5.18	104.25	111.50
1	g	115	ILE	CA-C-N	5.18	125.69	119.94
1	g	115	ILE	C-N-CA	5.18	125.69	119.94
1	v	115	ILE	CA-C-N	5.18	125.73	119.98
1	v	115	ILE	C-N-CA	5.18	125.73	119.98
1	gA	82	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	VC	85	PRO	CA-N-CD	-5.18	104.25	111.50
1	8D	147	PRO	CA-N-CD	-5.18	104.25	111.50
1	XE	173	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	60	GLY	CA-C-N	5.18	126.65	120.13
1	B	60	GLY	C-N-CA	5.18	126.65	120.13
1	vA	184	TRP	CB-CG-CD2	5.18	133.33	126.60
1	YB	173	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	aE	143	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	g	175	GLU	N-CA-C	5.17	116.92	111.28
1	wC	162	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	2C	173	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	WD	184	TRP	CB-CA-C	5.17	120.75	110.40
1	sD	154	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	7	122	PRO	CA-C-N	5.17	126.31	119.84
1	7	122	PRO	C-N-CA	5.17	126.31	119.84
1	oB	173	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	G	99	PRO	N-CA-C	5.17	119.21	111.14
1	N	99	PRO	N-CA-C	5.17	119.32	111.15
1	j	195	ASN	CA-CB-CG	5.17	117.77	112.60
1	IB	84	HIS	CA-C-N	5.17	131.58	117.10
1	HD	118	MET	CG-SD-CE	-5.17	91.93	100.20
1	nD	167	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	lC	167	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	9E	39	MET	CG-SD-CE	-5.17	91.93	100.20
1	e	189	LEU	N-CA-C	5.17	116.91	111.28
1	z	98	GLU	CA-C-N	5.17	126.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	z	98	GLU	C-N-CA	5.17	126.30	119.84
1	qA	145	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	CC	147	PRO	CA-N-CD	-5.17	104.27	111.50
1	EC	10	MET	CG-SD-CE	-5.17	91.93	100.20
1	HD	132	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	L	89	GLY	CA-C-N	5.17	126.30	119.84
1	L	89	GLY	C-N-CA	5.17	126.30	119.84
1	P	47	ALA	N-CA-C	5.17	118.28	110.64
1	k	195	ASN	CA-CB-CG	5.17	117.77	112.60
1	4C	184	TRP	CA-CB-CG	5.17	123.51	113.70
1	dB	144	MET	CG-SD-CE	-5.16	91.94	100.20
1	JC	184	TRP	CA-CB-CG	5.16	123.51	113.70
1	0C	143	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	aD	169	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	LA	154	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	6A	82	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	kA	147	PRO	N-CA-C	5.16	125.52	112.10
1	DB	154	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	QC	184	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	CD	184	TRP	CA-CB-CG	5.16	123.51	113.70
1	YD	147	PRO	CA-N-CD	-5.16	104.27	111.50
1	HE	167	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	vC	162	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	7	195	ASN	CA-C-N	5.16	124.60	119.24
1	7	195	ASN	C-N-CA	5.16	124.60	119.24
1	IB	97	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	S	183	ASN	CA-C-N	5.16	127.61	120.29
1	S	183	ASN	C-N-CA	5.16	127.61	120.29
1	bA	167	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	CB	82	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	5B	100	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	QA	97	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	s	192	GLN	N-CA-C	5.15	116.90	111.28
1	u	171	THR	CA-C-N	5.15	127.18	120.28
1	u	171	THR	C-N-CA	5.15	127.18	120.28
1	EA	229	ARG	N-CA-C	5.15	124.91	111.00
1	MA	184	TRP	CB-CG-CD2	5.15	133.30	126.60
1	EA	167	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	zB	184	TRP	CA-CB-CG	5.15	123.49	113.70
1	WD	184	TRP	CA-CB-CG	5.15	123.49	113.70
1	AA	167	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	rA	184	TRP	N-CA-CB	-5.15	101.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	190	LEU	N-CA-C	5.15	117.56	111.33
1	rA	143	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	YB	184	TRP	CA-CB-CG	5.15	123.48	113.70
1	oB	147	PRO	CA-N-CD	-5.15	104.29	111.50
1	i	111	LEU	N-CA-C	5.14	116.57	111.07
1	2	189	LEU	N-CA-C	5.14	116.89	111.28
1	HB	97	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	5B	167	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	eD	184	TRP	CB-CA-C	5.14	120.69	110.40
1	2D	229	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	178	SER	N-CA-C	5.14	117.49	110.24
1	Z	184	TRP	CB-CA-C	5.14	119.27	110.01
1	hA	184	TRP	N-CA-CB	-5.14	101.34	110.60
1	CB	229	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	hD	162	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	K	44	SER	CA-C-N	5.14	128.51	120.75
1	K	44	SER	C-N-CA	5.14	128.51	120.75
1	R	48	THR	CA-C-N	5.14	124.59	119.24
1	R	48	THR	C-N-CA	5.14	124.59	119.24
1	u	107	THR	N-CA-C	5.14	116.88	111.28
1	RB	144	MET	CG-SD-CE	-5.14	91.97	100.20
1	XA	100	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	LB	132	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	4C	162	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	AE	97	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	J	28	GLU	CA-C-N	5.14	127.17	120.28
1	J	28	GLU	C-N-CA	5.14	127.17	120.28
1	R	111	LEU	N-CA-C	5.14	116.88	111.28
1	n	85	PRO	CA-C-N	5.14	127.49	120.35
1	n	85	PRO	C-N-CA	5.14	127.49	120.35
1	q	9	GLN	N-CA-C	5.14	117.33	110.35
1	GA	184	TRP	N-CA-CB	-5.14	101.35	110.60
1	vC	82	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	GD	162	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	EE	229	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	f	115	ILE	CA-C-N	5.13	125.78	120.03
1	f	115	ILE	C-N-CA	5.13	125.78	120.03
1	BD	96	MET	CG-SD-CE	-5.13	91.98	100.20
1	3D	167	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	K	111	LEU	N-CA-C	5.13	116.56	111.07
1	v	229	ARG	N-CA-C	5.13	116.92	110.91
1	2	6	LEU	CA-C-N	5.13	127.16	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	6	LEU	C-N-CA	5.13	127.16	120.28
1	uC	130	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	PE	229	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	d	33	SER	CA-C-N	5.13	125.42	119.47
1	d	33	SER	C-N-CA	5.13	125.42	119.47
1	sA	229	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	DB	4	GLN	N-CA-CB	5.13	119.84	110.60
1	RD	167	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	c	206	GLY	CA-C-N	5.13	125.12	119.89
1	c	206	GLY	C-N-CA	5.13	125.12	119.89
1	yA	184	TRP	CA-CB-CG	5.13	123.45	113.70
1	NE	229	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	E	122	PRO	N-CA-C	5.13	116.96	110.70
1	h	184	TRP	CA-CB-CG	5.13	123.34	113.60
1	UA	229	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	zC	154	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	cE	147	PRO	CA-N-CD	-5.13	104.32	111.50
1	j	198	CYS	CA-C-N	5.13	127.66	120.28
1	j	198	CYS	C-N-CA	5.13	127.66	120.28
1	AC	100	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	dE	167	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	W	206	GLY	CA-C-N	5.12	125.12	119.89
1	W	206	GLY	C-N-CA	5.12	125.12	119.89
1	3	61	GLY	N-CA-C	5.12	125.33	113.18
1	bB	173	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	k	59	VAL	N-CA-C	5.12	116.84	109.51
1	F	33	SER	CA-C-N	5.12	125.41	119.47
1	F	33	SER	C-N-CA	5.12	125.41	119.47
1	n	92	ALA	N-CA-C	5.12	116.96	109.84
1	x	10	MET	N-CA-C	5.12	117.46	110.24
1	PB	82	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	QB	132	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	oB	167	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	IE	184	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	fE	173	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	AA	229	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	AA	229	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	eD	143	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	BE	229	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	aE	18	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	EB	184	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	hE	184	TRP	CB-CG-CD2	5.12	133.25	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	oE	184	TRP	CA-CB-CG	5.12	123.42	113.70
1	v	184	TRP	CB-CG-CD1	-5.12	119.22	126.90
1	zB	84	HIS	CA-C-N	5.12	131.43	117.10
1	6D	162	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	dB	18	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	fC	132	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	0E	82	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	t	29	GLU	N-CA-C	5.11	116.93	111.36
1	fC	100	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	UD	173	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	lA	100	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	eB	154	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	2B	173	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	oE	184	TRP	N-CA-CB	-5.11	101.40	110.60
1	0	171	THR	CA-C-N	5.11	127.12	120.28
1	0	171	THR	C-N-CA	5.11	127.12	120.28
1	dB	97	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	hE	154	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	N	126	VAL	N-CA-C	5.11	115.83	110.62
1	U	10	MET	N-CA-C	5.11	117.63	110.23
1	kC	97	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	FF	130	TYR	CB-CG-CD1	5.11	124.06	121.00
1	QB	18	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	pA	96	MET	CG-SD-CE	-5.10	92.04	100.20
1	uD	229	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	rE	173	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	s	48	THR	CA-C-N	5.10	124.55	119.24
1	s	48	THR	C-N-CA	5.10	124.55	119.24
1	4	33	SER	N-CA-C	5.10	116.31	109.83
1	8B	154	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	OC	145	TYR	CB-CG-CD1	5.10	124.06	121.00
1	YE	184	TRP	CA-CB-CG	5.10	123.39	113.70
1	G	80	TRP	CA-C-N	5.10	127.11	120.28
1	G	80	TRP	C-N-CA	5.10	127.11	120.28
1	P	122	PRO	CA-C-N	5.10	126.21	119.84
1	P	122	PRO	C-N-CA	5.10	126.21	119.84
1	g	84	HIS	CA-CB-CG	-5.10	108.70	113.80
1	5	84	HIS	CA-CB-CG	-5.10	108.70	113.80
1	PC	18	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	oD	154	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	J	3	VAL	CA-C-N	5.10	131.28	121.54
1	J	3	VAL	C-N-CA	5.10	131.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aC	103	ASP	CB-CG-OD1	5.10	122.89	118.30
1	zC	184	TRP	CA-CB-CG	5.10	123.39	113.70
1	pB	184	TRP	CA-CB-CG	5.10	123.38	113.70
1	k	121	ASN	CA-C-N	5.09	125.63	120.38
1	k	121	ASN	C-N-CA	5.09	125.63	120.38
1	m	206	GLY	CA-C-N	5.09	125.37	119.92
1	m	206	GLY	C-N-CA	5.09	125.37	119.92
1	yA	154	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	Y	10	MET	N-CA-C	5.09	117.61	110.23
1	o	115	ILE	CA-C-N	5.09	125.59	119.94
1	o	115	ILE	C-N-CA	5.09	125.59	119.94
1	q	164	TYR	N-CA-C	5.09	116.52	111.07
1	hA	184	TRP	CA-CB-CG	5.09	123.37	113.70
1	GD	197	ASP	CB-CG-OD1	5.09	122.88	118.30
1	eD	167	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	8D	143	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	I	146	SER	N-CA-C	5.09	121.06	109.81
1	JC	229	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	VC	144	MET	CG-SD-CE	-5.09	92.06	100.20
1	AE	18	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	a	126	VAL	N-CA-C	5.09	115.81	110.62
1	y	150	ILE	N-CA-C	5.09	117.41	111.05
1	nB	167	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	YC	173	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	qE	167	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	AF	100	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	8	141	ILE	N-CA-C	5.08	115.81	110.62
1	JB	100	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	AC	100	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	J	31	ALA	N-CA-C	5.08	121.63	110.80
1	6B	184	TRP	N-CA-CB	-5.08	101.45	110.60
1	DD	82	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	QD	144	MET	CG-SD-CE	-5.08	92.07	100.20
1	bD	132	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	192	GLN	N-CA-C	5.08	116.82	111.28
1	P	36	VAL	CA-C-N	5.08	124.39	120.33
1	P	36	VAL	C-N-CA	5.08	124.39	120.33
1	k	58	THR	CA-C-N	5.08	127.50	120.49
1	k	58	THR	C-N-CA	5.08	127.50	120.49
1	SA	184	TRP	CA-CB-CG	5.08	123.35	113.70
1	PB	18	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	y	206	GLY	CA-C-N	5.08	125.07	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	206	GLY	C-N-CA	5.08	125.07	119.89
1	C	122	PRO	CA-C-N	5.08	126.19	119.84
1	C	122	PRO	C-N-CA	5.08	126.19	119.84
1	M	5	ASN	CA-CB-CG	5.08	117.68	112.60
1	Q	111	LEU	N-CA-C	5.08	117.20	111.11
1	Q	206	GLY	CA-C-N	5.08	126.19	119.84
1	Q	206	GLY	C-N-CA	5.08	126.19	119.84
1	r	60	GLY	CA-C-N	5.08	125.73	119.99
1	r	60	GLY	C-N-CA	5.08	125.73	119.99
1	5C	154	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	K	122	PRO	N-CA-C	5.08	116.89	110.70
1	KA	229	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	4	126	VAL	N-CA-C	5.08	115.80	110.62
1	9A	97	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	VB	154	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	T	122	PRO	CA-C-N	5.07	126.18	119.84
1	T	122	PRO	C-N-CA	5.07	126.18	119.84
1	r	184	TRP	CB-CA-C	5.07	119.47	110.85
1	TC	82	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	0C	162	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	7C	184	TRP	N-CA-CB	-5.07	101.47	110.60
1	xD	97	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	SE	229	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	1	183	ASN	CA-C-N	5.07	127.08	120.28
1	1	183	ASN	C-N-CA	5.07	127.08	120.28
1	4E	229	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	H	61	GLY	N-CA-C	5.07	118.77	112.64
1	S	36	VAL	CA-C-N	5.07	123.43	120.24
1	S	36	VAL	C-N-CA	5.07	123.43	120.24
1	g	111	LEU	N-CA-C	5.07	116.49	111.07
1	x	99	PRO	N-CA-C	5.07	119.52	111.26
1	a	98	GLU	CA-C-N	5.07	126.17	119.84
1	a	98	GLU	C-N-CA	5.07	126.17	119.84
1	d	33	SER	N-CA-C	5.07	116.08	109.64
1	2A	162	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	yC	68	MET	CG-SD-CE	-5.07	92.09	100.20
1	PD	143	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	K	112	GLN	CA-C-N	5.07	127.07	120.28
1	K	112	GLN	C-N-CA	5.07	127.07	120.28
1	S	31	ALA	N-CA-C	5.07	121.59	110.80
1	yD	132	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	Q	89	GLY	CA-C-N	5.06	125.06	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	89	GLY	C-N-CA	5.06	125.06	119.89
1	mA	184	TRP	CA-CB-CG	5.06	123.32	113.70
1	xD	18	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	HE	184	TRP	CB-CG-CD1	5.06	133.58	127.00
1	g	226	HIS	N-CA-C	5.06	117.24	110.35
1	MA	103	ASP	CB-CG-OD1	5.06	122.86	118.30
1	TC	154	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	cD	184	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	iD	100	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	LA	100	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	SA	145	TYR	CB-CG-CD1	5.06	124.03	121.00
1	X	106	GLY	CA-C-N	5.05	127.05	120.28
1	X	106	GLY	C-N-CA	5.05	127.05	120.28
1	X	206	GLY	CA-C-N	5.05	126.16	119.84
1	X	206	GLY	C-N-CA	5.05	126.16	119.84
1	sC	147	PRO	CA-N-CD	-5.05	104.42	111.50
1	DF	197	ASP	CB-CG-OD2	5.05	122.85	118.30
1	a	189	LEU	N-CA-C	5.05	116.48	111.07
1	k	99	PRO	N-CA-C	5.05	122.88	112.47
1	dB	18	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	2C	162	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	5D	143	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	BE	173	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	iE	162	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	v	89	GLY	CA-C-N	5.05	126.15	119.84
1	v	89	GLY	C-N-CA	5.05	126.15	119.84
1	SC	143	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	pA	144	MET	CG-SD-CE	-5.05	92.12	100.20
1	JB	143	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	t	98	GLU	CA-C-N	5.05	126.15	119.84
1	t	98	GLU	C-N-CA	5.05	126.15	119.84
1	bC	100	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	f	225	GLY	CA-C-N	5.05	131.18	121.54
1	f	225	GLY	C-N-CA	5.05	131.18	121.54
1	W	16	SER	CA-C-N	5.04	125.07	119.32
1	W	16	SER	C-N-CA	5.04	125.07	119.32
1	jA	169	TYR	CB-CG-CD2	5.04	124.03	121.00
1	H	9	GLN	CA-C-N	5.04	128.82	121.31
1	H	9	GLN	C-N-CA	5.04	128.82	121.31
1	S	184	TRP	CA-CB-CG	5.04	123.18	113.60
1	V	225	GLY	N-CA-C	-5.04	106.89	112.04
1	f	175	GLU	N-CA-C	5.04	116.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	126	VAL	N-CA-C	5.04	115.76	110.62
1	yA	173	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	GE	130	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	l	183	ASN	CA-CB-CG	5.04	117.64	112.60
1	2	58	THR	CA-C-N	5.04	127.45	120.49
1	2	58	THR	C-N-CA	5.04	127.45	120.49
1	8	121	ASN	CA-C-N	5.04	125.57	120.38
1	8	121	ASN	C-N-CA	5.04	125.57	120.38
1	qA	145	TYR	CB-CG-CD1	5.04	124.03	121.00
1	qC	100	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	j	177	ALA	N-CA-C	5.04	117.35	110.55
1	I	48	THR	CA-C-N	5.04	124.48	119.24
1	I	48	THR	C-N-CA	5.04	124.48	119.24
1	V	121	ASN	CA-C-O	-5.04	116.60	121.08
1	f	219	GLN	N-CA-C	5.04	116.46	111.07
1	BA	162	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	hB	173	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	WE	145	TYR	CB-CG-CD1	5.04	124.02	121.00
1	F	34	PRO	N-CA-C	5.04	121.11	113.81
1	FA	167	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	T	88	ALA	N-CA-C	5.04	117.20	110.35
1	d	122	PRO	CA-C-N	5.04	126.14	119.84
1	d	122	PRO	C-N-CA	5.04	126.14	119.84
1	8	28	GLU	N-CA-C	5.04	116.58	111.14
1	OD	173	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	uC	154	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	eD	82	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	R	156	GLY	CA-C-N	5.03	125.06	119.32
1	R	156	GLY	C-N-CA	5.03	125.06	119.32
1	b	145	TYR	N-CA-C	5.03	116.45	111.07
1	mB	144	MET	CG-SD-CE	-5.03	92.15	100.20
1	lC	100	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	w	122	PRO	CA-C-N	5.03	126.13	119.84
1	w	122	PRO	C-N-CA	5.03	126.13	119.84
1	x	31	ALA	N-CA-C	5.03	119.67	111.37
1	KB	100	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	gC	97	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	225	GLY	CA-C-N	5.03	131.15	121.54
1	C	225	GLY	C-N-CA	5.03	131.15	121.54
1	w	206	GLY	CA-C-N	5.03	126.13	119.84
1	w	206	GLY	C-N-CA	5.03	126.13	119.84
1	MA	145	TYR	CB-CG-CD2	-5.03	117.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3B	143	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	tE	173	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	t	62	HIS	CA-C-N	5.03	127.02	120.28
1	t	62	HIS	C-N-CA	5.03	127.02	120.28
1	wC	4	GLN	N-CA-CB	5.03	119.64	110.60
1	FE	184	TRP	N-CA-CB	-5.03	101.55	110.60
1	PE	229	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	j	219	GLN	N-CA-C	5.02	116.76	111.28
1	m	189	LEU	N-CA-C	5.02	116.76	111.28
1	0	31	ALA	N-CA-C	5.02	117.41	111.33
1	SA	145	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	H	4	GLN	N-CA-CB	5.02	118.98	110.49
1	L	120	HIS	N-CA-C	5.02	116.75	111.28
1	V	171	THR	CA-C-N	5.02	127.51	120.28
1	V	171	THR	C-N-CA	5.02	127.51	120.28
1	7A	167	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	9A	167	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	dA	132	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	2	145	TYR	N-CA-C	5.02	116.44	111.07
1	SE	68	MET	CG-SD-CE	-5.02	92.17	100.20
1	CC	163	ASP	CB-CG-OD2	5.02	122.82	118.30
1	ZD	143	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	RE	167	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	bE	18	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	I	115	ILE	CA-C-N	5.02	125.66	119.99
1	I	115	ILE	C-N-CA	5.02	125.66	119.99
1	5	156	GLY	CA-C-N	5.02	126.11	119.84
1	5	156	GLY	C-N-CA	5.02	126.11	119.84
1	h	122	PRO	CA-C-N	5.01	126.11	119.84
1	h	122	PRO	C-N-CA	5.01	126.11	119.84
1	x	30	LYS	CA-C-N	5.01	128.34	120.82
1	x	30	LYS	C-N-CA	5.01	128.34	120.82
1	y	10	MET	N-CA-C	5.01	121.48	110.80
1	GA	184	TRP	CA-CB-CG	5.01	123.23	113.70
1	HB	144	MET	CG-SD-CE	-5.01	92.18	100.20
1	4D	229	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	b	68	MET	CA-C-N	5.01	127.00	120.28
1	b	68	MET	C-N-CA	5.01	127.00	120.28
1	j	74	ASN	CA-C-N	5.01	126.96	120.44
1	j	74	ASN	C-N-CA	5.01	126.96	120.44
1	lA	173	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	rC	144	MET	CG-SD-CE	-5.01	92.18	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	132	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	TA	167	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	QC	173	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	m	175	GLU	N-CA-C	5.01	116.74	111.28
1	t	36	VAL	CA-C-N	5.01	124.34	120.33
1	t	36	VAL	C-N-CA	5.01	124.34	120.33
1	2	92	ALA	N-CA-C	5.01	116.00	109.64
1	8C	162	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	g	136	LEU	CA-C-N	5.01	125.51	120.00
1	g	136	LEU	C-N-CA	5.01	125.51	120.00
1	XA	162	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	6A	162	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	180	GLU	CA-C-N	5.01	126.87	120.56
1	C	180	GLU	C-N-CA	5.01	126.87	120.56
1	C	191	VAL	CA-C-N	5.01	126.99	120.28
1	C	191	VAL	C-N-CA	5.01	126.99	120.28
1	D	228	ALA	N-CA-C	5.01	117.06	108.90
1	N	88	ALA	N-CA-C	5.01	117.16	110.35
1	V	198	CYS	CA-C-N	5.01	126.99	120.28
1	V	198	CYS	C-N-CA	5.01	126.99	120.28
1	s	195	ASN	CA-CB-CG	5.01	117.61	112.60
1	BF	229	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	1	202	LEU	CA-C-N	5.00	126.98	120.28
1	1	202	LEU	C-N-CA	5.00	126.98	120.28
1	RC	18	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	AF	173	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	vA	184	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	QB	162	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	wB	143	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	eE	18	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	82	ARG	Sidechain
1	A	130	TYR	Sidechain
1	A	229	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	130	TYR	Sidechain
1	C	97	ARG	Sidechain
1	D	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	143	ARG	Sidechain
1	D	173	ARG	Sidechain
1	F	97	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	154	ARG	Sidechain
1	H	97	ARG	Sidechain
1	H	169	TYR	Sidechain
1	I	173	ARG	Sidechain
1	J	18	ARG	Sidechain
1	J	100	ARG	Sidechain
1	J	162	ARG	Sidechain
1	J	229	ARG	Sidechain
1	K	143	ARG	Sidechain
1	K	162	ARG	Sidechain
1	L	132	ARG	Sidechain
1	M	97	ARG	Sidechain
1	M	167	ARG	Sidechain
1	M	229	ARG	Sidechain
1	N	100	ARG	Sidechain
1	O	82	ARG	Sidechain
1	O	100	ARG	Sidechain
1	O	162	ARG	Sidechain
1	O	229	ARG	Sidechain
1	P	18	ARG	Sidechain
1	P	97	ARG	Sidechain
1	P	100	ARG	Sidechain
1	P	132	ARG	Sidechain
1	P	167	ARG	Sidechain
1	Q	82	ARG	Sidechain
1	R	18	ARG	Sidechain
1	R	173	ARG	Sidechain
1	R	229	ARG	Sidechain
1	S	97	ARG	Sidechain
1	S	143	ARG	Sidechain
1	T	100	ARG	Sidechain
1	T	154	ARG	Sidechain
1	U	97	ARG	Sidechain
1	U	162	ARG	Sidechain
1	U	229	ARG	Sidechain
1	W	18	ARG	Sidechain
1	X	100	ARG	Sidechain
1	X	167	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	X	229	ARG	Sidechain
1	Y	97	ARG	Sidechain
1	Y	173	ARG	Sidechain
1	a	97	ARG	Sidechain
1	a	100	ARG	Sidechain
1	a	132	ARG	Sidechain
1	b	132	ARG	Sidechain
1	b	167	ARG	Sidechain
1	b	173	ARG	Sidechain
1	d	167	ARG	Sidechain
1	e	100	ARG	Sidechain
1	e	143	ARG	Sidechain
1	e	167	ARG	Sidechain
1	f	100	ARG	Sidechain
1	f	143	ARG	Sidechain
1	f	229	ARG	Sidechain
1	g	100	ARG	Sidechain
1	g	143	ARG	Sidechain
1	i	229	ARG	Sidechain
1	j	100	ARG	Sidechain
1	j	154	ARG	Sidechain
1	j	229	ARG	Sidechain
1	k	143	ARG	Sidechain
1	k	162	ARG	Sidechain
1	k	173	ARG	Sidechain
1	l	132	ARG	Sidechain
1	l	143	ARG	Sidechain
1	l	169	TYR	Sidechain
1	m	97	ARG	Sidechain
1	m	229	ARG	Sidechain
1	n	100	ARG	Sidechain
1	n	143	ARG	Sidechain
1	n	173	ARG	Sidechain
1	o	154	ARG	Sidechain
1	p	167	ARG	Sidechain
1	q	97	ARG	Sidechain
1	q	143	ARG	Sidechain
1	q	154	ARG	Sidechain
1	r	18	ARG	Sidechain
1	r	100	ARG	Sidechain
1	r	143	ARG	Sidechain
1	r	162	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	r	229	ARG	Sidechain
1	s	100	ARG	Sidechain
1	s	173	ARG	Sidechain
1	t	100	ARG	Sidechain
1	u	164	TYR	Sidechain
1	v	18	ARG	Sidechain
1	v	100	ARG	Sidechain
1	v	164	TYR	Sidechain
1	w	100	ARG	Sidechain
1	x	143	ARG	Sidechain
1	y	154	ARG	Sidechain
1	z	82	ARG	Sidechain
1	z	132	ARG	Sidechain
1	0	132	ARG	Sidechain
1	0	143	ARG	Sidechain
1	0	226	HIS	Sidechain
1	0	229	ARG	Sidechain
1	1	18	ARG	Sidechain
1	1	97	ARG	Sidechain
1	1	162	ARG	Sidechain
1	2	97	ARG	Sidechain
1	2	143	ARG	Sidechain
1	2	164	TYR	Sidechain
1	2	173	ARG	Sidechain
1	2	229	ARG	Sidechain
1	3	97	ARG	Sidechain
1	3	169	TYR	Sidechain
1	3	229	ARG	Sidechain
1	4	18	ARG	Sidechain
1	4	143	ARG	Sidechain
1	5	82	ARG	Sidechain
1	5	169	TYR	Sidechain
1	6	154	ARG	Sidechain
1	6	164	TYR	Sidechain
1	8	18	ARG	Sidechain
1	8	173	ARG	Sidechain
1	8	229	ARG	Sidechain
1	9	18	ARG	Sidechain
1	9	97	ARG	Sidechain
1	9	169	TYR	Sidechain
1	9	229	ARG	Sidechain
1	AA	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	100	ARG	Sidechain
1	CA	100	ARG	Sidechain
1	CA	229	ARG	Sidechain
1	DA	82	ARG	Sidechain
1	DA	97	ARG	Sidechain
1	DA	132	ARG	Sidechain
1	DA	162	ARG	Sidechain
1	DA	229	ARG	Sidechain
1	EA	162	ARG	Sidechain
1	EA	173	ARG	Sidechain
1	EA	229	ARG	Sidechain
1	FA	100	ARG	Sidechain
1	GA	18	ARG	Sidechain
1	GA	100	ARG	Sidechain
1	GA	154	ARG	Sidechain
1	GA	173	ARG	Sidechain
1	GA	229	ARG	Sidechain
1	HA	18	ARG	Sidechain
1	IA	97	ARG	Sidechain
1	IA	229	ARG	Sidechain
1	JA	132	ARG	Sidechain
1	JA	173	ARG	Sidechain
1	KA	82	ARG	Sidechain
1	KA	100	ARG	Sidechain
1	KA	143	ARG	Sidechain
1	KA	229	ARG	Sidechain
1	LA	100	ARG	Sidechain
1	MA	97	ARG	Sidechain
1	NA	229	ARG	Sidechain
1	OA	82	ARG	Sidechain
1	OA	143	ARG	Sidechain
1	OA	229	ARG	Sidechain
1	PA	229	ARG	Sidechain
1	RA	100	ARG	Sidechain
1	SA	18	ARG	Sidechain
1	SA	97	ARG	Sidechain
1	SA	132	ARG	Sidechain
1	SA	143	ARG	Sidechain
1	TA	100	ARG	Sidechain
1	UA	132	ARG	Sidechain
1	VA	229	ARG	Sidechain
1	WA	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	XA	154	ARG	Sidechain
1	XA	167	ARG	Sidechain
1	YA	97	ARG	Sidechain
1	YA	162	ARG	Sidechain
1	ZA	167	ARG	Sidechain
1	aA	143	ARG	Sidechain
1	aA	169	TYR	Sidechain
1	bA	18	ARG	Sidechain
1	cA	100	ARG	Sidechain
1	cA	173	ARG	Sidechain
1	cA	229	ARG	Sidechain
1	dA	82	ARG	Sidechain
1	dA	132	ARG	Sidechain
1	eA	132	ARG	Sidechain
1	fA	18	ARG	Sidechain
1	fA	173	ARG	Sidechain
1	hA	18	ARG	Sidechain
1	hA	100	ARG	Sidechain
1	hA	130	TYR	Sidechain
1	iA	100	ARG	Sidechain
1	iA	132	ARG	Sidechain
1	iA	173	ARG	Sidechain
1	iA	229	ARG	Sidechain
1	jA	18	ARG	Sidechain
1	jA	162	ARG	Sidechain
1	jA	169	TYR	Sidechain
1	kA	100	ARG	Sidechain
1	kA	162	ARG	Sidechain
1	kA	229	ARG	Sidechain
1	lA	143	ARG	Sidechain
1	nA	18	ARG	Sidechain
1	nA	97	ARG	Sidechain
1	nA	132	ARG	Sidechain
1	nA	229	ARG	Sidechain
1	oA	229	ARG	Sidechain
1	pA	18	ARG	Sidechain
1	pA	132	ARG	Sidechain
1	qA	82	ARG	Sidechain
1	qA	229	ARG	Sidechain
1	rA	97	ARG	Sidechain
1	rA	167	ARG	Sidechain
1	rA	169	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	rA	229	ARG	Sidechain
1	sA	154	ARG	Sidechain
1	sA	162	ARG	Sidechain
1	uA	18	ARG	Sidechain
1	uA	154	ARG	Sidechain
1	vA	97	ARG	Sidechain
1	vA	154	ARG	Sidechain
1	wA	143	ARG	Sidechain
1	wA	154	ARG	Sidechain
1	wA	173	ARG	Sidechain
1	wA	226	HIS	Sidechain
1	xA	132	ARG	Sidechain
1	yA	100	ARG	Sidechain
1	yA	164	TYR	Sidechain
1	zA	100	ARG	Sidechain
1	zA	162	ARG	Sidechain
1	zA	167	ARG	Sidechain
1	zA	229	ARG	Sidechain
1	0A	143	ARG	Sidechain
1	0A	154	ARG	Sidechain
1	0A	229	ARG	Sidechain
1	2A	97	ARG	Sidechain
1	3A	100	ARG	Sidechain
1	3A	143	ARG	Sidechain
1	3A	229	ARG	Sidechain
1	4A	97	ARG	Sidechain
1	4A	162	ARG	Sidechain
1	4A	229	ARG	Sidechain
1	5A	18	ARG	Sidechain
1	5A	229	ARG	Sidechain
1	6A	18	ARG	Sidechain
1	6A	100	ARG	Sidechain
1	6A	229	ARG	Sidechain
1	8A	82	ARG	Sidechain
1	8A	97	ARG	Sidechain
1	9A	97	ARG	Sidechain
1	9A	100	ARG	Sidechain
1	9A	143	ARG	Sidechain
1	BB	132	ARG	Sidechain
1	BB	169	TYR	Sidechain
1	BB	173	ARG	Sidechain
1	BB	229	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	CB	132	ARG	Sidechain
1	CB	229	ARG	Sidechain
1	DB	82	ARG	Sidechain
1	EB	173	ARG	Sidechain
1	FB	100	ARG	Sidechain
1	FB	145	TYR	Sidechain
1	FB	229	ARG	Sidechain
1	HB	18	ARG	Sidechain
1	HB	154	ARG	Sidechain
1	HB	173	ARG	Sidechain
1	HB	229	ARG	Sidechain
1	IB	154	ARG	Sidechain
1	IB	167	ARG	Sidechain
1	IB	226	HIS	Sidechain
1	JB	18	ARG	Sidechain
1	JB	100	ARG	Sidechain
1	KB	100	ARG	Sidechain
1	KB	143	ARG	Sidechain
1	MB	154	ARG	Sidechain
1	NB	100	ARG	Sidechain
1	OB	97	ARG	Sidechain
1	PB	18	ARG	Sidechain
1	PB	173	ARG	Sidechain
1	PB	229	ARG	Sidechain
1	QB	97	ARG	Sidechain
1	QB	169	TYR	Sidechain
1	RB	82	ARG	Sidechain
1	RB	143	ARG	Sidechain
1	RB	229	ARG	Sidechain
1	SB	132	ARG	Sidechain
1	SB	154	ARG	Sidechain
1	TB	100	ARG	Sidechain
1	TB	173	ARG	Sidechain
1	TB	226	HIS	Sidechain
1	UB	82	ARG	Sidechain
1	UB	173	ARG	Sidechain
1	VB	18	ARG	Sidechain
1	VB	154	ARG	Sidechain
1	VB	229	ARG	Sidechain
1	WB	18	ARG	Sidechain
1	WB	100	ARG	Sidechain
1	XB	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	XB	162	ARG	Sidechain
1	XB	229	ARG	Sidechain
1	YB	154	ARG	Sidechain
1	ZB	97	ARG	Sidechain
1	ZB	132	ARG	Sidechain
1	ZB	143	ARG	Sidechain
1	ZB	154	ARG	Sidechain
1	ZB	167	ARG	Sidechain
1	aB	97	ARG	Sidechain
1	aB	100	ARG	Sidechain
1	aB	143	ARG	Sidechain
1	bB	100	ARG	Sidechain
1	bB	162	ARG	Sidechain
1	cB	97	ARG	Sidechain
1	dB	18	ARG	Sidechain
1	eB	154	ARG	Sidechain
1	fB	154	ARG	Sidechain
1	fB	173	ARG	Sidechain
1	fB	229	ARG	Sidechain
1	gB	18	ARG	Sidechain
1	gB	97	ARG	Sidechain
1	hB	100	ARG	Sidechain
1	hB	162	ARG	Sidechain
1	iB	18	ARG	Sidechain
1	iB	97	ARG	Sidechain
1	iB	100	ARG	Sidechain
1	iB	154	ARG	Sidechain
1	jB	18	ARG	Sidechain
1	jB	100	ARG	Sidechain
1	jB	162	ARG	Sidechain
1	kB	100	ARG	Sidechain
1	kB	132	ARG	Sidechain
1	kB	143	ARG	Sidechain
1	lB	18	ARG	Sidechain
1	lB	173	ARG	Sidechain
1	mB	167	ARG	Sidechain
1	nB	169	TYR	Sidechain
1	oB	18	ARG	Sidechain
1	oB	97	ARG	Sidechain
1	pB	100	ARG	Sidechain
1	pB	143	ARG	Sidechain
1	pB	164	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	sB	132	ARG	Sidechain
1	tB	18	ARG	Sidechain
1	tB	97	ARG	Sidechain
1	tB	143	ARG	Sidechain
1	tB	154	ARG	Sidechain
1	uB	18	ARG	Sidechain
1	uB	97	ARG	Sidechain
1	uB	100	ARG	Sidechain
1	uB	132	ARG	Sidechain
1	uB	145	TYR	Sidechain
1	uB	173	ARG	Sidechain
1	vB	154	ARG	Sidechain
1	wB	100	ARG	Sidechain
1	wB	143	ARG	Sidechain
1	xB	173	ARG	Sidechain
1	yB	82	ARG	Sidechain
1	yB	97	ARG	Sidechain
1	yB	100	ARG	Sidechain
1	yB	130	TYR	Sidechain
1	yB	154	ARG	Sidechain
1	yB	229	ARG	Sidechain
1	zB	132	ARG	Sidechain
1	zB	143	ARG	Sidechain
1	zB	162	ARG	Sidechain
1	0B	97	ARG	Sidechain
1	0B	143	ARG	Sidechain
1	1B	18	ARG	Sidechain
1	1B	100	ARG	Sidechain
1	1B	173	ARG	Sidechain
1	2B	18	ARG	Sidechain
1	2B	229	ARG	Sidechain
1	3B	132	ARG	Sidechain
1	5B	226	HIS	Sidechain
1	6B	97	ARG	Sidechain
1	6B	100	ARG	Sidechain
1	8B	154	ARG	Sidechain
1	8B	229	ARG	Sidechain
1	9B	132	ARG	Sidechain
1	9B	154	ARG	Sidechain
1	9B	167	ARG	Sidechain
1	AC	82	ARG	Sidechain
1	AC	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	AC	132	ARG	Sidechain
1	BC	100	ARG	Sidechain
1	BC	229	ARG	Sidechain
1	CC	18	ARG	Sidechain
1	CC	154	ARG	Sidechain
1	CC	229	ARG	Sidechain
1	DC	97	ARG	Sidechain
1	DC	100	ARG	Sidechain
1	EC	100	ARG	Sidechain
1	EC	143	ARG	Sidechain
1	EC	229	ARG	Sidechain
1	FC	97	ARG	Sidechain
1	FC	100	ARG	Sidechain
1	FC	162	ARG	Sidechain
1	FC	229	ARG	Sidechain
1	GC	97	ARG	Sidechain
1	GC	167	ARG	Sidechain
1	HC	18	ARG	Sidechain
1	HC	100	ARG	Sidechain
1	IC	132	ARG	Sidechain
1	IC	162	ARG	Sidechain
1	KC	18	ARG	Sidechain
1	LC	132	ARG	Sidechain
1	MC	97	ARG	Sidechain
1	MC	229	ARG	Sidechain
1	NC	97	ARG	Sidechain
1	NC	100	ARG	Sidechain
1	NC	143	ARG	Sidechain
1	OC	82	ARG	Sidechain
1	OC	97	ARG	Sidechain
1	OC	100	ARG	Sidechain
1	OC	229	ARG	Sidechain
1	PC	132	ARG	Sidechain
1	PC	143	ARG	Sidechain
1	PC	229	ARG	Sidechain
1	QC	167	ARG	Sidechain
1	RC	167	ARG	Sidechain
1	TC	100	ARG	Sidechain
1	TC	154	ARG	Sidechain
1	UC	100	ARG	Sidechain
1	UC	143	ARG	Sidechain
1	UC	145	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	UC	167	ARG	Sidechain
1	UC	229	ARG	Sidechain
1	VC	82	ARG	Sidechain
1	VC	100	ARG	Sidechain
1	VC	229	ARG	Sidechain
1	WC	18	ARG	Sidechain
1	WC	229	ARG	Sidechain
1	XC	167	ARG	Sidechain
1	ZC	100	ARG	Sidechain
1	ZC	143	ARG	Sidechain
1	ZC	162	ARG	Sidechain
1	ZC	229	ARG	Sidechain
1	aC	100	ARG	Sidechain
1	aC	143	ARG	Sidechain
1	aC	162	ARG	Sidechain
1	aC	167	ARG	Sidechain
1	aC	229	ARG	Sidechain
1	bC	143	ARG	Sidechain
1	cC	97	ARG	Sidechain
1	cC	130	TYR	Sidechain
1	cC	143	ARG	Sidechain
1	dC	18	ARG	Sidechain
1	dC	82	ARG	Sidechain
1	dC	97	ARG	Sidechain
1	dC	173	ARG	Sidechain
1	fC	100	ARG	Sidechain
1	fC	143	ARG	Sidechain
1	fC	154	ARG	Sidechain
1	gC	18	ARG	Sidechain
1	gC	97	ARG	Sidechain
1	gC	100	ARG	Sidechain
1	hC	229	ARG	Sidechain
1	iC	82	ARG	Sidechain
1	iC	100	ARG	Sidechain
1	iC	154	ARG	Sidechain
1	iC	162	ARG	Sidechain
1	jC	18	ARG	Sidechain
1	jC	162	ARG	Sidechain
1	jC	173	ARG	Sidechain
1	kC	97	ARG	Sidechain
1	kC	100	ARG	Sidechain
1	kC	229	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	lC	18	ARG	Sidechain
1	lC	82	ARG	Sidechain
1	lC	143	ARG	Sidechain
1	lC	154	ARG	Sidechain
1	lC	162	ARG	Sidechain
1	nC	18	ARG	Sidechain
1	nC	100	ARG	Sidechain
1	nC	145	TYR	Sidechain
1	nC	154	ARG	Sidechain
1	oC	100	ARG	Sidechain
1	oC	143	ARG	Sidechain
1	oC	162	ARG	Sidechain
1	pC	132	ARG	Sidechain
1	qC	167	ARG	Sidechain
1	rC	18	ARG	Sidechain
1	rC	100	ARG	Sidechain
1	sC	100	ARG	Sidechain
1	tC	100	ARG	Sidechain
1	tC	229	ARG	Sidechain
1	uC	100	ARG	Sidechain
1	uC	132	ARG	Sidechain
1	vC	18	ARG	Sidechain
1	vC	167	ARG	Sidechain
1	wC	82	ARG	Sidechain
1	wC	100	ARG	Sidechain
1	wC	154	ARG	Sidechain
1	wC	167	ARG	Sidechain
1	xC	100	ARG	Sidechain
1	yC	132	ARG	Sidechain
1	yC	154	ARG	Sidechain
1	yC	173	ARG	Sidechain
1	zC	18	ARG	Sidechain
1	zC	97	ARG	Sidechain
1	1C	143	ARG	Sidechain
1	1C	162	ARG	Sidechain
1	2C	97	ARG	Sidechain
1	2C	100	ARG	Sidechain
1	2C	143	ARG	Sidechain
1	4C	18	ARG	Sidechain
1	4C	97	ARG	Sidechain
1	4C	100	ARG	Sidechain
1	5C	154	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	5C	167	ARG	Sidechain
1	6C	143	ARG	Sidechain
1	6C	229	ARG	Sidechain
1	7C	167	ARG	Sidechain
1	7C	173	ARG	Sidechain
1	8C	18	ARG	Sidechain
1	8C	97	ARG	Sidechain
1	9C	18	ARG	Sidechain
1	AD	18	ARG	Sidechain
1	AD	62	HIS	Sidechain
1	BD	162	ARG	Sidechain
1	CD	18	ARG	Sidechain
1	CD	164	TYR	Sidechain
1	CD	229	ARG	Sidechain
1	DD	18	ARG	Sidechain
1	DD	82	ARG	Sidechain
1	DD	229	ARG	Sidechain
1	ED	97	ARG	Sidechain
1	ED	130	TYR	Sidechain
1	ED	145	TYR	Sidechain
1	ED	167	ARG	Sidechain
1	ED	229	ARG	Sidechain
1	FD	143	ARG	Sidechain
1	FD	229	ARG	Sidechain
1	GD	82	ARG	Sidechain
1	GD	100	ARG	Sidechain
1	GD	173	ARG	Sidechain
1	HD	18	ARG	Sidechain
1	HD	100	ARG	Sidechain
1	HD	145	TYR	Sidechain
1	HD	162	ARG	Sidechain
1	HD	164	TYR	Sidechain
1	HD	167	ARG	Sidechain
1	ID	18	ARG	Sidechain
1	ID	100	ARG	Sidechain
1	ID	132	ARG	Sidechain
1	ID	154	ARG	Sidechain
1	JD	18	ARG	Sidechain
1	JD	100	ARG	Sidechain
1	LD	169	TYR	Sidechain
1	MD	82	ARG	Sidechain
1	MD	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	OD	100	ARG	Sidechain
1	OD	164	TYR	Sidechain
1	PD	18	ARG	Sidechain
1	PD	229	ARG	Sidechain
1	QD	229	ARG	Sidechain
1	SD	82	ARG	Sidechain
1	SD	97	ARG	Sidechain
1	SD	132	ARG	Sidechain
1	SD	229	ARG	Sidechain
1	TD	100	ARG	Sidechain
1	TD	229	ARG	Sidechain
1	UD	162	ARG	Sidechain
1	VD	132	ARG	Sidechain
1	VD	229	ARG	Sidechain
1	WD	97	ARG	Sidechain
1	XD	97	ARG	Sidechain
1	XD	100	ARG	Sidechain
1	YD	18	ARG	Sidechain
1	YD	173	ARG	Sidechain
1	ZD	169	TYR	Sidechain
1	aD	132	ARG	Sidechain
1	bD	18	ARG	Sidechain
1	bD	162	ARG	Sidechain
1	bD	167	ARG	Sidechain
1	cD	97	ARG	Sidechain
1	dD	97	ARG	Sidechain
1	dD	143	ARG	Sidechain
1	eD	100	ARG	Sidechain
1	fD	173	ARG	Sidechain
1	hD	97	ARG	Sidechain
1	hD	143	ARG	Sidechain
1	hD	162	ARG	Sidechain
1	hD	167	ARG	Sidechain
1	hD	226	HIS	Sidechain
1	iD	100	ARG	Sidechain
1	iD	173	ARG	Sidechain
1	iD	229	ARG	Sidechain
1	jD	229	ARG	Sidechain
1	kD	97	ARG	Sidechain
1	kD	143	ARG	Sidechain
1	kD	162	ARG	Sidechain
1	nD	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	nD	229	ARG	Sidechain
1	oD	97	ARG	Sidechain
1	pD	18	ARG	Sidechain
1	pD	97	ARG	Sidechain
1	qD	173	ARG	Sidechain
1	rD	97	ARG	Sidechain
1	rD	143	ARG	Sidechain
1	rD	169	TYR	Sidechain
1	sD	143	ARG	Sidechain
1	sD	229	ARG	Sidechain
1	tD	97	ARG	Sidechain
1	tD	100	ARG	Sidechain
1	tD	143	ARG	Sidechain
1	tD	173	ARG	Sidechain
1	uD	97	ARG	Sidechain
1	vD	82	ARG	Sidechain
1	wD	18	ARG	Sidechain
1	wD	132	ARG	Sidechain
1	xD	167	ARG	Sidechain
1	yD	82	ARG	Sidechain
1	yD	154	ARG	Sidechain
1	zD	97	ARG	Sidechain
1	zD	100	ARG	Sidechain
1	0D	145	TYR	Sidechain
1	0D	154	ARG	Sidechain
1	0D	229	ARG	Sidechain
1	1D	164	TYR	Sidechain
1	1D	229	ARG	Sidechain
1	2D	18	ARG	Sidechain
1	2D	82	ARG	Sidechain
1	2D	167	ARG	Sidechain
1	3D	132	ARG	Sidechain
1	3D	154	ARG	Sidechain
1	4D	154	ARG	Sidechain
1	5D	143	ARG	Sidechain
1	6D	97	ARG	Sidechain
1	6D	143	ARG	Sidechain
1	7D	154	ARG	Sidechain
1	7D	162	ARG	Sidechain
1	7D	229	ARG	Sidechain
1	8D	97	ARG	Sidechain
1	9D	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	9D	132	ARG	Sidechain
1	9D	167	ARG	Sidechain
1	9D	229	ARG	Sidechain
1	BE	100	ARG	Sidechain
1	BE	154	ARG	Sidechain
1	CE	162	ARG	Sidechain
1	DE	97	ARG	Sidechain
1	EE	100	ARG	Sidechain
1	FE	100	ARG	Sidechain
1	FE	167	ARG	Sidechain
1	HE	100	ARG	Sidechain
1	HE	143	ARG	Sidechain
1	HE	173	ARG	Sidechain
1	HE	229	ARG	Sidechain
1	IE	18	ARG	Sidechain
1	IE	97	ARG	Sidechain
1	JE	100	ARG	Sidechain
1	JE	162	ARG	Sidechain
1	KE	100	ARG	Sidechain
1	LE	100	ARG	Sidechain
1	ME	132	ARG	Sidechain
1	OE	173	ARG	Sidechain
1	OE	229	ARG	Sidechain
1	PE	162	ARG	Sidechain
1	QE	97	ARG	Sidechain
1	QE	169	TYR	Sidechain
1	RE	100	ARG	Sidechain
1	RE	229	ARG	Sidechain
1	SE	143	ARG	Sidechain
1	TE	132	ARG	Sidechain
1	TE	145	TYR	Sidechain
1	TE	229	ARG	Sidechain
1	UE	97	ARG	Sidechain
1	UE	229	ARG	Sidechain
1	VE	100	ARG	Sidechain
1	WE	154	ARG	Sidechain
1	WE	229	ARG	Sidechain
1	XE	162	ARG	Sidechain
1	YE	100	ARG	Sidechain
1	YE	229	ARG	Sidechain
1	aE	97	ARG	Sidechain
1	aE	162	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	aE	164	TYR	Sidechain
1	bE	100	ARG	Sidechain
1	cE	143	ARG	Sidechain
1	cE	169	TYR	Sidechain
1	dE	97	ARG	Sidechain
1	dE	100	ARG	Sidechain
1	eE	100	ARG	Sidechain
1	fE	18	ARG	Sidechain
1	fE	162	ARG	Sidechain
1	gE	97	ARG	Sidechain
1	gE	132	ARG	Sidechain
1	hE	97	ARG	Sidechain
1	hE	169	TYR	Sidechain
1	iE	97	ARG	Sidechain
1	iE	130	TYR	Sidechain
1	iE	162	ARG	Sidechain
1	iE	167	ARG	Sidechain
1	jE	18	ARG	Sidechain
1	jE	154	ARG	Sidechain
1	jE	226	HIS	Sidechain
1	kE	100	ARG	Sidechain
1	kE	143	ARG	Sidechain
1	lE	18	ARG	Sidechain
1	lE	132	ARG	Sidechain
1	lE	167	ARG	Sidechain
1	lE	229	ARG	Sidechain
1	mE	82	ARG	Sidechain
1	mE	100	ARG	Sidechain
1	mE	229	ARG	Sidechain
1	oE	132	ARG	Sidechain
1	oE	143	ARG	Sidechain
1	oE	162	ARG	Sidechain
1	pE	18	ARG	Sidechain
1	pE	100	ARG	Sidechain
1	pE	143	ARG	Sidechain
1	pE	154	ARG	Sidechain
1	pE	164	TYR	Sidechain
1	pE	167	ARG	Sidechain
1	qE	100	ARG	Sidechain
1	qE	154	ARG	Sidechain
1	qE	164	TYR	Sidechain
1	rE	169	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	rE	229	ARG	Sidechain
1	sE	18	ARG	Sidechain
1	sE	97	ARG	Sidechain
1	sE	173	ARG	Sidechain
1	sE	229	ARG	Sidechain
1	tE	100	ARG	Sidechain
1	uE	82	ARG	Sidechain
1	vE	18	ARG	Sidechain
1	vE	173	ARG	Sidechain
1	wE	100	ARG	Sidechain
1	wE	143	ARG	Sidechain
1	wE	162	ARG	Sidechain
1	xE	167	ARG	Sidechain
1	yE	143	ARG	Sidechain
1	0E	97	ARG	Sidechain
1	0E	143	ARG	Sidechain
1	0E	173	ARG	Sidechain
1	0E	229	ARG	Sidechain
1	1E	82	ARG	Sidechain
1	1E	162	ARG	Sidechain
1	2E	100	ARG	Sidechain
1	3E	162	ARG	Sidechain
1	3E	173	ARG	Sidechain
1	5E	100	ARG	Sidechain
1	5E	145	TYR	Sidechain
1	5E	229	ARG	Sidechain
1	6E	97	ARG	Sidechain
1	6E	100	ARG	Sidechain
1	7E	18	ARG	Sidechain
1	7E	130	TYR	Sidechain
1	7E	143	ARG	Sidechain
1	8E	82	ARG	Sidechain
1	8E	132	ARG	Sidechain
1	8E	169	TYR	Sidechain
1	8E	229	ARG	Sidechain
1	9E	132	ARG	Sidechain
1	9E	162	ARG	Sidechain
1	AF	62	HIS	Sidechain
1	BF	100	ARG	Sidechain
1	BF	226	HIS	Sidechain
1	CF	82	ARG	Sidechain
1	CF	143	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	CF	229	ARG	Sidechain
1	DF	100	ARG	Sidechain
1	DF	164	TYR	Sidechain
1	DF	229	ARG	Sidechain
1	EF	18	ARG	Sidechain
1	EF	100	ARG	Sidechain
1	EF	229	ARG	Sidechain
1	FF	97	ARG	Sidechain
1	FF	100	ARG	Sidechain
1	FF	143	ARG	Sidechain
1	FF	167	ARG	Sidechain
1	FF	173	ARG	Sidechain

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	1E	1795	1801	1801	1
1	2B	1795	1801	1801	1
1	3	1795	1801	1801	1
1	3C	1795	1801	1801	2
1	4C	1795	1801	1801	2
1	5E	1795	1801	1801	1
1	7	1795	1801	1801	1
1	7D	1795	1801	1801	1
1	8B	1795	1801	1801	1
1	9	1795	1801	1801	1
1	9A	1795	1801	1801	1
1	AB	1795	1801	1801	1
1	BC	1795	1801	1801	1
1	D	1795	1801	1801	1
1	EC	1795	1801	1801	2
1	FD	1795	1801	1801	1
1	GB	1795	1801	1801	2
1	H	1795	1801	1801	2
1	HD	1795	1801	1801	2
1	JB	1795	1801	1801	2
1	JD	1795	1801	1801	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	JE	1795	1801	1801	1
1	KD	1795	1801	1801	1
1	KE	1795	1801	1801	1
1	LA	1795	1801	1801	3
1	LB	1795	1801	1801	1
1	LC	1795	1801	1801	1
1	LD	1795	1801	1801	1
1	MB	1795	1801	1801	2
1	OA	1795	1801	1801	1
1	P	1795	1801	1801	1
1	PA	1795	1801	1801	1
1	QB	1795	1801	1801	1
1	RA	1795	1801	1801	1
1	SA	1795	1801	1801	1
1	SE	1795	1801	1801	1
1	TC	1795	1801	1801	3
1	UA	1795	1801	1801	1
1	VB	1795	1801	1801	1
1	VD	1795	1801	1801	2
1	W	1795	1801	1801	1
1	XA	1795	1801	1801	2
1	YD	1795	1801	1801	1
1	bB	1795	1801	1801	1
1	c	1795	1801	1801	2
1	dD	1795	1801	1801	1
1	f	1795	1801	1801	2
1	gD	1795	1801	1801	2
1	hB	1795	1801	1801	1
1	i	1795	1801	1801	3
1	iC	1795	1801	1801	3
1	kE	1795	1801	1801	1
1	lA	1795	1801	1801	1
1	lE	1795	1801	1801	1
1	mD	1795	1801	1801	1
1	nE	1795	1801	1801	2
1	o	1795	1801	1801	1
1	oB	1795	1801	1801	1
1	oE	1795	1801	1801	1
1	qB	1795	1801	1801	1
1	t	1795	1801	1801	1
1	tB	1795	1801	1801	2
1	uC	1795	1801	1801	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	vD	1795	1801	1801	2
1	xC	1795	1801	1801	2
1	zB	1795	1801	1801	2
All	All	678510	680778	680778	92

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:xC:87:HIS:CG	1:xC:88:ALA:H	0.63	2.11
1:JB:87:HIS:CG	1:JB:88:ALA:H	0.59	2.16
1:LA:87:HIS:CG	1:LA:88:ALA:H	0.58	2.17
1:zB:87:HIS:CG	1:zB:88:ALA:H	0.57	2.17
1:HD:60:GLY:H	1:HD:62:HIS:CE1	0.56	2.18
1:GB:87:HIS:CG	1:GB:88:ALA:H	0.56	2.18
1:3C:87:HIS:CG	1:3C:88:ALA:H	0.56	2.19
1:JD:59:VAL:HG23	1:JD:62:HIS:CD2	0.56	2.35
1:VD:226:HIS:CG	1:VD:227:LYS:H	0.54	2.20
1:bB:87:HIS:CG	1:bB:88:ALA:H	0.53	2.21
1:uC:87:HIS:CD2	1:uC:89:GLY:H	0.53	2.22
1:RA:87:HIS:CG	1:RA:88:ALA:H	0.53	2.21
1:xC:87:HIS:CG	1:xC:88:ALA:N	0.52	2.77
1:i:87:HIS:CG	1:i:88:ALA:H	0.51	2.23
1:XA:87:HIS:CG	1:XA:88:ALA:H	0.51	2.24
1:f:87:HIS:CG	1:f:88:ALA:H	0.51	2.22
1:tB:226:HIS:CG	1:tB:227:LYS:N	0.50	2.78
1:i:87:HIS:CG	1:i:88:ALA:N	0.50	2.79
1:c:87:HIS:CG	1:c:88:ALA:H	0.50	2.24
1:UA:226:HIS:CG	1:UA:227:LYS:N	0.50	2.79
1:H:87:HIS:CG	1:H:88:ALA:H	0.49	2.25
1:f:87:HIS:CG	1:f:88:ALA:N	0.49	2.81
1:c:87:HIS:CG	1:c:88:ALA:N	0.48	2.82
1:MB:87:HIS:CD2	1:MB:89:GLY:H	0.47	2.27
1:lA:87:HIS:CD2	1:lA:89:GLY:H	0.47	2.27
1:LA:87:HIS:CG	1:LA:88:ALA:N	0.47	2.83
1:vD:87:HIS:CG	1:vD:88:ALA:H	0.47	2.27
1:1E:116:GLY:HA2	1:1E:120:HIS:CD2	0.46	2.45
1:nE:87:HIS:CG	1:nE:88:ALA:H	0.46	2.28
1:EC:87:HIS:CD2	1:EC:89:GLY:H	0.46	2.27
1:7D:87:HIS:CG	1:7D:88:ALA:H	0.46	2.29
1:P:226:HIS:CG	1:P:227:LYS:H	0.46	2.27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:GB:87:HIS:CG	1:GB:88:ALA:N	0.46	2.83
1:4C:87:HIS:CG	1:4C:88:ALA:H	0.46	2.29
1:OA:226:HIS:CG	1:OA:227:LYS:N	0.46	2.84
1:mD:27:VAL:HG13	1:mD:62:HIS:CE1	0.46	2.46
1:VB:31:ALA:HB1	1:VB:62:HIS:CE1	0.45	2.46
1:EC:27:VAL:HG13	1:EC:62:HIS:CE1	0.45	2.46
1:2B:201:ILE:HD11	1:2B:226:HIS:H	0.45	1.72
1:MB:87:HIS:CG	1:MB:88:ALA:N	0.45	2.85
1:vD:87:HIS:CG	1:vD:88:ALA:N	0.45	2.85
1:nE:87:HIS:CG	1:nE:88:ALA:N	0.45	2.85
1:qB:2:ILE:H	1:qB:2:ILE:HD13	0.45	1.70
1:dD:87:HIS:CG	1:dD:88:ALA:H	0.45	2.30
1:hB:87:HIS:CG	1:hB:88:ALA:H	0.44	2.30
1:5E:87:HIS:CG	1:5E:88:ALA:H	0.44	2.30
1:JB:87:HIS:CG	1:JB:88:ALA:N	0.44	2.84
1:kE:87:HIS:CG	1:kE:88:ALA:N	0.44	2.85
1:8B:87:HIS:CD2	1:8B:89:GLY:H	0.44	2.30
1:AB:87:HIS:CD2	1:AB:89:GLY:H	0.44	2.31
1:KE:201:ILE:H	1:KE:201:ILE:HD12	0.44	1.72
1:lE:28:GLU:HA	1:lE:62:HIS:CE1	0.44	2.48
1:QB:226:HIS:O	1:QB:226:HIS:CG	0.44	2.71
1:zB:87:HIS:CG	1:zB:88:ALA:N	0.44	2.85
1:LC:226:HIS:CG	1:LC:227:LYS:H	0.44	2.31
1:iC:87:HIS:CD2	1:iC:89:GLY:H	0.44	2.30
1:W:87:HIS:CD2	1:W:89:GLY:H	0.44	2.31
1:iC:87:HIS:CG	1:iC:88:ALA:N	0.44	2.86
1:9:27:VAL:HG13	1:9:62:HIS:CE1	0.43	2.48
1:VD:226:HIS:CG	1:VD:227:LYS:N	0.43	2.85
1:o:87:HIS:CG	1:o:88:ALA:N	0.43	2.86
1:iC:226:HIS:CE1	1:iC:228:ALA:HB3	0.43	2.49
1:TC:87:HIS:CG	1:TC:88:ALA:N	0.42	2.87
1:gD:27:VAL:HG13	1:gD:62:HIS:CE1	0.42	2.50
1:LA:87:HIS:CD2	1:LA:88:ALA:H	0.42	2.33
1:uC:87:HIS:CG	1:uC:88:ALA:N	0.42	2.87
1:TC:87:HIS:CG	1:TC:88:ALA:H	0.42	2.33
1:BC:27:VAL:HG13	1:BC:62:HIS:CE1	0.42	2.49
1:3C:87:HIS:CG	1:3C:88:ALA:N	0.42	2.87
1:i:80:TRP:CZ3	1:i:84:HIS:CD2	0.41	3.07
1:7:12:HIS:CE1	1:7:51:ASP:OD2	0.41	2.73
1:FD:87:HIS:CG	1:FD:88:ALA:H	0.41	2.32
1:HD:59:VAL:HG23	1:HD:62:HIS:CD2	0.41	2.50
1:JE:31:ALA:HB1	1:JE:62:HIS:CE1	0.41	2.50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:D:1:PRO:HA	1:D:12:HIS:CE1	0.41	2.49
1:oB:1:PRO:HA	1:oB:12:HIS:CE1	0.41	2.51
1:tB:226:HIS:CG	1:tB:227:LYS:H	0.41	2.32
1:YD:226:HIS:CG	1:YD:227:LYS:H	0.41	2.33
1:gD:87:HIS:CD2	1:gD:89:GLY:H	0.41	2.34
1:TC:27:VAL:HG13	1:TC:62:HIS:CE1	0.41	2.50
1:4C:80:TRP:CE3	1:4C:84:HIS:CD2	0.41	3.09
1:t:27:VAL:HG13	1:t:62:HIS:CE1	0.40	2.51
1:LD:27:VAL:HG13	1:LD:62:HIS:CE1	0.40	2.52
1:SA:87:HIS:CG	1:SA:88:ALA:H	0.40	2.35
1:LB:87:HIS:CE1	1:LB:98:GLU:O	0.40	2.74
1:PA:226:HIS:CG	1:PA:227:LYS:N	0.40	2.90
1:3:181:VAL:HG21	1:9A:184:TRP:CZ2	0.40	2.51
1:XA:87:HIS:CG	1:XA:88:ALA:N	0.40	2.88
1:H:87:HIS:CG	1:H:88:ALA:N	0.40	2.90
1:KD:226:HIS:CG	1:KD:227:LYS:N	0.40	2.90
1:SE:87:HIS:CD2	1:SE:89:GLY:H	0.40	2.35
1:oE:50:GLN:H	1:oE:50:GLN:CD	0.40	2.23

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	0	229/231 (99%)	208 (91%)	20 (9%)	1 (0%)	31	76
1	0A	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	7	47
1	0B	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	0C	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	0D	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	0E	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	9	53
1	1	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	1A	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	4	30
1	1B	229/231 (99%)	207 (90%)	12 (5%)	10 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1C	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	1D	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	7	47
1	1E	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	2	229/231 (99%)	215 (94%)	9 (4%)	5 (2%)	7	47
1	2A	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	2B	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	4	33
1	2C	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	2D	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	6	42
1	2E	229/231 (99%)	199 (87%)	27 (12%)	3 (1%)	12	60
1	3	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	4	33
1	3A	229/231 (99%)	213 (93%)	10 (4%)	6 (3%)	6	42
1	3B	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	9	53
1	3C	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	3D	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	3E	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	4	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	6	42
1	4A	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	4B	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	4C	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	4D	229/231 (99%)	203 (89%)	18 (8%)	8 (3%)	4	33
1	4E	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	5	37
1	5	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	12	60
1	5A	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	7	47
1	5B	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	5C	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	5D	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	5E	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	6	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	6A	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	9	53
1	6B	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	9	53
1	6C	229/231 (99%)	200 (87%)	23 (10%)	6 (3%)	6	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6D	229/231 (99%)	215 (94%)	10 (4%)	4 (2%)	9	53
1	6E	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	6	42
1	7	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	4	33
1	7A	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	12	60
1	7B	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	7C	229/231 (99%)	205 (90%)	15 (7%)	9 (4%)	4	30
1	7D	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	7E	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	5	37
1	8	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	8A	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	12	60
1	8B	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	8C	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	12	60
1	8D	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	8E	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	5	37
1	9	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	7	47
1	9A	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	9B	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	7	47
1	9C	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	9D	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	12	60
1	9E	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	12	60
1	A	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	6	42
1	AA	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	16	66
1	AB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	AC	229/231 (99%)	215 (94%)	12 (5%)	2 (1%)	16	66
1	AD	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	AE	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	6	42
1	AF	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	B	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	16	66
1	BA	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	BB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	BC	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	5	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	7	47
1	BE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	BF	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	5	37
1	C	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	CA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	CB	229/231 (99%)	214 (93%)	12 (5%)	3 (1%)	12	60
1	CC	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	7	47
1	CD	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	12	60
1	CE	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	CF	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	D	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	DA	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	DB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	DC	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	DD	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	4	30
1	DE	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	DF	229/231 (99%)	200 (87%)	21 (9%)	8 (3%)	4	33
1	E	229/231 (99%)	206 (90%)	14 (6%)	9 (4%)	4	30
1	EA	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	EB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	EC	229/231 (99%)	200 (87%)	24 (10%)	5 (2%)	7	47
1	ED	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	7	47
1	EE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	EF	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	5	37
1	F	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	FA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	FB	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	FC	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	FD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	FE	229/231 (99%)	213 (93%)	12 (5%)	4 (2%)	9	53
1	FF	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	5	37
1	GA	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	9	53
1	GB	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	GC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	GD	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	GE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	H	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	HA	229/231 (99%)	199 (87%)	22 (10%)	8 (3%)	4	33
1	HB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	HC	229/231 (99%)	201 (88%)	21 (9%)	7 (3%)	5	37
1	HD	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	HE	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	I	229/231 (99%)	201 (88%)	25 (11%)	3 (1%)	12	60
1	IA	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	IB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	IC	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	16	66
1	ID	229/231 (99%)	202 (88%)	21 (9%)	6 (3%)	6	42
1	IE	229/231 (99%)	207 (90%)	20 (9%)	2 (1%)	16	66
1	J	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	JA	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	JB	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	5	37
1	JC	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	JD	229/231 (99%)	210 (92%)	17 (7%)	2 (1%)	16	66
1	JE	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	K	229/231 (99%)	205 (90%)	16 (7%)	8 (3%)	4	33
1	KA	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	7	47
1	KB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	KC	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	KD	229/231 (99%)	211 (92%)	17 (7%)	1 (0%)	31	76
1	KE	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	L	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	12	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	LB	229/231 (99%)	206 (90%)	14 (6%)	9 (4%)	4	30
1	LC	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	4	33
1	LD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	LE	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	M	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	MA	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	9	53
1	MB	229/231 (99%)	210 (92%)	17 (7%)	2 (1%)	16	66
1	MC	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	9	53
1	MD	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	12	60
1	ME	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	N	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	9	53
1	NA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	NB	229/231 (99%)	205 (90%)	15 (7%)	9 (4%)	4	30
1	NC	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	4	33
1	ND	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	60
1	NE	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	12	60
1	O	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	7	47
1	OA	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	7	47
1	OB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	OC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	OD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	OE	229/231 (99%)	217 (95%)	8 (3%)	4 (2%)	9	53
1	P	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	PA	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	12	60
1	PB	229/231 (99%)	204 (89%)	16 (7%)	9 (4%)	4	30
1	PC	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	PD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	PE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	Q	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	QA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QB	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	12	60
1	QC	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	QD	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	QE	229/231 (99%)	209 (91%)	11 (5%)	9 (4%)	4	30
1	R	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	9	53
1	RA	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	9	53
1	RB	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	9	53
1	RC	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	RD	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	RE	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	S	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	SA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	60
1	SB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	SC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	SD	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	SE	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	9	53
1	T	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	TA	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	TB	229/231 (99%)	210 (92%)	12 (5%)	7 (3%)	5	37
1	TC	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	TD	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	TE	229/231 (99%)	213 (93%)	12 (5%)	4 (2%)	9	53
1	U	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	6	42
1	UA	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	12	60
1	UB	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	9	53
1	UC	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	7	47
1	UD	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	UE	229/231 (99%)	205 (90%)	22 (10%)	2 (1%)	16	66
1	V	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	VA	229/231 (99%)	209 (91%)	10 (4%)	10 (4%)	3	27
1	VB	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	VC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	VD	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	VE	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	12	60
1	W	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	9	53
1	WA	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	9	53
1	WB	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	WC	229/231 (99%)	203 (89%)	25 (11%)	1 (0%)	31	76
1	WD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	7	47
1	WE	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	X	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	6	42
1	XA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	XB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	XC	229/231 (99%)	211 (92%)	9 (4%)	9 (4%)	4	30
1	XD	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	12	60
1	XE	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	Y	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	YA	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	12	60
1	YB	229/231 (99%)	202 (88%)	21 (9%)	6 (3%)	6	42
1	YC	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	YD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	YE	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	Z	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	ZA	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	ZB	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	9	53
1	ZC	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	ZD	229/231 (99%)	209 (91%)	18 (8%)	2 (1%)	16	66
1	ZE	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	a	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	aA	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	aB	229/231 (99%)	206 (90%)	21 (9%)	2 (1%)	16	66
1	aC	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aD	229/231 (99%)	206 (90%)	15 (7%)	8 (3%)	4	33
1	aE	229/231 (99%)	204 (89%)	23 (10%)	2 (1%)	16	66
1	b	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	4	30
1	bA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	bB	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	9	53
1	bC	229/231 (99%)	203 (89%)	16 (7%)	10 (4%)	3	27
1	bD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	bE	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	c	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	cA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	60
1	cB	229/231 (99%)	205 (90%)	16 (7%)	8 (3%)	4	33
1	cC	229/231 (99%)	202 (88%)	20 (9%)	7 (3%)	5	37
1	cD	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	9	53
1	cE	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	d	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	7	47
1	dA	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	dB	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	6	42
1	dC	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	dD	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	6	42
1	dE	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	9	53
1	e	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	12	60
1	eA	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	eB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	eC	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	16	66
1	eD	229/231 (99%)	215 (94%)	10 (4%)	4 (2%)	9	53
1	eE	229/231 (99%)	206 (90%)	15 (7%)	8 (3%)	4	33
1	f	229/231 (99%)	205 (90%)	17 (7%)	7 (3%)	5	37
1	fA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	fB	229/231 (99%)	209 (91%)	18 (8%)	2 (1%)	16	66
1	fC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	fD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	fE	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	g	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	7	47
1	gA	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	4	33
1	gB	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	12	60
1	gC	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	16	66
1	gD	229/231 (99%)	203 (89%)	18 (8%)	8 (3%)	4	33
1	gE	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	9	53
1	h	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	hA	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	7	47
1	hB	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	16	66
1	hC	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	16	66
1	hD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	hE	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	16	66
1	i	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	iA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	60
1	iB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	5	37
1	iC	229/231 (99%)	209 (91%)	11 (5%)	9 (4%)	4	30
1	iD	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	7	47
1	iE	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	16	66
1	j	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	jA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	jB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	jC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	jD	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	jE	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	k	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	12	60
1	kA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	kB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	kC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	kD	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	kE	229/231 (99%)	207 (90%)	13 (6%)	9 (4%)	4	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	l	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	6	42
1	lA	229/231 (99%)	209 (91%)	19 (8%)	1 (0%)	31	76
1	lB	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	lC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	lD	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	lE	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	12	60
1	m	229/231 (99%)	204 (89%)	17 (7%)	8 (3%)	4	33
1	mA	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	7	47
1	mB	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	mC	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	6	42
1	mD	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	mE	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	9	53
1	n	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	7	47
1	nA	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	nB	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	7	47
1	nC	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	nD	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	nE	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	7	47
1	o	229/231 (99%)	208 (91%)	13 (6%)	8 (3%)	4	33
1	oA	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	oB	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	9	53
1	oC	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	5	37
1	oD	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	12	60
1	oE	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	12	60
1	p	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	pA	229/231 (99%)	201 (88%)	25 (11%)	3 (1%)	12	60
1	pB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	pC	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	pD	229/231 (99%)	209 (91%)	12 (5%)	8 (3%)	4	33
1	pE	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	9	53
1	q	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	5	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	qA	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	5	37
1	qB	229/231 (99%)	203 (89%)	20 (9%)	6 (3%)	6	42
1	qC	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	5	37
1	qD	229/231 (99%)	212 (93%)	11 (5%)	6 (3%)	6	42
1	qE	229/231 (99%)	201 (88%)	23 (10%)	5 (2%)	7	47
1	r	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	9	53
1	rA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	5	37
1	rB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	rC	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	rD	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	rE	229/231 (99%)	207 (90%)	13 (6%)	9 (4%)	4	30
1	s	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	12	60
1	sA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	sB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	16	66
1	sC	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	sD	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	sE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	t	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	9	53
1	tA	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	9	53
1	tB	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	4	33
1	tC	229/231 (99%)	200 (87%)	21 (9%)	8 (3%)	4	33
1	tD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	tE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	12	60
1	u	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	9	53
1	uA	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	6	42
1	uB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	9	53
1	uC	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	12	60
1	uD	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	uE	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	9	53
1	v	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	5	37
1	vA	229/231 (99%)	207 (90%)	20 (9%)	2 (1%)	16	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	vB	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	9	53
1	vC	229/231 (99%)	210 (92%)	12 (5%)	7 (3%)	5	37
1	vD	229/231 (99%)	201 (88%)	21 (9%)	7 (3%)	5	37
1	vE	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	w	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	wA	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	9	53
1	wB	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	wC	229/231 (99%)	214 (93%)	10 (4%)	5 (2%)	7	47
1	wD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	7	47
1	wE	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	16	66
1	x	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	60
1	xA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	7	47
1	xB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	6	42
1	xC	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	12	60
1	xD	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	xE	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	6	42
1	y	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	7	47
1	yA	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	12	60
1	yB	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	16	66
1	yC	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	6	42
1	yD	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	9	53
1	yE	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	9	53
1	z	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	7	47
1	zA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	6	42
1	zB	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	12	60
1	zC	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	5	37
1	zD	229/231 (99%)	212 (93%)	11 (5%)	6 (3%)	6	42
1	zE	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	12	60
All	All	86562/87318 (99%)	78634 (91%)	6023 (7%)	1905 (2%)	7	47

All 1905 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	4	GLN
1	A	60	GLY
1	A	85	PRO
1	A	89	GLY
1	A	146	SER
1	A	176	GLN
1	B	4	GLN
1	B	146	SER
1	C	4	GLN
1	C	97	ARG
1	C	122	PRO
1	C	147	PRO
1	C	226	HIS
1	D	31	ALA
1	D	47	ALA
1	D	85	PRO
1	D	98	GLU
1	D	147	PRO
1	D	175	GLU
1	E	4	GLN
1	E	10	MET
1	E	31	ALA
1	E	61	GLY
1	E	85	PRO
1	E	98	GLU
1	E	122	PRO
1	E	123	PRO
1	E	146	SER
1	F	4	GLN
1	F	85	PRO
1	F	98	GLU
1	F	207	PRO
1	F	223	GLY
1	F	226	HIS
1	G	4	GLN
1	G	31	ALA
1	G	47	ALA
1	G	85	PRO
1	G	97	ARG
1	G	147	PRO
1	G	226	HIS
1	H	4	GLN
1	H	224	PRO

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Mol	Chain	Res	Type
1	H	227	LYS
1	I	4	GLN
1	I	63	GLN
1	I	147	PRO
1	J	4	GLN
1	J	31	ALA
1	J	47	ALA
1	J	88	ALA
1	J	99	PRO
1	K	4	GLN
1	K	31	ALA
1	K	87	HIS
1	K	98	GLU
1	K	147	PRO
1	K	210	THR
1	K	226	HIS
1	K	227	LYS
1	L	4	GLN
1	L	98	GLU
1	L	226	HIS
1	M	4	GLN
1	M	85	PRO
1	M	147	PRO
1	M	223	GLY
1	N	4	GLN
1	N	31	ALA
1	N	87	HIS
1	N	121	ASN
1	O	5	ASN
1	O	47	ALA
1	O	147	PRO
1	O	176	GLN
1	O	230	VAL
1	P	4	GLN
1	P	85	PRO
1	P	88	ALA
1	P	98	GLU
1	P	150	ILE
1	P	228	ALA
1	Q	4	GLN
1	Q	10	MET
1	Q	62	HIS

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Mol	Chain	Res	Type
1	Q	98	GLU
1	Q	122	PRO
1	Q	207	PRO
1	Q	228	ALA
1	R	31	ALA
1	R	63	GLN
1	R	98	GLU
1	R	209	ALA
1	S	4	GLN
1	S	5	ASN
1	S	31	ALA
1	S	97	ARG
1	S	176	GLN
1	S	226	HIS
1	T	4	GLN
1	T	224	PRO
1	T	226	HIS
1	U	4	GLN
1	U	31	ALA
1	U	97	ARG
1	U	145	TYR
1	U	147	PRO
1	U	207	PRO
1	V	4	GLN
1	V	61	GLY
1	V	98	GLU
1	V	147	PRO
1	V	227	LYS
1	W	4	GLN
1	W	97	ARG
1	W	98	GLU
1	W	224	PRO
1	X	4	GLN
1	X	85	PRO
1	X	96	MET
1	X	98	GLU
1	X	223	GLY
1	X	230	VAL
1	Y	4	GLN
1	Y	31	ALA
1	Y	61	GLY
1	Y	222	GLY

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Mol	Chain	Res	Type
1	Y	224	PRO
1	Y	228	ALA
1	Z	4	GLN
1	Z	14	ALA
1	Z	30	LYS
1	Z	119	THR
1	Z	122	PRO
1	Z	226	HIS
1	a	10	MET
1	a	97	ARG
1	a	147	PRO
1	a	226	HIS
1	a	229	ARG
1	b	2	ILE
1	b	4	GLN
1	b	10	MET
1	b	61	GLY
1	b	85	PRO
1	b	88	ALA
1	b	98	GLU
1	b	147	PRO
1	b	230	VAL
1	c	4	GLN
1	c	31	ALA
1	c	96	MET
1	c	98	GLU
1	c	123	PRO
1	c	227	LYS
1	d	4	GLN
1	d	98	GLU
1	d	228	ALA
1	d	229	ARG
1	d	230	VAL
1	e	4	GLN
1	e	31	ALA
1	e	61	GLY
1	f	4	GLN
1	f	31	ALA
1	f	61	GLY
1	f	97	ARG
1	f	119	THR
1	f	222	GLY

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Mol	Chain	Res	Type
1	f	226	HIS
1	g	4	GLN
1	g	87	HIS
1	g	97	ARG
1	g	147	PRO
1	g	227	LYS
1	h	4	GLN
1	h	98	GLU
1	h	146	SER
1	h	223	GLY
1	h	229	ARG
1	i	4	GLN
1	i	97	ARG
1	i	146	SER
1	i	206	GLY
1	j	85	PRO
1	j	98	GLU
1	j	99	PRO
1	j	226	HIS
1	k	4	GLN
1	k	120	HIS
1	k	123	PRO
1	l	4	GLN
1	l	31	ALA
1	l	87	HIS
1	l	121	ASN
1	l	147	PRO
1	l	226	HIS
1	m	5	ASN
1	m	47	ALA
1	m	60	GLY
1	m	62	HIS
1	m	97	ARG
1	m	119	THR
1	m	147	PRO
1	m	226	HIS
1	n	4	GLN
1	n	31	ALA
1	n	85	PRO
1	n	98	GLU
1	n	146	SER
1	o	4	GLN

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Mol	Chain	Res	Type
1	o	97	ARG
1	o	98	GLU
1	o	122	PRO
1	o	147	PRO
1	o	176	GLN
1	o	227	LYS
1	o	229	ARG
1	p	4	GLN
1	p	31	ALA
1	p	98	GLU
1	p	120	HIS
1	p	147	PRO
1	p	209	ALA
1	p	223	GLY
1	q	4	GLN
1	q	10	MET
1	q	31	ALA
1	q	47	ALA
1	q	85	PRO
1	q	147	PRO
1	q	224	PRO
1	r	4	GLN
1	r	122	PRO
1	r	147	PRO
1	r	150	ILE
1	s	4	GLN
1	s	97	ARG
1	s	147	PRO
1	t	4	GLN
1	t	47	ALA
1	t	84	HIS
1	t	147	PRO
1	u	4	GLN
1	u	89	GLY
1	u	96	MET
1	u	147	PRO
1	v	4	GLN
1	v	31	ALA
1	v	60	GLY
1	v	85	PRO
1	v	98	GLU
1	v	147	PRO

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Mol	Chain	Res	Type
1	v	224	PRO
1	w	4	GLN
1	w	10	MET
1	w	31	ALA
1	w	85	PRO
1	w	147	PRO
1	w	176	GLN
1	x	4	GLN
1	x	47	ALA
1	x	176	GLN
1	y	10	MET
1	y	85	PRO
1	y	97	ARG
1	y	146	SER
1	y	147	PRO
1	z	4	GLN
1	z	31	ALA
1	z	61	GLY
1	z	99	PRO
1	z	228	ALA
1	0	4	GLN
1	1	4	GLN
1	1	61	GLY
1	1	85	PRO
1	1	98	GLU
1	1	121	ASN
1	1	176	GLN
1	1	224	PRO
1	2	8	GLY
1	2	47	ALA
1	2	85	PRO
1	2	123	PRO
1	2	150	ILE
1	3	4	GLN
1	3	31	ALA
1	3	45	GLU
1	3	47	ALA
1	3	61	GLY
1	3	89	GLY
1	3	123	PRO
1	3	147	PRO
1	4	4	GLN

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Mol	Chain	Res	Type
1	4	97	ARG
1	4	119	THR
1	4	147	PRO
1	4	222	GLY
1	4	226	HIS
1	5	61	GLY
1	5	121	ASN
1	5	226	HIS
1	6	4	GLN
1	6	47	ALA
1	6	98	GLU
1	6	123	PRO
1	6	147	PRO
1	6	224	PRO
1	6	228	ALA
1	7	4	GLN
1	7	85	PRO
1	7	98	GLU
1	7	123	PRO
1	7	150	ILE
1	7	176	GLN
1	7	209	ALA
1	7	224	PRO
1	8	4	GLN
1	8	47	ALA
1	8	88	ALA
1	8	97	ARG
1	8	147	PRO
1	8	229	ARG
1	9	4	GLN
1	9	47	ALA
1	9	176	GLN
1	9	223	GLY
1	9	224	PRO
1	AA	4	GLN
1	AA	147	PRO
1	BA	4	GLN
1	BA	10	MET
1	BA	85	PRO
1	BA	86	VAL
1	BA	98	GLU
1	BA	222	GLY

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Mol	Chain	Res	Type
1	CA	4	GLN
1	CA	61	GLY
1	CA	98	GLU
1	CA	123	PRO
1	CA	146	SER
1	CA	224	PRO
1	DA	4	GLN
1	DA	84	HIS
1	DA	98	GLU
1	DA	147	PRO
1	DA	223	GLY
1	EA	4	GLN
1	EA	85	PRO
1	EA	97	ARG
1	EA	147	PRO
1	EA	176	GLN
1	EA	229	ARG
1	FA	4	GLN
1	FA	31	ALA
1	FA	87	HIS
1	FA	97	ARG
1	FA	122	PRO
1	FA	147	PRO
1	FA	224	PRO
1	GA	4	GLN
1	GA	87	HIS
1	GA	147	PRO
1	GA	148	THR
1	HA	4	GLN
1	HA	61	GLY
1	HA	85	PRO
1	HA	98	GLU
1	HA	147	PRO
1	HA	221	VAL
1	HA	228	ALA
1	HA	229	ARG
1	IA	31	ALA
1	IA	98	GLU
1	IA	123	PRO
1	IA	224	PRO
1	IA	229	ARG
1	JA	4	GLN

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Mol	Chain	Res	Type
1	JA	98	GLU
1	JA	146	SER
1	JA	209	ALA
1	KA	4	GLN
1	KA	31	ALA
1	KA	47	ALA
1	KA	61	GLY
1	KA	230	VAL
1	LA	4	GLN
1	LA	31	ALA
1	LA	226	HIS
1	MA	10	MET
1	MA	60	GLY
1	MA	147	PRO
1	MA	226	HIS
1	NA	45	GLU
1	NA	85	PRO
1	NA	98	GLU
1	NA	150	ILE
1	NA	175	GLU
1	OA	4	GLN
1	OA	98	GLU
1	OA	149	SER
1	OA	226	HIS
1	OA	228	ALA
1	PA	15	ILE
1	PA	98	GLU
1	PA	209	ALA
1	QA	31	ALA
1	QA	97	ARG
1	QA	226	HIS
1	QA	227	LYS
1	RA	4	GLN
1	RA	47	ALA
1	RA	97	ARG
1	RA	123	PRO
1	SA	4	GLN
1	SA	85	PRO
1	SA	147	PRO
1	TA	4	GLN
1	TA	44	SER
1	TA	85	PRO

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Mol	Chain	Res	Type
1	TA	121	ASN
1	TA	150	ILE
1	UA	4	GLN
1	UA	98	GLU
1	UA	147	PRO
1	VA	4	GLN
1	VA	10	MET
1	VA	60	GLY
1	VA	62	HIS
1	VA	85	PRO
1	VA	93	PRO
1	VA	98	GLU
1	VA	147	PRO
1	VA	176	GLN
1	VA	226	HIS
1	WA	4	GLN
1	WA	31	ALA
1	WA	47	ALA
1	WA	224	PRO
1	XA	4	GLN
1	XA	31	ALA
1	XA	61	GLY
1	XA	123	PRO
1	YA	47	ALA
1	YA	97	ARG
1	YA	147	PRO
1	ZA	4	GLN
1	ZA	5	ASN
1	ZA	31	ALA
1	ZA	61	GLY
1	ZA	85	PRO
1	ZA	98	GLU
1	ZA	123	PRO
1	aA	4	GLN
1	aA	98	GLU
1	aA	123	PRO
1	bA	4	GLN
1	bA	85	PRO
1	bA	98	GLU
1	bA	147	PRO
1	cA	4	GLN
1	cA	31	ALA

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Mol	Chain	Res	Type
1	cA	47	ALA
1	dA	4	GLN
1	dA	61	GLY
1	dA	123	PRO
1	eA	4	GLN
1	eA	85	PRO
1	eA	87	HIS
1	eA	119	THR
1	eA	147	PRO
1	fA	4	GLN
1	fA	85	PRO
1	fA	150	ILE
1	fA	175	GLU
1	fA	226	HIS
1	gA	4	GLN
1	gA	31	ALA
1	gA	85	PRO
1	gA	87	HIS
1	gA	98	GLU
1	gA	146	SER
1	gA	223	GLY
1	gA	224	PRO
1	hA	4	GLN
1	hA	31	ALA
1	hA	98	GLU
1	hA	223	GLY
1	hA	229	ARG
1	iA	60	GLY
1	iA	223	GLY
1	iA	224	PRO
1	jA	4	GLN
1	jA	31	ALA
1	jA	61	GLY
1	jA	85	PRO
1	jA	87	HIS
1	jA	120	HIS
1	jA	147	PRO
1	kA	10	MET
1	kA	90	PRO
1	kA	97	ARG
1	kA	147	PRO
1	kA	176	GLN

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Mol	Chain	Res	Type
1	kA	223	GLY
1	lA	150	ILE
1	mA	4	GLN
1	mA	47	ALA
1	mA	98	GLU
1	mA	146	SER
1	mA	227	LYS
1	nA	4	GLN
1	nA	10	MET
1	nA	47	ALA
1	nA	98	GLU
1	nA	119	THR
1	nA	224	PRO
1	oA	147	PRO
1	oA	175	GLU
1	oA	222	GLY
1	pA	4	GLN
1	pA	88	ALA
1	pA	146	SER
1	qA	4	GLN
1	qA	87	HIS
1	qA	147	PRO
1	qA	206	GLY
1	qA	222	GLY
1	qA	226	HIS
1	qA	228	ALA
1	rA	4	GLN
1	rA	31	ALA
1	rA	85	PRO
1	rA	123	PRO
1	rA	150	ILE
1	rA	178	SER
1	rA	226	HIS
1	sA	85	PRO
1	sA	98	GLU
1	sA	119	THR
1	sA	122	PRO
1	sA	146	SER
1	tA	4	GLN
1	tA	10	MET
1	tA	31	ALA
1	tA	146	SER

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Mol	Chain	Res	Type
1	uA	31	ALA
1	uA	47	ALA
1	uA	88	ALA
1	uA	120	HIS
1	uA	147	PRO
1	uA	176	GLN
1	vA	4	GLN
1	vA	88	ALA
1	wA	4	GLN
1	wA	31	ALA
1	wA	61	GLY
1	wA	147	PRO
1	xA	4	GLN
1	xA	47	ALA
1	xA	85	PRO
1	xA	99	PRO
1	xA	147	PRO
1	yA	4	GLN
1	yA	31	ALA
1	yA	230	VAL
1	zA	4	GLN
1	zA	9	GLN
1	zA	31	ALA
1	zA	176	GLN
1	zA	207	PRO
1	zA	229	ARG
1	0A	4	GLN
1	0A	31	ALA
1	0A	47	ALA
1	0A	85	PRO
1	0A	121	ASN
1	1A	4	GLN
1	1A	10	MET
1	1A	31	ALA
1	1A	84	HIS
1	1A	87	HIS
1	1A	88	ALA
1	1A	97	ARG
1	1A	123	PRO
1	1A	147	PRO
1	2A	4	GLN
1	2A	10	MET

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Mol	Chain	Res	Type
1	2A	63	GLN
1	2A	97	ARG
1	2A	147	PRO
1	3A	45	GLU
1	3A	47	ALA
1	3A	85	PRO
1	3A	98	GLU
1	3A	147	PRO
1	3A	178	SER
1	4A	4	GLN
1	4A	31	ALA
1	4A	98	GLU
1	5A	4	GLN
1	5A	14	ALA
1	5A	85	PRO
1	5A	147	PRO
1	5A	226	HIS
1	6A	47	ALA
1	6A	150	ILE
1	6A	176	GLN
1	6A	224	PRO
1	7A	4	GLN
1	7A	10	MET
1	7A	207	PRO
1	8A	85	PRO
1	8A	97	ARG
1	8A	147	PRO
1	9A	4	GLN
1	9A	88	ALA
1	9A	99	PRO
1	9A	146	SER
1	9A	174	ALA
1	AB	4	GLN
1	AB	31	ALA
1	AB	85	PRO
1	AB	96	MET
1	AB	97	ARG
1	AB	98	GLU
1	AB	224	PRO
1	BB	4	GLN
1	BB	64	ALA
1	BB	98	GLU

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Mol	Chain	Res	Type
1	BB	209	ALA
1	BB	223	GLY
1	CB	31	ALA
1	CB	123	PRO
1	CB	147	PRO
1	DB	4	GLN
1	DB	5	ASN
1	DB	47	ALA
1	DB	85	PRO
1	DB	122	PRO
1	DB	147	PRO
1	DB	230	VAL
1	EB	4	GLN
1	EB	85	PRO
1	EB	87	HIS
1	EB	97	ARG
1	EB	147	PRO
1	FB	10	MET
1	FB	31	ALA
1	FB	85	PRO
1	FB	98	GLU
1	FB	147	PRO
1	GB	4	GLN
1	GB	60	GLY
1	GB	98	GLU
1	GB	120	HIS
1	GB	122	PRO
1	HB	4	GLN
1	HB	47	ALA
1	HB	85	PRO
1	HB	98	GLU
1	HB	226	HIS
1	IB	84	HIS
1	IB	147	PRO
1	IB	150	ILE
1	IB	228	ALA
1	JB	4	GLN
1	JB	61	GLY
1	JB	147	PRO
1	JB	223	GLY
1	JB	224	PRO
1	JB	228	ALA

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Mol	Chain	Res	Type
1	JB	229	ARG
1	KB	31	ALA
1	KB	47	ALA
1	KB	87	HIS
1	KB	147	PRO
1	LB	4	GLN
1	LB	31	ALA
1	LB	85	PRO
1	LB	96	MET
1	LB	98	GLU
1	LB	99	PRO
1	LB	123	PRO
1	LB	147	PRO
1	LB	175	GLU
1	MB	4	GLN
1	MB	31	ALA
1	NB	4	GLN
1	NB	63	GLN
1	NB	97	ARG
1	NB	98	GLU
1	NB	147	PRO
1	NB	209	ALA
1	NB	222	GLY
1	NB	228	ALA
1	NB	230	VAL
1	OB	4	GLN
1	OB	47	ALA
1	OB	85	PRO
1	OB	97	ARG
1	OB	147	PRO
1	OB	176	GLN
1	OB	224	PRO
1	PB	4	GLN
1	PB	47	ALA
1	PB	85	PRO
1	PB	97	ARG
1	PB	147	PRO
1	PB	176	GLN
1	PB	223	GLY
1	PB	224	PRO
1	PB	227	LYS
1	QB	4	GLN

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Mol	Chain	Res	Type
1	QB	147	PRO
1	QB	224	PRO
1	RB	4	GLN
1	RB	85	PRO
1	RB	98	GLU
1	RB	150	ILE
1	SB	4	GLN
1	SB	98	GLU
1	SB	150	ILE
1	SB	228	ALA
1	SB	230	VAL
1	TB	4	GLN
1	TB	10	MET
1	TB	31	ALA
1	TB	64	ALA
1	TB	97	ARG
1	TB	147	PRO
1	TB	209	ALA
1	UB	4	GLN
1	UB	47	ALA
1	UB	147	PRO
1	UB	223	GLY
1	VB	4	GLN
1	VB	31	ALA
1	VB	61	GLY
1	VB	147	PRO
1	VB	228	ALA
1	WB	10	MET
1	WB	47	ALA
1	WB	85	PRO
1	WB	87	HIS
1	WB	97	ARG
1	WB	147	PRO
1	XB	10	MET
1	XB	85	PRO
1	XB	99	PRO
1	XB	123	PRO
1	XB	147	PRO
1	XB	207	PRO
1	YB	4	GLN
1	YB	62	HIS
1	YB	85	PRO

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Mol	Chain	Res	Type
1	YB	87	HIS
1	YB	98	GLU
1	YB	176	GLN
1	ZB	4	GLN
1	ZB	31	ALA
1	ZB	98	GLU
1	ZB	146	SER
1	aB	10	MET
1	aB	230	VAL
1	bB	4	GLN
1	bB	31	ALA
1	bB	85	PRO
1	bB	147	PRO
1	cB	10	MET
1	cB	87	HIS
1	cB	120	HIS
1	cB	122	PRO
1	cB	123	PRO
1	cB	147	PRO
1	cB	227	LYS
1	cB	228	ALA
1	dB	4	GLN
1	dB	47	ALA
1	dB	85	PRO
1	dB	121	ASN
1	dB	147	PRO
1	dB	176	GLN
1	eB	4	GLN
1	eB	31	ALA
1	eB	61	GLY
1	eB	85	PRO
1	eB	97	ARG
1	eB	98	GLU
1	eB	224	PRO
1	fB	64	ALA
1	fB	85	PRO
1	gB	97	ARG
1	gB	147	PRO
1	gB	227	LYS
1	hB	31	ALA
1	hB	224	PRO
1	iB	10	MET

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Mol	Chain	Res	Type
1	iB	31	ALA
1	iB	47	ALA
1	iB	97	ARG
1	iB	121	ASN
1	iB	147	PRO
1	iB	222	GLY
1	jB	4	GLN
1	jB	47	ALA
1	jB	86	VAL
1	jB	98	GLU
1	jB	147	PRO
1	jB	230	VAL
1	kB	4	GLN
1	kB	31	ALA
1	kB	97	ARG
1	kB	98	GLU
1	kB	146	SER
1	kB	209	ALA
1	kB	210	THR
1	lB	4	GLN
1	lB	85	PRO
1	lB	98	GLU
1	lB	147	PRO
1	lB	176	GLN
1	lB	209	ALA
1	lB	225	GLY
1	mB	4	GLN
1	mB	85	PRO
1	mB	119	THR
1	mB	147	PRO
1	nB	4	GLN
1	nB	97	ARG
1	nB	119	THR
1	nB	146	SER
1	nB	176	GLN
1	oB	85	PRO
1	oB	87	HIS
1	oB	147	PRO
1	oB	226	HIS
1	pB	5	ASN
1	pB	61	GLY
1	pB	99	PRO

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Mol	Chain	Res	Type
1	pB	146	SER
1	pB	227	LYS
1	qB	4	GLN
1	qB	98	GLU
1	qB	120	HIS
1	qB	147	PRO
1	qB	176	GLN
1	qB	209	ALA
1	rB	4	GLN
1	rB	31	ALA
1	rB	98	GLU
1	rB	121	ASN
1	rB	147	PRO
1	sB	85	PRO
1	sB	97	ARG
1	tB	4	GLN
1	tB	10	MET
1	tB	31	ALA
1	tB	62	HIS
1	tB	85	PRO
1	tB	123	PRO
1	tB	147	PRO
1	tB	224	PRO
1	uB	31	ALA
1	uB	47	ALA
1	uB	87	HIS
1	uB	147	PRO
1	vB	4	GLN
1	vB	98	GLU
1	vB	99	PRO
1	vB	227	LYS
1	wB	4	GLN
1	wB	85	PRO
1	wB	87	HIS
1	wB	98	GLU
1	wB	223	GLY
1	wB	229	ARG
1	xB	4	GLN
1	xB	98	GLU
1	xB	106	GLY
1	xB	176	GLN
1	xB	222	GLY

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Mol	Chain	Res	Type
1	xB	226	HIS
1	yB	4	GLN
1	yB	146	SER
1	zB	5	ASN
1	zB	84	HIS
1	zB	97	ARG
1	0B	84	HIS
1	0B	87	HIS
1	0B	147	PRO
1	0B	224	PRO
1	0B	228	ALA
1	1B	4	GLN
1	1B	31	ALA
1	1B	61	GLY
1	1B	62	HIS
1	1B	85	PRO
1	1B	90	PRO
1	1B	98	GLU
1	1B	99	PRO
1	1B	123	PRO
1	1B	146	SER
1	2B	4	GLN
1	2B	31	ALA
1	2B	87	HIS
1	2B	96	MET
1	2B	98	GLU
1	2B	122	PRO
1	2B	147	PRO
1	2B	223	GLY
1	3B	4	GLN
1	3B	47	ALA
1	3B	98	GLU
1	3B	120	HIS
1	4B	4	GLN
1	4B	31	ALA
1	4B	85	PRO
1	4B	147	PRO
1	5B	4	GLN
1	5B	87	HIS
1	5B	122	PRO
1	5B	229	ARG
1	6B	4	GLN

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Mol	Chain	Res	Type
1	6B	87	HIS
1	6B	97	ARG
1	6B	147	PRO
1	7B	4	GLN
1	7B	47	ALA
1	7B	98	GLU
1	7B	146	SER
1	8B	4	GLN
1	8B	63	GLN
1	8B	146	SER
1	8B	223	GLY
1	9B	4	GLN
1	9B	85	PRO
1	9B	88	ALA
1	9B	98	GLU
1	9B	122	PRO
1	AC	4	GLN
1	AC	147	PRO
1	BC	4	GLN
1	BC	85	PRO
1	BC	97	ARG
1	BC	119	THR
1	BC	122	PRO
1	BC	146	SER
1	BC	178	SER
1	CC	10	MET
1	CC	85	PRO
1	CC	122	PRO
1	CC	147	PRO
1	CC	226	HIS
1	DC	10	MET
1	DC	60	GLY
1	DC	92	ALA
1	DC	99	PRO
1	EC	4	GLN
1	EC	176	GLN
1	EC	223	GLY
1	EC	226	HIS
1	EC	229	ARG
1	FC	4	GLN
1	FC	64	ALA
1	FC	85	PRO

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Mol	Chain	Res	Type
1	FC	207	PRO
1	FC	209	ALA
1	GC	4	GLN
1	GC	31	ALA
1	GC	47	ALA
1	GC	88	ALA
1	GC	97	ARG
1	GC	147	PRO
1	HC	4	GLN
1	HC	10	MET
1	HC	31	ALA
1	HC	47	ALA
1	HC	222	GLY
1	HC	223	GLY
1	HC	227	LYS
1	IC	47	ALA
1	IC	147	PRO
1	JC	4	GLN
1	JC	47	ALA
1	JC	98	GLU
1	JC	123	PRO
1	JC	224	PRO
1	KC	4	GLN
1	KC	47	ALA
1	KC	61	GLY
1	KC	98	GLU
1	KC	123	PRO
1	KC	209	ALA
1	KC	224	PRO
1	LC	4	GLN
1	LC	31	ALA
1	LC	60	GLY
1	LC	98	GLU
1	LC	123	PRO
1	LC	146	SER
1	LC	147	PRO
1	LC	226	HIS
1	MC	4	GLN
1	MC	47	ALA
1	MC	97	ARG
1	MC	229	ARG
1	NC	4	GLN

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Mol	Chain	Res	Type
1	NC	87	HIS
1	NC	97	ARG
1	NC	147	PRO
1	NC	175	GLU
1	NC	224	PRO
1	NC	225	GLY
1	NC	228	ALA
1	OC	4	GLN
1	OC	10	MET
1	OC	31	ALA
1	OC	47	ALA
1	OC	119	THR
1	OC	147	PRO
1	PC	4	GLN
1	PC	30	LYS
1	PC	85	PRO
1	PC	90	PRO
1	PC	147	PRO
1	PC	150	ILE
1	QC	4	GLN
1	QC	44	SER
1	QC	47	ALA
1	QC	87	HIS
1	QC	98	GLU
1	RC	4	GLN
1	RC	31	ALA
1	RC	85	PRO
1	RC	98	GLU
1	RC	146	SER
1	RC	228	ALA
1	SC	93	PRO
1	SC	120	HIS
1	SC	226	HIS
1	SC	230	VAL
1	TC	4	GLN
1	TC	31	ALA
1	TC	47	ALA
1	TC	85	PRO
1	UC	4	GLN
1	UC	47	ALA
1	UC	123	PRO
1	UC	147	PRO

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Mol	Chain	Res	Type
1	UC	228	ALA
1	VC	47	ALA
1	VC	61	GLY
1	VC	85	PRO
1	VC	92	ALA
1	VC	98	GLU
1	VC	147	PRO
1	WC	31	ALA
1	XC	4	GLN
1	XC	31	ALA
1	XC	97	ARG
1	XC	98	GLU
1	XC	119	THR
1	XC	121	ASN
1	XC	150	ILE
1	XC	227	LYS
1	XC	228	ALA
1	YC	5	ASN
1	YC	122	PRO
1	YC	150	ILE
1	YC	178	SER
1	YC	222	GLY
1	YC	224	PRO
1	ZC	4	GLN
1	ZC	31	ALA
1	ZC	47	ALA
1	aC	5	ASN
1	aC	61	GLY
1	aC	87	HIS
1	aC	123	PRO
1	aC	147	PRO
1	aC	148	THR
1	aC	224	PRO
1	bC	4	GLN
1	bC	31	ALA
1	bC	47	ALA
1	bC	85	PRO
1	bC	98	GLU
1	bC	119	THR
1	bC	123	PRO
1	bC	150	ILE
1	bC	175	GLU

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Mol	Chain	Res	Type
1	bC	226	HIS
1	cC	4	GLN
1	cC	31	ALA
1	cC	101	GLY
1	cC	121	ASN
1	cC	146	SER
1	cC	209	ALA
1	cC	224	PRO
1	dC	4	GLN
1	dC	10	MET
1	dC	85	PRO
1	dC	147	PRO
1	dC	226	HIS
1	eC	47	ALA
1	eC	150	ILE
1	fC	4	GLN
1	fC	8	GLY
1	fC	60	GLY
1	fC	87	HIS
1	fC	224	PRO
1	fC	226	HIS
1	gC	10	MET
1	gC	147	PRO
1	hC	4	GLN
1	hC	85	PRO
1	iC	4	GLN
1	iC	60	GLY
1	iC	97	ARG
1	iC	98	GLU
1	iC	123	PRO
1	iC	147	PRO
1	iC	176	GLN
1	iC	209	ALA
1	iC	226	HIS
1	jC	4	GLN
1	jC	31	ALA
1	jC	47	ALA
1	jC	97	ARG
1	kC	4	GLN
1	kC	31	ALA
1	kC	85	PRO
1	kC	147	PRO

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Mol	Chain	Res	Type
1	lC	4	GLN
1	lC	47	ALA
1	lC	97	ARG
1	lC	227	LYS
1	mC	10	MET
1	mC	97	ARG
1	mC	122	PRO
1	mC	147	PRO
1	mC	175	GLU
1	mC	226	HIS
1	nC	4	GLN
1	nC	85	PRO
1	nC	97	ARG
1	nC	98	GLU
1	nC	150	ILE
1	oC	4	GLN
1	oC	61	GLY
1	oC	85	PRO
1	oC	97	ARG
1	oC	98	GLU
1	oC	176	GLN
1	oC	206	GLY
1	pC	31	ALA
1	pC	47	ALA
1	pC	85	PRO
1	pC	98	GLU
1	pC	147	PRO
1	pC	229	ARG
1	qC	4	GLN
1	qC	31	ALA
1	qC	85	PRO
1	qC	123	PRO
1	qC	147	PRO
1	qC	224	PRO
1	qC	226	HIS
1	rC	31	ALA
1	rC	44	SER
1	rC	61	GLY
1	rC	87	HIS
1	rC	97	ARG
1	rC	122	PRO
1	sC	47	ALA

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Mol	Chain	Res	Type
1	sC	85	PRO
1	sC	147	PRO
1	sC	224	PRO
1	tC	4	GLN
1	tC	31	ALA
1	tC	61	GLY
1	tC	85	PRO
1	tC	98	GLU
1	tC	121	ASN
1	tC	147	PRO
1	tC	175	GLU
1	uC	4	GLN
1	uC	98	GLU
1	uC	229	ARG
1	vC	4	GLN
1	vC	31	ALA
1	vC	47	ALA
1	vC	85	PRO
1	vC	98	GLU
1	vC	147	PRO
1	vC	209	ALA
1	wC	4	GLN
1	wC	31	ALA
1	wC	59	VAL
1	wC	147	PRO
1	wC	150	ILE
1	xC	31	ALA
1	xC	61	GLY
1	xC	122	PRO
1	yC	4	GLN
1	yC	47	ALA
1	yC	87	HIS
1	yC	147	PRO
1	yC	206	GLY
1	yC	226	HIS
1	zC	4	GLN
1	zC	10	MET
1	zC	45	GLU
1	zC	47	ALA
1	zC	85	PRO
1	zC	146	SER
1	zC	226	HIS

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Mol	Chain	Res	Type
1	0C	4	GLN
1	0C	87	HIS
1	0C	98	GLU
1	0C	123	PRO
1	0C	224	PRO
1	1C	5	ASN
1	1C	31	ALA
1	1C	47	ALA
1	1C	98	GLU
1	1C	122	PRO
1	1C	209	ALA
1	1C	223	GLY
1	2C	4	GLN
1	2C	97	ARG
1	2C	147	PRO
1	2C	224	PRO
1	2C	228	ALA
1	3C	4	GLN
1	3C	31	ALA
1	3C	146	SER
1	3C	223	GLY
1	4C	47	ALA
1	4C	84	HIS
1	4C	97	ARG
1	4C	119	THR
1	4C	122	PRO
1	4C	147	PRO
1	5C	4	GLN
1	5C	85	PRO
1	5C	98	GLU
1	5C	150	ILE
1	5C	227	LYS
1	5C	229	ARG
1	6C	4	GLN
1	6C	31	ALA
1	6C	85	PRO
1	6C	123	PRO
1	6C	150	ILE
1	6C	226	HIS
1	7C	4	GLN
1	7C	44	SER
1	7C	85	PRO

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Mol	Chain	Res	Type
1	7C	98	GLU
1	7C	119	THR
1	7C	147	PRO
1	7C	176	GLN
1	7C	209	ALA
1	7C	224	PRO
1	8C	4	GLN
1	8C	47	ALA
1	8C	226	HIS
1	9C	97	ARG
1	9C	147	PRO
1	9C	222	GLY
1	9C	230	VAL
1	AD	4	GLN
1	AD	44	SER
1	AD	47	ALA
1	AD	90	PRO
1	AD	147	PRO
1	BD	4	GLN
1	BD	10	MET
1	BD	31	ALA
1	BD	85	PRO
1	BD	98	GLU
1	CD	4	GLN
1	CD	97	ARG
1	CD	228	ALA
1	DD	4	GLN
1	DD	31	ALA
1	DD	85	PRO
1	DD	97	ARG
1	DD	98	GLU
1	DD	119	THR
1	DD	147	PRO
1	DD	221	VAL
1	DD	229	ARG
1	ED	4	GLN
1	ED	31	ALA
1	ED	47	ALA
1	ED	147	PRO
1	ED	224	PRO
1	FD	4	GLN
1	FD	31	ALA

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Mol	Chain	Res	Type
1	FD	122	PRO
1	FD	230	VAL
1	GD	4	GLN
1	GD	61	GLY
1	GD	85	PRO
1	GD	97	ARG
1	GD	122	PRO
1	GD	147	PRO
1	GD	176	GLN
1	HD	10	MET
1	HD	90	PRO
1	HD	98	GLU
1	HD	147	PRO
1	HD	176	GLN
1	ID	4	GLN
1	ID	47	ALA
1	ID	63	GLN
1	ID	209	ALA
1	ID	224	PRO
1	ID	229	ARG
1	JD	98	GLU
1	JD	176	GLN
1	KD	176	GLN
1	LD	4	GLN
1	LD	31	ALA
1	LD	61	GLY
1	LD	226	HIS
1	MD	10	MET
1	MD	97	ARG
1	MD	147	PRO
1	ND	85	PRO
1	ND	98	GLU
1	ND	119	THR
1	OD	4	GLN
1	OD	31	ALA
1	OD	146	SER
1	OD	176	GLN
1	PD	4	GLN
1	PD	10	MET
1	PD	31	ALA
1	PD	98	GLU
1	PD	147	PRO

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Mol	Chain	Res	Type
1	PD	209	ALA
1	QD	4	GLN
1	QD	46	GLY
1	QD	85	PRO
1	QD	97	ARG
1	QD	147	PRO
1	RD	4	GLN
1	RD	47	ALA
1	RD	61	GLY
1	RD	97	ARG
1	RD	227	LYS
1	SD	4	GLN
1	SD	147	PRO
1	SD	224	PRO
1	TD	31	ALA
1	TD	98	GLU
1	TD	147	PRO
1	TD	150	ILE
1	TD	223	GLY
1	UD	4	GLN
1	UD	61	GLY
1	UD	63	GLN
1	UD	98	GLU
1	UD	123	PRO
1	UD	226	HIS
1	VD	4	GLN
1	VD	47	ALA
1	VD	147	PRO
1	VD	176	GLN
1	VD	223	GLY
1	WD	4	GLN
1	WD	85	PRO
1	WD	97	ARG
1	WD	121	ASN
1	WD	147	PRO
1	XD	4	GLN
1	XD	5	ASN
1	XD	178	SER
1	YD	5	ASN
1	YD	85	PRO
1	YD	97	ARG
1	YD	146	SER

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Mol	Chain	Res	Type
1	YD	147	PRO
1	YD	148	THR
1	ZD	4	GLN
1	ZD	98	GLU
1	aD	4	GLN
1	aD	31	ALA
1	aD	47	ALA
1	aD	87	HIS
1	aD	98	GLU
1	aD	210	THR
1	aD	225	GLY
1	aD	226	HIS
1	bD	10	MET
1	bD	84	HIS
1	bD	98	GLU
1	bD	123	PRO
1	bD	176	GLN
1	bD	224	PRO
1	cD	4	GLN
1	cD	31	ALA
1	cD	150	ILE
1	cD	226	HIS
1	dD	4	GLN
1	dD	98	GLU
1	dD	99	PRO
1	dD	147	PRO
1	dD	206	GLY
1	dD	225	GLY
1	eD	4	GLN
1	eD	87	HIS
1	eD	97	ARG
1	eD	122	PRO
1	fD	4	GLN
1	fD	85	PRO
1	fD	98	GLU
1	fD	119	THR
1	fD	122	PRO
1	fD	147	PRO
1	gD	4	GLN
1	gD	85	PRO
1	gD	97	ARG
1	gD	98	GLU

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Mol	Chain	Res	Type
1	gD	176	GLN
1	gD	209	ALA
1	gD	223	GLY
1	gD	228	ALA
1	hD	4	GLN
1	hD	98	GLU
1	hD	146	SER
1	hD	224	PRO
1	hD	229	ARG
1	hD	230	VAL
1	iD	4	GLN
1	iD	31	ALA
1	iD	60	GLY
1	iD	85	PRO
1	iD	120	HIS
1	jD	4	GLN
1	jD	85	PRO
1	jD	87	HIS
1	jD	97	ARG
1	kD	4	GLN
1	kD	44	SER
1	kD	147	PRO
1	kD	176	GLN
1	lD	4	GLN
1	lD	9	GLN
1	lD	10	MET
1	lD	31	ALA
1	lD	61	GLY
1	lD	87	HIS
1	lD	98	GLU
1	mD	4	GLN
1	mD	147	PRO
1	mD	223	GLY
1	nD	4	GLN
1	nD	47	ALA
1	nD	63	GLN
1	nD	85	PRO
1	nD	98	GLU
1	nD	209	ALA
1	nD	224	PRO
1	oD	4	GLN
1	oD	31	ALA

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Mol	Chain	Res	Type
1	oD	47	ALA
1	pD	30	LYS
1	pD	31	ALA
1	pD	87	HIS
1	pD	89	GLY
1	pD	97	ARG
1	pD	147	PRO
1	pD	150	ILE
1	pD	176	GLN
1	qD	4	GLN
1	qD	10	MET
1	qD	85	PRO
1	qD	87	HIS
1	qD	97	ARG
1	qD	147	PRO
1	rD	31	ALA
1	rD	47	ALA
1	rD	60	GLY
1	rD	85	PRO
1	sD	4	GLN
1	sD	84	HIS
1	sD	87	HIS
1	sD	98	GLU
1	sD	229	ARG
1	tD	4	GLN
1	tD	62	HIS
1	tD	86	VAL
1	tD	98	GLU
1	tD	121	ASN
1	tD	224	PRO
1	uD	31	ALA
1	uD	106	GLY
1	uD	123	PRO
1	uD	228	ALA
1	uD	229	ARG
1	vD	4	GLN
1	vD	61	GLY
1	vD	87	HIS
1	vD	122	PRO
1	vD	147	PRO
1	vD	150	ILE
1	vD	226	HIS

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Mol	Chain	Res	Type
1	wD	4	GLN
1	wD	85	PRO
1	wD	97	ARG
1	wD	123	PRO
1	wD	147	PRO
1	xD	4	GLN
1	xD	85	PRO
1	xD	89	GLY
1	xD	123	PRO
1	xD	228	ALA
1	yD	4	GLN
1	yD	98	GLU
1	yD	209	ALA
1	yD	224	PRO
1	zD	4	GLN
1	zD	47	ALA
1	zD	85	PRO
1	zD	97	ARG
1	zD	98	GLU
1	zD	209	ALA
1	0D	4	GLN
1	0D	31	ALA
1	0D	85	PRO
1	0D	147	PRO
1	0D	229	ARG
1	0D	230	VAL
1	1D	4	GLN
1	1D	87	HIS
1	1D	97	ARG
1	1D	147	PRO
1	1D	224	PRO
1	2D	5	ASN
1	2D	31	ALA
1	2D	44	SER
1	2D	147	PRO
1	2D	223	GLY
1	2D	229	ARG
1	3D	4	GLN
1	3D	85	PRO
1	3D	98	GLU
1	3D	150	ILE
1	4D	4	GLN

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Mol	Chain	Res	Type
1	4D	63	GLN
1	4D	87	HIS
1	4D	98	GLU
1	4D	99	PRO
1	4D	122	PRO
1	4D	223	GLY
1	4D	226	HIS
1	5D	4	GLN
1	5D	85	PRO
1	5D	121	ASN
1	5D	146	SER
1	6D	4	GLN
1	6D	47	ALA
1	6D	106	GLY
1	6D	147	PRO
1	7D	4	GLN
1	7D	98	GLU
1	7D	147	PRO
1	7D	226	HIS
1	8D	4	GLN
1	8D	97	ARG
1	8D	147	PRO
1	9D	4	GLN
1	9D	98	GLU
1	9D	147	PRO
1	AE	4	GLN
1	AE	63	GLN
1	AE	84	HIS
1	AE	123	PRO
1	AE	147	PRO
1	AE	224	PRO
1	BE	98	GLU
1	BE	209	ALA
1	BE	224	PRO
1	CE	4	GLN
1	CE	31	ALA
1	CE	47	ALA
1	CE	88	ALA
1	CE	147	PRO
1	DE	4	GLN
1	DE	5	ASN
1	DE	47	ALA

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Mol	Chain	Res	Type
1	DE	61	GLY
1	DE	230	VAL
1	EE	4	GLN
1	EE	10	MET
1	EE	47	ALA
1	EE	147	PRO
1	FE	4	GLN
1	FE	47	ALA
1	FE	88	ALA
1	FE	147	PRO
1	GE	4	GLN
1	GE	98	GLU
1	GE	146	SER
1	HE	4	GLN
1	HE	97	ARG
1	HE	121	ASN
1	HE	224	PRO
1	IE	4	GLN
1	IE	147	PRO
1	JE	4	GLN
1	JE	5	ASN
1	JE	31	ALA
1	JE	61	GLY
1	JE	146	SER
1	JE	226	HIS
1	KE	3	VAL
1	KE	10	MET
1	KE	87	HIS
1	KE	119	THR
1	KE	147	PRO
1	LE	4	GLN
1	LE	31	ALA
1	LE	61	GLY
1	LE	85	PRO
1	ME	4	GLN
1	ME	98	GLU
1	ME	120	HIS
1	ME	122	PRO
1	ME	223	GLY
1	ME	224	PRO
1	NE	4	GLN
1	NE	98	GLU

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Mol	Chain	Res	Type
1	NE	229	ARG
1	OE	4	GLN
1	OE	31	ALA
1	OE	123	PRO
1	OE	230	VAL
1	PE	4	GLN
1	PE	47	ALA
1	PE	147	PRO
1	PE	178	SER
1	QE	4	GLN
1	QE	10	MET
1	QE	47	ALA
1	QE	85	PRO
1	QE	97	ARG
1	QE	121	ASN
1	QE	147	PRO
1	QE	222	GLY
1	QE	226	HIS
1	RE	4	GLN
1	RE	47	ALA
1	RE	97	ARG
1	RE	150	ILE
1	SE	4	GLN
1	SE	61	GLY
1	SE	97	ARG
1	SE	146	SER
1	TE	4	GLN
1	TE	31	ALA
1	TE	98	GLU
1	TE	121	ASN
1	UE	4	GLN
1	UE	226	HIS
1	VE	31	ALA
1	VE	224	PRO
1	VE	226	HIS
1	WE	4	GLN
1	WE	85	PRO
1	WE	147	PRO
1	WE	223	GLY
1	WE	224	PRO
1	XE	4	GLN
1	XE	47	ALA

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Mol	Chain	Res	Type
1	XE	84	HIS
1	XE	147	PRO
1	XE	221	VAL
1	YE	4	GLN
1	YE	85	PRO
1	YE	147	PRO
1	YE	210	THR
1	YE	230	VAL
1	ZE	64	ALA
1	ZE	85	PRO
1	ZE	98	GLU
1	ZE	99	PRO
1	ZE	121	ASN
1	ZE	222	GLY
1	aE	85	PRO
1	aE	222	GLY
1	bE	4	GLN
1	bE	87	HIS
1	bE	121	ASN
1	bE	146	SER
1	cE	2	ILE
1	cE	31	ALA
1	cE	85	PRO
1	cE	87	HIS
1	cE	97	ARG
1	cE	147	PRO
1	dE	2	ILE
1	dE	4	GLN
1	dE	47	ALA
1	dE	98	GLU
1	eE	4	GLN
1	eE	31	ALA
1	eE	63	GLN
1	eE	87	HIS
1	eE	119	THR
1	eE	223	GLY
1	eE	228	ALA
1	eE	229	ARG
1	fE	4	GLN
1	fE	8	GLY
1	fE	47	ALA
1	fE	97	ARG

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Mol	Chain	Res	Type
1	fE	209	ALA
1	gE	4	GLN
1	gE	88	ALA
1	gE	192	GLN
1	gE	229	ARG
1	hE	4	GLN
1	hE	224	PRO
1	iE	87	HIS
1	iE	147	PRO
1	jE	4	GLN
1	jE	31	ALA
1	jE	61	GLY
1	jE	85	PRO
1	jE	98	GLU
1	jE	119	THR
1	kE	4	GLN
1	kE	10	MET
1	kE	61	GLY
1	kE	85	PRO
1	kE	87	HIS
1	kE	97	ARG
1	kE	98	GLU
1	kE	224	PRO
1	kE	227	LYS
1	lE	4	GLN
1	lE	106	GLY
1	lE	146	SER
1	mE	4	GLN
1	mE	59	VAL
1	mE	62	HIS
1	mE	97	ARG
1	nE	4	GLN
1	nE	31	ALA
1	nE	123	PRO
1	nE	147	PRO
1	nE	176	GLN
1	oE	4	GLN
1	oE	87	HIS
1	oE	147	PRO
1	pE	4	GLN
1	pE	30	LYS
1	pE	85	PRO

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Mol	Chain	Res	Type
1	pE	98	GLU
1	qE	4	GLN
1	qE	47	ALA
1	qE	98	GLU
1	qE	106	GLY
1	qE	227	LYS
1	rE	4	GLN
1	rE	10	MET
1	rE	47	ALA
1	rE	62	HIS
1	rE	98	GLU
1	rE	207	PRO
1	rE	224	PRO
1	rE	226	HIS
1	rE	229	ARG
1	sE	4	GLN
1	sE	88	ALA
1	sE	147	PRO
1	sE	150	ILE
1	tE	4	GLN
1	tE	226	HIS
1	tE	230	VAL
1	uE	10	MET
1	uE	62	HIS
1	uE	87	HIS
1	uE	147	PRO
1	vE	4	GLN
1	vE	85	PRO
1	vE	98	GLU
1	vE	99	PRO
1	vE	121	ASN
1	vE	175	GLU
1	wE	4	GLN
1	wE	63	GLN
1	xE	4	GLN
1	xE	62	HIS
1	xE	122	PRO
1	xE	147	PRO
1	xE	228	ALA
1	xE	229	ARG
1	yE	4	GLN
1	yE	97	ARG

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Mol	Chain	Res	Type
1	yE	147	PRO
1	yE	226	HIS
1	zE	5	ASN
1	zE	122	PRO
1	zE	178	SER
1	0E	4	GLN
1	0E	47	ALA
1	0E	119	THR
1	0E	147	PRO
1	1E	2	ILE
1	1E	47	ALA
1	1E	85	PRO
1	1E	119	THR
1	1E	176	GLN
1	2E	4	GLN
1	2E	98	GLU
1	2E	224	PRO
1	3E	4	GLN
1	3E	85	PRO
1	3E	97	ARG
1	3E	98	GLU
1	3E	119	THR
1	4E	4	GLN
1	4E	10	MET
1	4E	85	PRO
1	4E	97	ARG
1	4E	122	PRO
1	4E	147	PRO
1	4E	228	ALA
1	5E	4	GLN
1	5E	85	PRO
1	5E	97	ARG
1	5E	123	PRO
1	5E	147	PRO
1	5E	226	HIS
1	6E	46	GLY
1	6E	61	GLY
1	6E	87	HIS
1	6E	123	PRO
1	6E	147	PRO
1	6E	223	GLY
1	7E	4	GLN

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Mol	Chain	Res	Type
1	7E	47	ALA
1	7E	85	PRO
1	7E	150	ILE
1	7E	222	GLY
1	7E	226	HIS
1	7E	227	LYS
1	8E	4	GLN
1	8E	31	ALA
1	8E	98	GLU
1	8E	147	PRO
1	8E	176	GLN
1	8E	209	ALA
1	8E	223	GLY
1	9E	85	PRO
1	9E	147	PRO
1	9E	227	LYS
1	AF	4	GLN
1	AF	31	ALA
1	AF	85	PRO
1	AF	122	PRO
1	AF	176	GLN
1	AF	224	PRO
1	BF	4	GLN
1	BF	31	ALA
1	BF	87	HIS
1	BF	97	ARG
1	BF	120	HIS
1	BF	146	SER
1	BF	230	VAL
1	CF	4	GLN
1	CF	47	ALA
1	CF	84	HIS
1	CF	85	PRO
1	CF	97	ARG
1	CF	147	PRO
1	DF	4	GLN
1	DF	15	ILE
1	DF	31	ALA
1	DF	47	ALA
1	DF	85	PRO
1	DF	98	GLU
1	DF	147	PRO

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Mol	Chain	Res	Type
1	DF	230	VAL
1	EF	4	GLN
1	EF	62	HIS
1	EF	85	PRO
1	EF	98	GLU
1	EF	176	GLN
1	EF	226	HIS
1	EF	229	ARG
1	FF	4	GLN
1	FF	10	MET
1	FF	47	ALA
1	FF	85	PRO
1	FF	147	PRO
1	FF	207	PRO

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	0	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	0A	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	0B	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	0C	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	0D	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	0E	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	1	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	1A	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	1B	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	1C	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	1D	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	1E	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	2	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	2A	194/194 (100%)	192 (99%)	2 (1%)	65	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2B	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	2C	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	2D	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	2E	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	3	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	3A	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	3B	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	3C	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	3D	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	3E	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	4	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	4A	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	4B	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	4C	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	4D	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	4E	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	5	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	5A	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	5B	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	5C	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	5D	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	5E	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	6	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	6A	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	6B	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	6C	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	6D	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	6E	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	7	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	7A	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	7B	194/194 (100%)	189 (97%)	5 (3%)	41	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7C	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	7D	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	7E	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	8	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	8A	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	8B	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	8C	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	8D	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	8E	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	9	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	9A	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	9B	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	9C	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	9D	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	9E	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	A	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	AA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	AB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	AC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	AD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	AE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	AF	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	B	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	BA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	BB	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	BC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	BD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	BE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	BF	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	C	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	CA	194/194 (100%)	191 (98%)	3 (2%)	55	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	CC	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	CD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	CE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	CF	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	D	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	DA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	DB	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	DC	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	DD	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	DE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	DF	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	E	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	EA	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	EB	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	EC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	ED	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	EE	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	EF	194/194 (100%)	194 (100%)	0 (0%)	100	100
1	F	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	FA	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	FB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	FC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	FD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	FE	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	FF	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	G	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	GA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	GB	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	GC	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	GD	194/194 (100%)	184 (95%)	10 (5%)	22	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	H	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	HA	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	HB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	HC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	HD	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	HE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	I	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	IA	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	IB	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	IC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	ID	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	IE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	J	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	JA	194/194 (100%)	194 (100%)	0 (0%)	100	100
1	JB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	JC	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	JD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	JE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	K	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	KA	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	KB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	KC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	KD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	KE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	L	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	LA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	LB	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	LC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	LD	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	LE	194/194 (100%)	187 (96%)	7 (4%)	32	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	MA	194/194 (100%)	183 (94%)	11 (6%)	20	70
1	MB	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	MC	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	MD	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	ME	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	N	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	NA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	NB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	NC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	ND	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	NE	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	O	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	OA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	OB	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	OC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	OD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	OE	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	P	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	PA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	PB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	PC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	PD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	PE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	Q	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	QA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	QB	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	QC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	QD	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	QE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	R	194/194 (100%)	188 (97%)	6 (3%)	36	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RA	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	RB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	RC	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	RD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	RE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	S	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	SA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	SB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	SC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	SD	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	SE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	T	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	TA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	TB	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	TC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	TD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	TE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	U	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	UA	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	UB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	UC	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	UD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	UE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	V	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	VA	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	VB	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	VC	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	VD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	VE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	W	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	WA	194/194 (100%)	190 (98%)	4 (2%)	46	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	WC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	WD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	WE	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	X	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	XA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	XB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	XC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	XD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	XE	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	Y	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	YA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	YB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	YC	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	YD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	YE	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	Z	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	ZA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	ZB	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	ZC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	ZD	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	ZE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	a	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	aA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	aB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	aC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	aD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	aE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	b	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	bA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	bB	194/194 (100%)	190 (98%)	4 (2%)	46	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	bD	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	bE	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	c	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	cA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	cB	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	cC	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	cD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	cE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	d	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	dA	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	dB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	dC	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	dD	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	dE	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	e	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	eA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	eB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	eC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	eD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	eE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	f	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	fA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	fB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	fC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	fD	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	fE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	g	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	gA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	gB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	gC	194/194 (100%)	186 (96%)	8 (4%)	28	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	gD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	gE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	h	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	hA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	hB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	hC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	hD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	hE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	i	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	iA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	iB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	iC	194/194 (100%)	194 (100%)	0 (0%)	100	100
1	iD	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	iE	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	j	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	jA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	jB	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	jC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	jD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	jE	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	k	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	kA	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	kB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	kC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	kD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	kE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	l	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	lA	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	lB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	lC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	lD	194/194 (100%)	188 (97%)	6 (3%)	36	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	lE	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	m	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	mA	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	mB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	mC	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	mD	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	mE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	n	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	nA	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	nB	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	nC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	nD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	nE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	o	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	oA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	oB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	oC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	oD	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	oE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	p	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	pA	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	pB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	pC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	pD	194/194 (100%)	194 (100%)	0 (0%)	100	100
1	pE	194/194 (100%)	183 (94%)	11 (6%)	20	70
1	q	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	qA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	qB	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	qC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	qD	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	qE	194/194 (100%)	190 (98%)	4 (2%)	46	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	rA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	rB	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	rC	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	rD	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	rE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	s	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	sA	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	sB	194/194 (100%)	183 (94%)	11 (6%)	20	70
1	sC	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	sD	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	sE	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	t	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	tA	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	tB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	tC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	tD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	tE	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	u	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	uA	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	uB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	uC	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	uD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	uE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	v	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	vA	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	vB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	vC	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	vD	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	vE	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	w	194/194 (100%)	191 (98%)	3 (2%)	55	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	wA	194/194 (100%)	184 (95%)	10 (5%)	22	72
1	wB	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	wC	194/194 (100%)	190 (98%)	4 (2%)	46	90
1	wD	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	wE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	x	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	xA	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	xB	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	xC	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	xD	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	xE	194/194 (100%)	188 (97%)	6 (3%)	36	85
1	y	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	yA	194/194 (100%)	185 (95%)	9 (5%)	25	76
1	yB	194/194 (100%)	187 (96%)	7 (4%)	32	82
1	yC	194/194 (100%)	192 (99%)	2 (1%)	65	95
1	yD	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	yE	194/194 (100%)	191 (98%)	3 (2%)	55	93
1	z	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	zA	194/194 (100%)	193 (99%)	1 (1%)	78	96
1	zB	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	zC	194/194 (100%)	186 (96%)	8 (4%)	28	79
1	zD	194/194 (100%)	189 (97%)	5 (3%)	41	88
1	zE	194/194 (100%)	186 (96%)	8 (4%)	28	79
All	All	73332/73332 (100%)	71326 (97%)	2006 (3%)	40	87

All 2006 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	1	PRO
1	A	69	LEU
1	A	72	THR
1	A	99	PRO
1	A	108	THR

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Mol	Chain	Res	Type
1	A	184	TRP
1	A	200	THR
1	B	2	ILE
1	B	63	GLN
1	B	108	THR
1	C	15	ILE
1	C	72	THR
1	C	96	MET
1	C	97	ARG
1	C	112	GLN
1	C	119	THR
1	C	142	VAL
1	C	147	PRO
1	C	165	VAL
1	C	184	TRP
1	D	5	ASN
1	D	119	THR
1	D	121	ASN
1	D	148	THR
1	D	175	GLU
1	E	2	ILE
1	E	58	THR
1	E	69	LEU
1	E	85	PRO
1	E	117	TRP
1	E	148	THR
1	F	48	THR
1	F	54	THR
1	F	97	ARG
1	F	108	THR
1	F	148	THR
1	F	184	TRP
1	G	85	PRO
1	G	97	ARG
1	G	184	TRP
1	H	3	VAL
1	H	4	GLN
1	H	10	MET
1	H	54	THR
1	H	141	ILE
1	H	175	GLU
1	I	72	THR

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Mol	Chain	Res	Type
1	I	96	MET
1	I	108	THR
1	I	141	ILE
1	I	147	PRO
1	I	195	ASN
1	J	1	PRO
1	J	10	MET
1	J	66	MET
1	J	108	THR
1	J	195	ASN
1	J	231	LEU
1	K	108	THR
1	K	184	TRP
1	K	214	MET
1	L	2	ILE
1	L	72	THR
1	L	107	THR
1	L	148	THR
1	L	154	ARG
1	L	184	TRP
1	M	54	THR
1	M	72	THR
1	M	107	THR
1	M	108	THR
1	N	53	ASN
1	N	54	THR
1	N	74	ASN
1	N	81	ASP
1	N	139	ASN
1	N	184	TRP
1	O	63	GLN
1	O	96	MET
1	O	108	THR
1	O	147	PRO
1	O	192	GLN
1	O	226	HIS
1	P	108	THR
1	P	148	THR
1	Q	10	MET
1	Q	67	GLN
1	Q	72	THR
1	Q	86	VAL

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Mol	Chain	Res	Type
1	Q	184	TRP
1	Q	200	THR
1	R	4	GLN
1	R	30	LYS
1	R	96	MET
1	R	184	TRP
1	R	200	THR
1	R	226	HIS
1	S	10	MET
1	S	54	THR
1	S	107	THR
1	S	108	THR
1	S	122	PRO
1	S	158	LYS
1	S	184	TRP
1	S	195	ASN
1	T	58	THR
1	T	96	MET
1	T	108	THR
1	T	148	THR
1	T	154	ARG
1	T	184	TRP
1	U	96	MET
1	U	108	THR
1	U	147	PRO
1	U	186	THR
1	V	1	PRO
1	V	9	GLN
1	V	15	ILE
1	V	85	PRO
1	V	96	MET
1	V	121	ASN
1	V	182	LYS
1	V	184	TRP
1	W	96	MET
1	W	150	ILE
1	W	205	LEU
1	X	72	THR
1	X	96	MET
1	X	107	THR
1	X	108	THR
1	X	219	GLN

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Mol	Chain	Res	Type
1	Y	54	THR
1	Y	107	THR
1	Y	108	THR
1	Z	58	THR
1	Z	107	THR
1	Z	108	THR
1	Z	175	GLU
1	Z	184	TRP
1	a	9	GLN
1	a	10	MET
1	a	96	MET
1	a	108	THR
1	a	123	PRO
1	a	147	PRO
1	a	184	TRP
1	b	48	THR
1	b	99	PRO
1	b	108	THR
1	b	114	GLN
1	b	121	ASN
1	b	184	TRP
1	b	188	THR
1	b	221	VAL
1	b	230	VAL
1	c	2	ILE
1	c	69	LEU
1	c	112	GLN
1	c	196	PRO
1	d	63	GLN
1	d	72	THR
1	d	110	THR
1	d	145	TYR
1	e	96	MET
1	e	108	THR
1	e	121	ASN
1	e	184	TRP
1	f	54	THR
1	f	58	THR
1	f	72	THR
1	f	96	MET
1	f	110	THR
1	g	15	ILE

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Mol	Chain	Res	Type
1	g	48	THR
1	g	67	GLN
1	g	72	THR
1	g	96	MET
1	g	108	THR
1	g	147	PRO
1	g	175	GLU
1	g	197	ASP
1	g	219	GLN
1	h	10	MET
1	h	58	THR
1	h	69	LEU
1	h	95	GLN
1	h	121	ASN
1	h	148	THR
1	h	176	GLN
1	h	184	TRP
1	i	188	THR
1	j	2	ILE
1	j	4	GLN
1	j	63	GLN
1	j	108	THR
1	j	230	VAL
1	k	54	THR
1	k	72	THR
1	k	96	MET
1	k	99	PRO
1	k	108	THR
1	k	115	ILE
1	k	143	ARG
1	k	175	GLU
1	k	184	TRP
1	l	48	THR
1	l	69	LEU
1	l	95	GLN
1	l	96	MET
1	l	108	THR
1	l	184	TRP
1	l	185	MET
1	m	48	THR
1	m	59	VAL
1	m	142	VAL

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Mol	Chain	Res	Type
1	m	147	PRO
1	m	175	GLU
1	m	188	THR
1	n	48	THR
1	n	108	THR
1	n	119	THR
1	n	121	ASN
1	n	162	ARG
1	n	196	PRO
1	o	3	VAL
1	o	62	HIS
1	o	96	MET
1	o	107	THR
1	p	2	ILE
1	p	69	LEU
1	p	107	THR
1	p	184	TRP
1	p	229	ARG
1	q	4	GLN
1	q	25	LYS
1	q	54	THR
1	q	69	LEU
1	q	85	PRO
1	q	108	THR
1	q	188	THR
1	r	2	ILE
1	r	96	MET
1	r	99	PRO
1	r	184	TRP
1	s	48	THR
1	s	50	GLN
1	s	72	THR
1	s	85	PRO
1	s	96	MET
1	s	147	PRO
1	s	188	THR
1	t	72	THR
1	t	121	ASN
1	t	148	THR
1	t	150	ILE
1	t	184	TRP
1	t	216	THR

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Mol	Chain	Res	Type
1	t	230	VAL
1	u	184	TRP
1	u	211	LEU
1	v	72	THR
1	v	97	ARG
1	v	108	THR
1	v	184	TRP
1	v	195	ASN
1	v	205	LEU
1	w	72	THR
1	w	85	PRO
1	w	108	THR
1	x	30	LYS
1	x	69	LEU
1	x	108	THR
1	x	145	TYR
1	x	226	HIS
1	y	53	ASN
1	y	58	THR
1	y	72	THR
1	y	96	MET
1	y	107	THR
1	y	110	THR
1	y	147	PRO
1	y	184	TRP
1	z	48	THR
1	z	96	MET
1	z	110	THR
1	z	121	ASN
1	z	171	THR
1	0	69	LEU
1	0	72	THR
1	0	195	ASN
1	1	15	ILE
1	1	63	GLN
1	1	72	THR
1	1	96	MET
1	1	107	THR
1	1	182	LYS
1	2	15	ILE
1	2	154	ARG
1	2	158	LYS

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Mol	Chain	Res	Type
1	2	184	TRP
1	3	25	LYS
1	3	107	THR
1	4	7	GLN
1	4	30	LYS
1	4	66	MET
1	4	96	MET
1	4	108	THR
1	4	142	VAL
1	4	147	PRO
1	5	72	THR
1	5	96	MET
1	5	107	THR
1	5	112	GLN
1	5	184	TRP
1	6	10	MET
1	6	19	THR
1	6	80	TRP
1	6	84	HIS
1	6	184	TRP
1	6	205	LEU
1	7	4	GLN
1	7	97	ARG
1	7	107	THR
1	7	184	TRP
1	7	195	ASN
1	8	25	LYS
1	8	96	MET
1	8	107	THR
1	8	145	TYR
1	8	175	GLU
1	8	184	TRP
1	9	10	MET
1	9	66	MET
1	9	96	MET
1	9	108	THR
1	9	171	THR
1	9	175	GLU
1	9	179	GLN
1	AA	21	ASN
1	AA	147	PRO
1	AA	184	TRP

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Mol	Chain	Res	Type
1	BA	10	MET
1	BA	30	LYS
1	BA	108	THR
1	BA	148	THR
1	BA	196	PRO
1	CA	2	ILE
1	CA	54	THR
1	CA	69	LEU
1	DA	69	LEU
1	DA	97	ARG
1	DA	184	TRP
1	DA	192	GLN
1	DA	201	ILE
1	DA	227	LYS
1	EA	2	ILE
1	EA	96	MET
1	EA	108	THR
1	EA	227	LYS
1	FA	62	HIS
1	FA	69	LEU
1	FA	72	THR
1	FA	108	THR
1	GA	2	ILE
1	GA	54	THR
1	GA	96	MET
1	GA	184	TRP
1	GA	229	ARG
1	HA	15	ILE
1	HA	85	PRO
1	IA	66	MET
1	IA	148	THR
1	KA	54	THR
1	KA	99	PRO
1	KA	107	THR
1	KA	139	ASN
1	KA	175	GLU
1	KA	184	TRP
1	KA	221	VAL
1	LA	10	MET
1	LA	48	THR
1	LA	108	THR
1	LA	175	GLU

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Mol	Chain	Res	Type
1	LA	184	TRP
1	LA	195	ASN
1	MA	48	THR
1	MA	72	THR
1	MA	84	HIS
1	MA	107	THR
1	MA	108	THR
1	MA	122	PRO
1	MA	147	PRO
1	MA	184	TRP
1	MA	188	THR
1	MA	207	PRO
1	MA	229	ARG
1	NA	2	ILE
1	NA	48	THR
1	NA	58	THR
1	NA	113	GLU
1	NA	148	THR
1	NA	188	THR
1	OA	2	ILE
1	OA	25	LYS
1	OA	121	ASN
1	OA	179	GLN
1	OA	203	LYS
1	PA	72	THR
1	PA	97	ARG
1	PA	200	THR
1	QA	10	MET
1	QA	48	THR
1	QA	96	MET
1	QA	107	THR
1	QA	149	SER
1	QA	195	ASN
1	RA	4	GLN
1	RA	48	THR
1	RA	71	GLU
1	RA	96	MET
1	RA	108	THR
1	RA	148	THR
1	RA	175	GLU
1	SA	54	THR
1	SA	72	THR

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Mol	Chain	Res	Type
1	SA	96	MET
1	SA	147	PRO
1	SA	172	LEU
1	SA	184	TRP
1	TA	69	LEU
1	TA	72	THR
1	TA	85	PRO
1	UA	2	ILE
1	UA	107	THR
1	VA	4	GLN
1	VA	28	GLU
1	VA	54	THR
1	VA	72	THR
1	VA	107	THR
1	VA	184	TRP
1	VA	192	GLN
1	VA	195	ASN
1	WA	10	MET
1	WA	72	THR
1	WA	115	ILE
1	WA	184	TRP
1	XA	67	GLN
1	XA	108	THR
1	XA	110	THR
1	YA	48	THR
1	YA	96	MET
1	YA	108	THR
1	YA	147	PRO
1	YA	171	THR
1	YA	229	ARG
1	ZA	15	ILE
1	ZA	85	PRO
1	ZA	107	THR
1	ZA	119	THR
1	ZA	184	TRP
1	ZA	213	GLU
1	aA	2	ILE
1	aA	72	THR
1	aA	74	ASN
1	bA	2	ILE
1	bA	72	THR
1	bA	96	MET

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Mol	Chain	Res	Type
1	bA	107	THR
1	bA	108	THR
1	bA	195	ASN
1	cA	54	THR
1	cA	96	MET
1	cA	97	ARG
1	cA	107	THR
1	cA	111	LEU
1	cA	184	TRP
1	dA	10	MET
1	dA	32	PHE
1	dA	80	TRP
1	dA	96	MET
1	dA	107	THR
1	dA	108	THR
1	dA	175	GLU
1	dA	196	PRO
1	eA	2	ILE
1	eA	108	THR
1	eA	147	PRO
1	eA	175	GLU
1	eA	184	TRP
1	eA	200	THR
1	fA	15	ILE
1	fA	30	LYS
1	fA	68	MET
1	fA	85	PRO
1	fA	121	ASN
1	gA	48	THR
1	gA	184	TRP
1	gA	205	LEU
1	hA	45	GLU
1	hA	54	THR
1	hA	95	GLN
1	hA	148	THR
1	hA	184	TRP
1	iA	107	THR
1	iA	154	ARG
1	iA	195	ASN
1	jA	2	ILE
1	jA	107	THR
1	jA	108	THR

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Mol	Chain	Res	Type
1	jA	165	VAL
1	jA	184	TRP
1	jA	214	MET
1	kA	1	PRO
1	kA	15	ILE
1	kA	108	THR
1	kA	147	PRO
1	lA	1	PRO
1	lA	10	MET
1	lA	48	THR
1	lA	150	ILE
1	mA	54	THR
1	mA	84	HIS
1	mA	107	THR
1	mA	188	THR
1	mA	195	ASN
1	nA	50	GLN
1	nA	96	MET
1	oA	96	MET
1	oA	97	ARG
1	oA	108	THR
1	pA	54	THR
1	pA	96	MET
1	pA	97	ARG
1	pA	139	ASN
1	pA	148	THR
1	pA	195	ASN
1	pA	205	LEU
1	qA	108	THR
1	qA	147	PRO
1	qA	226	HIS
1	rA	54	THR
1	rA	72	THR
1	rA	95	GLN
1	rA	108	THR
1	rA	171	THR
1	rA	184	TRP
1	sA	4	GLN
1	sA	96	MET
1	sA	107	THR
1	sA	123	PRO
1	sA	128	GLU

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Mol	Chain	Res	Type
1	sA	148	THR
1	sA	179	GLN
1	sA	227	LYS
1	tA	5	ASN
1	tA	72	THR
1	tA	107	THR
1	tA	121	ASN
1	uA	107	THR
1	uA	108	THR
1	uA	184	TRP
1	vA	96	MET
1	vA	97	ARG
1	vA	99	PRO
1	vA	108	THR
1	vA	113	GLU
1	vA	148	THR
1	vA	229	ARG
1	vA	230	VAL
1	wA	72	THR
1	wA	85	PRO
1	wA	96	MET
1	wA	99	PRO
1	wA	108	THR
1	wA	140	LYS
1	wA	141	ILE
1	wA	147	PRO
1	wA	182	LYS
1	wA	184	TRP
1	xA	2	ILE
1	xA	48	THR
1	xA	96	MET
1	xA	121	ASN
1	xA	188	THR
1	xA	231	LEU
1	yA	3	VAL
1	yA	63	GLN
1	yA	66	MET
1	yA	72	THR
1	yA	84	HIS
1	yA	107	THR
1	yA	148	THR
1	yA	184	TRP

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Mol	Chain	Res	Type
1	yA	196	PRO
1	zA	108	THR
1	0A	10	MET
1	0A	108	THR
1	0A	110	THR
1	0A	171	THR
1	0A	184	TRP
1	0A	229	ARG
1	1A	54	THR
1	1A	69	LEU
1	1A	96	MET
1	1A	108	THR
1	1A	141	ILE
1	1A	189	LEU
1	1A	226	HIS
1	2A	147	PRO
1	2A	184	TRP
1	3A	1	PRO
1	3A	69	LEU
1	3A	72	THR
1	3A	85	PRO
1	3A	96	MET
1	3A	108	THR
1	3A	121	ASN
1	3A	184	TRP
1	4A	148	THR
1	4A	149	SER
1	4A	184	TRP
1	5A	10	MET
1	5A	72	THR
1	5A	81	ASP
1	5A	118	MET
1	5A	184	TRP
1	6A	1	PRO
1	6A	30	LYS
1	6A	72	THR
1	6A	96	MET
1	6A	108	THR
1	6A	171	THR
1	6A	184	TRP
1	7A	48	THR
1	7A	139	ASN

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Mol	Chain	Res	Type
1	7A	175	GLU
1	7A	184	TRP
1	7A	205	LEU
1	8A	15	ILE
1	8A	48	THR
1	8A	96	MET
1	8A	108	THR
1	8A	147	PRO
1	8A	203	LYS
1	9A	10	MET
1	9A	99	PRO
1	9A	121	ASN
1	9A	171	THR
1	9A	200	THR
1	AB	10	MET
1	AB	15	ILE
1	AB	72	THR
1	AB	96	MET
1	AB	107	THR
1	AB	148	THR
1	AB	184	TRP
1	BB	4	GLN
1	BB	96	MET
1	BB	108	THR
1	CB	5	ASN
1	CB	72	THR
1	CB	108	THR
1	CB	119	THR
1	CB	184	TRP
1	CB	186	THR
1	DB	54	THR
1	DB	96	MET
1	DB	107	THR
1	DB	162	ARG
1	EB	63	GLN
1	EB	188	THR
1	EB	203	LYS
1	FB	72	THR
1	FB	82	ARG
1	FB	121	ASN
1	FB	175	GLU
1	FB	182	LYS

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Mol	Chain	Res	Type
1	FB	184	TRP
1	FB	195	ASN
1	GB	72	THR
1	GB	148	THR
1	GB	184	TRP
1	GB	188	THR
1	HB	4	GLN
1	HB	48	THR
1	HB	72	THR
1	HB	97	ARG
1	HB	108	THR
1	HB	184	TRP
1	IB	96	MET
1	IB	165	VAL
1	JB	96	MET
1	JB	108	THR
1	JB	148	THR
1	JB	186	THR
1	JB	227	LYS
1	KB	48	THR
1	KB	75	GLU
1	KB	81	ASP
1	KB	147	PRO
1	KB	175	GLU
1	LB	1	PRO
1	LB	10	MET
1	LB	48	THR
1	LB	85	PRO
1	LB	96	MET
1	LB	97	ARG
1	LB	108	THR
1	LB	171	THR
1	LB	175	GLU
1	MB	10	MET
1	MB	84	HIS
1	MB	107	THR
1	NB	72	THR
1	NB	87	HIS
1	NB	96	MET
1	NB	184	TRP
1	NB	205	LEU
1	OB	4	GLN

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Mol	Chain	Res	Type
1	OB	72	THR
1	OB	96	MET
1	OB	108	THR
1	OB	112	GLN
1	OB	148	THR
1	OB	179	GLN
1	OB	216	THR
1	PB	30	LYS
1	PB	96	MET
1	PB	108	THR
1	PB	148	THR
1	PB	180	GLU
1	QB	1	PRO
1	QB	7	GLN
1	QB	15	ILE
1	QB	96	MET
1	QB	108	THR
1	QB	119	THR
1	QB	147	PRO
1	QB	180	GLU
1	QB	184	TRP
1	QB	195	ASN
1	RB	10	MET
1	RB	15	ILE
1	RB	48	THR
1	RB	71	GLU
1	RB	121	ASN
1	SB	15	ILE
1	SB	63	GLN
1	SB	72	THR
1	SB	96	MET
1	SB	107	THR
1	SB	119	THR
1	SB	148	THR
1	TB	72	THR
1	TB	107	THR
1	TB	184	TRP
1	TB	219	GLN
1	UB	107	THR
1	UB	108	THR
1	UB	184	TRP
1	UB	187	GLU

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Mol	Chain	Res	Type
1	UB	200	THR
1	UB	229	ARG
1	VB	10	MET
1	WB	58	THR
1	WB	72	THR
1	WB	108	THR
1	WB	147	PRO
1	WB	184	TRP
1	XB	30	LYS
1	XB	48	THR
1	XB	85	PRO
1	XB	99	PRO
1	XB	121	ASN
1	XB	171	THR
1	YB	69	LEU
1	YB	110	THR
1	YB	122	PRO
1	YB	171	THR
1	YB	184	TRP
1	ZB	4	GLN
1	ZB	69	LEU
1	ZB	72	THR
1	ZB	96	MET
1	aB	96	MET
1	aB	97	ARG
1	aB	107	THR
1	aB	119	THR
1	aB	184	TRP
1	bB	10	MET
1	bB	96	MET
1	bB	108	THR
1	bB	175	GLU
1	cB	10	MET
1	cB	48	THR
1	cB	96	MET
1	cB	108	THR
1	cB	122	PRO
1	cB	147	PRO
1	cB	200	THR
1	cB	230	VAL
1	dB	10	MET
1	dB	85	PRO

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Mol	Chain	Res	Type
1	dB	95	GLN
1	dB	108	THR
1	dB	110	THR
1	eB	48	THR
1	eB	53	ASN
1	eB	72	THR
1	eB	107	THR
1	eB	148	THR
1	fB	54	THR
1	fB	58	THR
1	fB	121	ASN
1	fB	148	THR
1	fB	179	GLN
1	fB	184	TRP
1	fB	227	LYS
1	gB	95	GLN
1	gB	96	MET
1	gB	132	ARG
1	gB	175	GLU
1	gB	184	TRP
1	gB	226	HIS
1	hB	30	LYS
1	hB	67	GLN
1	hB	95	GLN
1	hB	108	THR
1	hB	162	ARG
1	hB	184	TRP
1	iB	96	MET
1	iB	108	THR
1	iB	147	PRO
1	iB	184	TRP
1	iB	230	VAL
1	jB	2	ILE
1	jB	66	MET
1	jB	67	GLN
1	jB	69	LEU
1	jB	96	MET
1	jB	99	PRO
1	jB	108	THR
1	jB	121	ASN
1	jB	171	THR
1	jB	230	VAL

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Mol	Chain	Res	Type
1	kB	69	LEU
1	kB	107	THR
1	kB	119	THR
1	kB	143	ARG
1	kB	201	ILE
1	lB	2	ILE
1	lB	72	THR
1	lB	97	ARG
1	lB	107	THR
1	lB	184	TRP
1	mB	48	THR
1	mB	96	MET
1	mB	108	THR
1	mB	175	GLU
1	mB	184	TRP
1	nB	139	ASN
1	oB	69	LEU
1	oB	72	THR
1	oB	91	ILE
1	oB	110	THR
1	oB	147	PRO
1	oB	184	TRP
1	oB	231	LEU
1	pB	30	LYS
1	pB	69	LEU
1	pB	95	GLN
1	pB	184	TRP
1	pB	195	ASN
1	pB	230	VAL
1	qB	2	ILE
1	qB	10	MET
1	qB	33	SER
1	qB	85	PRO
1	qB	148	THR
1	qB	176	GLN
1	rB	72	THR
1	rB	97	ARG
1	rB	184	TRP
1	sB	2	ILE
1	sB	66	MET
1	sB	72	THR
1	sB	85	PRO

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Mol	Chain	Res	Type
1	sB	96	MET
1	sB	108	THR
1	sB	122	PRO
1	sB	171	THR
1	sB	184	TRP
1	sB	200	THR
1	sB	207	PRO
1	tB	48	THR
1	tB	96	MET
1	tB	108	THR
1	tB	111	LEU
1	tB	171	THR
1	uB	1	PRO
1	uB	25	LYS
1	uB	75	GLU
1	uB	96	MET
1	uB	108	THR
1	uB	147	PRO
1	uB	179	GLN
1	vB	10	MET
1	vB	69	LEU
1	vB	108	THR
1	vB	121	ASN
1	vB	195	ASN
1	wB	69	LEU
1	wB	96	MET
1	wB	229	ARG
1	xB	54	THR
1	xB	72	THR
1	xB	96	MET
1	xB	97	ARG
1	xB	121	ASN
1	xB	148	THR
1	xB	227	LYS
1	xB	230	VAL
1	yB	43	LEU
1	yB	58	THR
1	yB	96	MET
1	yB	184	TRP
1	yB	192	GLN
1	yB	195	ASN
1	yB	230	VAL

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Mol	Chain	Res	Type
1	zB	30	LYS
1	zB	96	MET
1	zB	139	ASN
1	zB	162	ARG
1	zB	184	TRP
1	0B	58	THR
1	0B	63	GLN
1	0B	72	THR
1	0B	139	ASN
1	0B	184	TRP
1	0B	227	LYS
1	1B	56	LEU
1	1B	85	PRO
1	1B	108	THR
1	1B	175	GLU
1	2B	2	ILE
1	2B	96	MET
1	2B	122	PRO
1	2B	148	THR
1	3B	72	THR
1	3B	96	MET
1	3B	107	THR
1	4B	85	PRO
1	4B	96	MET
1	4B	107	THR
1	4B	108	THR
1	4B	182	LYS
1	5B	69	LEU
1	5B	107	THR
1	5B	108	THR
1	5B	122	PRO
1	5B	139	ASN
1	5B	148	THR
1	5B	229	ARG
1	6B	25	LYS
1	6B	48	THR
1	6B	107	THR
1	6B	108	THR
1	6B	147	PRO
1	6B	184	TRP
1	6B	230	VAL
1	7B	15	ILE

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Mol	Chain	Res	Type
1	7B	48	THR
1	7B	71	GLU
1	7B	99	PRO
1	7B	186	THR
1	8B	2	ILE
1	8B	3	VAL
1	8B	84	HIS
1	8B	107	THR
1	8B	148	THR
1	9B	96	MET
1	9B	148	THR
1	9B	184	TRP
1	AC	69	LEU
1	AC	91	ILE
1	AC	184	TRP
1	BC	54	THR
1	BC	96	MET
1	BC	108	THR
1	BC	171	THR
1	BC	175	GLU
1	CC	10	MET
1	CC	85	PRO
1	CC	96	MET
1	CC	107	THR
1	CC	108	THR
1	CC	122	PRO
1	CC	147	PRO
1	CC	175	GLU
1	CC	196	PRO
1	CC	231	LEU
1	DC	1	PRO
1	DC	10	MET
1	DC	107	THR
1	DC	108	THR
1	DC	121	ASN
1	DC	148	THR
1	DC	175	GLU
1	DC	200	THR
1	EC	62	HIS
1	EC	63	GLN
1	EC	107	THR
1	EC	148	THR

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Mol	Chain	Res	Type
1	EC	210	THR
1	EC	226	HIS
1	FC	10	MET
1	FC	72	THR
1	FC	97	ARG
1	FC	108	THR
1	FC	121	ASN
1	FC	184	TRP
1	GC	2	ILE
1	GC	48	THR
1	GC	69	LEU
1	GC	107	THR
1	GC	108	THR
1	GC	148	THR
1	GC	200	THR
1	HC	71	GLU
1	HC	108	THR
1	HC	150	ILE
1	IC	108	THR
1	IC	147	PRO
1	IC	171	THR
1	IC	180	GLU
1	IC	184	TRP
1	JC	1	PRO
1	JC	15	ILE
1	JC	19	THR
1	JC	81	ASP
1	JC	96	MET
1	JC	121	ASN
1	JC	171	THR
1	JC	184	TRP
1	JC	195	ASN
1	JC	213	GLU
1	KC	72	THR
1	KC	107	THR
1	KC	179	GLN
1	KC	184	TRP
1	LC	15	ILE
1	LC	58	THR
1	LC	63	GLN
1	LC	72	THR
1	LC	97	ARG

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Mol	Chain	Res	Type
1	LC	165	VAL
1	MC	96	MET
1	MC	107	THR
1	MC	108	THR
1	MC	122	PRO
1	MC	154	ARG
1	MC	171	THR
1	MC	179	GLN
1	NC	1	PRO
1	NC	30	LYS
1	NC	108	THR
1	NC	221	VAL
1	NC	227	LYS
1	OC	96	MET
1	OC	147	PRO
1	OC	166	ASP
1	OC	171	THR
1	OC	227	LYS
1	PC	19	THR
1	PC	85	PRO
1	PC	108	THR
1	PC	110	THR
1	PC	195	ASN
1	PC	201	ILE
1	QC	84	HIS
1	QC	91	ILE
1	QC	96	MET
1	QC	108	THR
1	QC	184	TRP
1	QC	200	THR
1	RC	72	THR
1	RC	96	MET
1	RC	97	ARG
1	RC	108	THR
1	RC	121	ASN
1	RC	148	THR
1	RC	184	TRP
1	SC	72	THR
1	SC	96	MET
1	SC	108	THR
1	SC	175	GLU
1	SC	184	TRP

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Mol	Chain	Res	Type
1	SC	230	VAL
1	TC	107	THR
1	TC	108	THR
1	TC	171	THR
1	TC	175	GLU
1	UC	15	ILE
1	UC	72	THR
1	UC	96	MET
1	UC	108	THR
1	UC	147	PRO
1	UC	171	THR
1	UC	184	TRP
1	VC	1	PRO
1	VC	35	GLU
1	VC	48	THR
1	VC	69	LEU
1	VC	85	PRO
1	VC	96	MET
1	VC	108	THR
1	VC	121	ASN
1	VC	195	ASN
1	VC	227	LYS
1	WC	4	GLN
1	WC	58	THR
1	WC	192	GLN
1	WC	227	LYS
1	XC	96	MET
1	XC	148	THR
1	XC	184	TRP
1	XC	230	VAL
1	YC	54	THR
1	YC	58	THR
1	YC	72	THR
1	YC	108	THR
1	YC	112	GLN
1	YC	142	VAL
1	YC	171	THR
1	YC	175	GLU
1	ZC	72	THR
1	ZC	108	THR
1	ZC	148	THR
1	ZC	175	GLU

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Mol	Chain	Res	Type
1	ZC	211	LEU
1	aC	72	THR
1	aC	107	THR
1	aC	147	PRO
1	aC	186	THR
1	bC	2	ILE
1	bC	10	MET
1	bC	72	THR
1	bC	108	THR
1	bC	175	GLU
1	cC	69	LEU
1	cC	96	MET
1	dC	18	ARG
1	dC	121	ASN
1	eC	30	LYS
1	eC	184	TRP
1	eC	188	THR
1	fC	25	LYS
1	fC	96	MET
1	fC	108	THR
1	fC	139	ASN
1	fC	175	GLU
1	gC	7	GLN
1	gC	48	THR
1	gC	63	GLN
1	gC	96	MET
1	gC	108	THR
1	gC	147	PRO
1	gC	148	THR
1	gC	184	TRP
1	hC	13	GLN
1	hC	71	GLU
1	hC	108	THR
1	hC	188	THR
1	hC	196	PRO
1	jC	4	GLN
1	jC	108	THR
1	jC	184	TRP
1	jC	192	GLN
1	jC	226	HIS
1	jC	230	VAL
1	kC	58	THR

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Mol	Chain	Res	Type
1	kC	96	MET
1	kC	107	THR
1	kC	171	THR
1	kC	188	THR
1	kC	229	ARG
1	lC	66	MET
1	lC	69	LEU
1	lC	96	MET
1	lC	108	THR
1	lC	162	ARG
1	lC	230	VAL
1	mC	1	PRO
1	mC	48	THR
1	mC	96	MET
1	mC	107	THR
1	mC	122	PRO
1	mC	147	PRO
1	mC	175	GLU
1	mC	215	MET
1	mC	227	LYS
1	nC	1	PRO
1	nC	48	THR
1	nC	85	PRO
1	nC	108	THR
1	nC	175	GLU
1	nC	196	PRO
1	oC	107	THR
1	oC	148	THR
1	oC	184	TRP
1	oC	205	LEU
1	oC	219	GLN
1	pC	4	GLN
1	pC	58	THR
1	pC	108	THR
1	qC	96	MET
1	qC	108	THR
1	qC	149	SER
1	rC	54	THR
1	rC	96	MET
1	rC	195	ASN
1	sC	66	MET
1	sC	72	THR

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Mol	Chain	Res	Type
1	sC	96	MET
1	sC	108	THR
1	sC	147	PRO
1	sC	184	TRP
1	sC	195	ASN
1	tC	1	PRO
1	tC	107	THR
1	tC	122	PRO
1	tC	148	THR
1	tC	179	GLN
1	uC	96	MET
1	uC	136	LEU
1	uC	162	ARG
1	uC	184	TRP
1	uC	207	PRO
1	vC	69	LEU
1	vC	97	ARG
1	vC	107	THR
1	vC	110	THR
1	vC	121	ASN
1	vC	192	GLN
1	wC	33	SER
1	wC	54	THR
1	wC	107	THR
1	wC	231	LEU
1	xC	112	GLN
1	xC	184	TRP
1	yC	147	PRO
1	yC	183	ASN
1	zC	1	PRO
1	zC	10	MET
1	zC	15	ILE
1	zC	33	SER
1	zC	107	THR
1	zC	184	TRP
1	zC	196	PRO
1	zC	229	ARG
1	0C	69	LEU
1	0C	108	THR
1	0C	148	THR
1	0C	200	THR
1	1C	96	MET

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Mol	Chain	Res	Type
1	1C	107	THR
1	1C	110	THR
1	1C	148	THR
1	1C	184	TRP
1	1C	205	LEU
1	2C	21	ASN
1	2C	66	MET
1	2C	96	MET
1	2C	108	THR
1	2C	184	TRP
1	2C	192	GLN
1	3C	96	MET
1	3C	108	THR
1	3C	122	PRO
1	3C	148	THR
1	4C	108	THR
1	4C	147	PRO
1	4C	184	TRP
1	4C	230	VAL
1	5C	10	MET
1	5C	33	SER
1	5C	67	GLN
1	5C	69	LEU
1	5C	72	THR
1	5C	85	PRO
1	5C	108	THR
1	5C	121	ASN
1	5C	123	PRO
1	5C	184	TRP
1	6C	85	PRO
1	7C	15	ILE
1	7C	30	LYS
1	7C	63	GLN
1	7C	96	MET
1	7C	97	ARG
1	7C	148	THR
1	7C	171	THR
1	8C	48	THR
1	8C	107	THR
1	8C	184	TRP
1	8C	195	ASN
1	8C	226	HIS

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Mol	Chain	Res	Type
1	9C	96	MET
1	9C	108	THR
1	9C	139	ASN
1	9C	195	ASN
1	AD	1	PRO
1	AD	2	ILE
1	AD	15	ILE
1	AD	72	THR
1	AD	147	PRO
1	AD	227	LYS
1	BD	69	LEU
1	BD	85	PRO
1	BD	148	THR
1	BD	184	TRP
1	CD	72	THR
1	CD	84	HIS
1	CD	96	MET
1	CD	107	THR
1	CD	215	MET
1	DD	72	THR
1	DD	82	ARG
1	DD	85	PRO
1	DD	90	PRO
1	DD	107	THR
1	DD	148	THR
1	DD	159	GLU
1	ED	54	THR
1	ED	99	PRO
1	ED	100	ARG
1	ED	107	THR
1	ED	182	LYS
1	ED	184	TRP
1	FD	10	MET
1	FD	107	THR
1	FD	182	LYS
1	GD	10	MET
1	GD	48	THR
1	GD	85	PRO
1	GD	96	MET
1	GD	108	THR
1	GD	142	VAL
1	GD	147	PRO

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Mol	Chain	Res	Type
1	GD	184	TRP
1	GD	188	THR
1	GD	230	VAL
1	HD	1	PRO
1	HD	3	VAL
1	HD	10	MET
1	HD	23	TRP
1	HD	48	THR
1	HD	99	PRO
1	HD	108	THR
1	HD	121	ASN
1	HD	195	ASN
1	ID	54	THR
1	ID	84	HIS
1	ID	184	TRP
1	JD	4	GLN
1	JD	54	THR
1	JD	148	THR
1	KD	53	ASN
1	KD	96	MET
1	KD	148	THR
1	KD	230	VAL
1	LD	25	LYS
1	LD	96	MET
1	LD	162	ARG
1	LD	171	THR
1	LD	200	THR
1	LD	221	VAL
1	LD	226	HIS
1	MD	53	ASN
1	MD	58	THR
1	MD	91	ILE
1	MD	107	THR
1	MD	108	THR
1	MD	147	PRO
1	MD	184	TRP
1	MD	195	ASN
1	MD	201	ILE
1	MD	226	HIS
1	ND	30	LYS
1	ND	85	PRO
1	ND	96	MET

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Mol	Chain	Res	Type
1	ND	148	THR
1	ND	182	LYS
1	ND	184	TRP
1	ND	188	THR
1	OD	63	GLN
1	OD	148	THR
1	OD	184	TRP
1	PD	48	THR
1	PD	96	MET
1	PD	107	THR
1	PD	108	THR
1	QD	54	THR
1	QD	58	THR
1	QD	63	GLN
1	QD	74	ASN
1	QD	108	THR
1	QD	171	THR
1	QD	184	TRP
1	RD	96	MET
1	RD	107	THR
1	RD	112	GLN
1	RD	139	ASN
1	RD	185	MET
1	RD	205	LEU
1	SD	48	THR
1	SD	58	THR
1	SD	72	THR
1	SD	108	THR
1	SD	147	PRO
1	SD	179	GLN
1	SD	184	TRP
1	SD	226	HIS
1	TD	48	THR
1	TD	62	HIS
1	TD	121	ASN
1	TD	148	THR
1	UD	2	ILE
1	UD	69	LEU
1	UD	126	VAL
1	UD	184	TRP
1	UD	192	GLN
1	VD	54	THR

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Mol	Chain	Res	Type
1	VD	58	THR
1	VD	108	THR
1	VD	184	TRP
1	VD	195	ASN
1	VD	227	LYS
1	WD	66	MET
1	WD	108	THR
1	WD	184	TRP
1	XD	10	MET
1	XD	108	THR
1	XD	175	GLU
1	XD	184	TRP
1	XD	195	ASN
1	YD	63	GLN
1	YD	108	THR
1	YD	147	PRO
1	YD	184	TRP
1	YD	216	THR
1	ZD	1	PRO
1	ZD	48	THR
1	ZD	99	PRO
1	ZD	108	THR
1	ZD	121	ASN
1	ZD	171	THR
1	ZD	184	TRP
1	ZD	196	PRO
1	ZD	221	VAL
1	aD	2	ILE
1	aD	58	THR
1	aD	69	LEU
1	aD	85	PRO
1	aD	107	THR
1	aD	148	THR
1	bD	4	GLN
1	bD	97	ARG
1	cD	54	THR
1	cD	96	MET
1	cD	108	THR
1	cD	184	TRP
1	dD	33	SER
1	dD	69	LEU
1	dD	95	GLN

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Mol	Chain	Res	Type
1	dD	97	ARG
1	dD	108	THR
1	dD	171	THR
1	dD	175	GLU
1	dD	184	TRP
1	eD	15	ILE
1	eD	48	THR
1	eD	66	MET
1	eD	96	MET
1	eD	184	TRP
1	eD	195	ASN
1	fD	54	THR
1	fD	85	PRO
1	fD	108	THR
1	fD	121	ASN
1	fD	148	THR
1	fD	150	ILE
1	fD	184	TRP
1	gD	69	LEU
1	gD	72	THR
1	gD	96	MET
1	gD	107	THR
1	gD	131	LYS
1	gD	184	TRP
1	hD	4	GLN
1	hD	96	MET
1	hD	97	ARG
1	hD	108	THR
1	iD	85	PRO
1	iD	96	MET
1	iD	97	ARG
1	iD	108	THR
1	iD	184	TRP
1	iD	188	THR
1	iD	230	VAL
1	jD	30	LYS
1	jD	108	THR
1	jD	139	ASN
1	kD	110	THR
1	kD	142	VAL
1	kD	147	PRO
1	kD	205	LEU

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Mol	Chain	Res	Type
1	lD	1	PRO
1	lD	54	THR
1	lD	72	THR
1	lD	96	MET
1	lD	148	THR
1	lD	196	PRO
1	mD	15	ILE
1	mD	48	THR
1	mD	69	LEU
1	mD	107	THR
1	nD	4	GLN
1	nD	63	GLN
1	nD	97	ARG
1	oD	66	MET
1	oD	184	TRP
1	qD	1	PRO
1	qD	48	THR
1	qD	72	THR
1	qD	107	THR
1	qD	141	ILE
1	qD	147	PRO
1	qD	175	GLU
1	qD	201	ILE
1	rD	9	GLN
1	rD	10	MET
1	rD	66	MET
1	rD	85	PRO
1	rD	91	ILE
1	rD	108	THR
1	rD	121	ASN
1	rD	148	THR
1	rD	182	LYS
1	sD	10	MET
1	sD	84	HIS
1	sD	107	THR
1	tD	2	ILE
1	tD	96	MET
1	tD	108	THR
1	tD	154	ARG
1	tD	188	THR
1	tD	229	ARG
1	uD	96	MET

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Mol	Chain	Res	Type
1	uD	108	THR
1	uD	182	LYS
1	uD	184	TRP
1	uD	230	VAL
1	vD	54	THR
1	vD	58	THR
1	vD	96	MET
1	vD	108	THR
1	vD	122	PRO
1	vD	171	THR
1	vD	184	TRP
1	vD	200	THR
1	vD	229	ARG
1	wD	25	LYS
1	wD	48	THR
1	wD	72	THR
1	wD	108	THR
1	wD	119	THR
1	wD	142	VAL
1	wD	147	PRO
1	wD	175	GLU
1	xD	10	MET
1	xD	19	THR
1	xD	30	LYS
1	xD	148	THR
1	xD	189	LEU
1	xD	231	LEU
1	yD	171	THR
1	zD	48	THR
1	zD	72	THR
1	zD	107	THR
1	zD	108	THR
1	zD	121	ASN
1	0D	96	MET
1	0D	108	THR
1	0D	145	TYR
1	0D	184	TRP
1	1D	96	MET
1	1D	108	THR
1	1D	119	THR
1	1D	148	THR
1	1D	175	GLU

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Mol	Chain	Res	Type
1	2D	15	ILE
1	2D	87	HIS
1	2D	96	MET
1	2D	113	GLU
1	2D	147	PRO
1	2D	184	TRP
1	3D	48	THR
1	3D	54	THR
1	3D	69	LEU
1	3D	87	HIS
1	3D	108	THR
1	3D	121	ASN
1	3D	148	THR
1	3D	175	GLU
1	3D	185	MET
1	4D	63	GLN
1	4D	96	MET
1	4D	143	ARG
1	4D	148	THR
1	4D	184	TRP
1	5D	4	GLN
1	5D	141	ILE
1	6D	54	THR
1	6D	58	THR
1	6D	86	VAL
1	6D	103	ASP
1	6D	108	THR
1	6D	148	THR
1	6D	184	TRP
1	7D	9	GLN
1	7D	30	LYS
1	7D	69	LEU
1	7D	108	THR
1	7D	175	GLU
1	7D	186	THR
1	8D	96	MET
1	8D	107	THR
1	8D	108	THR
1	8D	142	VAL
1	8D	147	PRO
1	8D	184	TRP
1	8D	229	ARG

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Mol	Chain	Res	Type
1	9D	10	MET
1	9D	48	THR
1	9D	96	MET
1	9D	99	PRO
1	9D	108	THR
1	9D	175	GLU
1	AE	2	ILE
1	AE	15	ILE
1	AE	69	LEU
1	AE	86	VAL
1	AE	148	THR
1	AE	192	GLN
1	BE	5	ASN
1	BE	63	GLN
1	BE	69	LEU
1	BE	72	THR
1	CE	10	MET
1	CE	58	THR
1	CE	108	THR
1	CE	112	GLN
1	CE	231	LEU
1	DE	54	THR
1	DE	139	ASN
1	DE	141	ILE
1	DE	184	TRP
1	EE	54	THR
1	EE	96	MET
1	EE	107	THR
1	EE	108	THR
1	EE	147	PRO
1	EE	179	GLN
1	EE	184	TRP
1	FE	30	LYS
1	FE	72	THR
1	FE	108	THR
1	FE	121	ASN
1	FE	148	THR
1	FE	165	VAL
1	FE	184	TRP
1	FE	200	THR
1	GE	54	THR
1	GE	96	MET

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Mol	Chain	Res	Type
1	GE	107	THR
1	GE	171	THR
1	GE	215	MET
1	HE	58	THR
1	HE	72	THR
1	HE	96	MET
1	HE	109	SER
1	IE	1	PRO
1	IE	184	TRP
1	IE	226	HIS
1	IE	229	ARG
1	JE	48	THR
1	JE	54	THR
1	JE	96	MET
1	JE	107	THR
1	JE	108	THR
1	JE	184	TRP
1	KE	30	LYS
1	KE	147	PRO
1	KE	184	TRP
1	KE	226	HIS
1	LE	48	THR
1	LE	72	THR
1	LE	85	PRO
1	LE	148	THR
1	LE	166	ASP
1	LE	182	LYS
1	LE	184	TRP
1	ME	10	MET
1	ME	71	GLU
1	ME	107	THR
1	ME	148	THR
1	NE	2	ILE
1	NE	195	ASN
1	OE	108	THR
1	OE	154	ARG
1	OE	184	TRP
1	PE	72	THR
1	PE	111	LEU
1	PE	119	THR
1	PE	122	PRO
1	PE	175	GLU

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Mol	Chain	Res	Type
1	PE	184	TRP
1	QE	66	MET
1	QE	72	THR
1	QE	141	ILE
1	QE	147	PRO
1	RE	10	MET
1	RE	69	LEU
1	RE	110	THR
1	RE	148	THR
1	RE	179	GLN
1	RE	184	TRP
1	SE	4	GLN
1	SE	58	THR
1	SE	72	THR
1	SE	74	ASN
1	SE	107	THR
1	SE	108	THR
1	TE	62	HIS
1	TE	96	MET
1	TE	108	THR
1	TE	119	THR
1	TE	184	TRP
1	UE	2	ILE
1	UE	107	THR
1	UE	108	THR
1	UE	184	TRP
1	UE	229	ARG
1	VE	30	LYS
1	VE	139	ASN
1	VE	148	THR
1	VE	226	HIS
1	VE	227	LYS
1	VE	229	ARG
1	WE	85	PRO
1	WE	87	HIS
1	WE	96	MET
1	WE	107	THR
1	WE	108	THR
1	WE	123	PRO
1	WE	147	PRO
1	WE	171	THR
1	WE	175	GLU

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Mol	Chain	Res	Type
1	WE	231	LEU
1	XE	10	MET
1	XE	30	LYS
1	XE	69	LEU
1	XE	96	MET
1	XE	107	THR
1	XE	108	THR
1	XE	121	ASN
1	XE	195	ASN
1	YE	95	GLN
1	YE	96	MET
1	YE	184	TRP
1	ZE	4	GLN
1	ZE	25	LYS
1	ZE	58	THR
1	ZE	107	THR
1	ZE	195	ASN
1	aE	69	LEU
1	aE	72	THR
1	aE	96	MET
1	aE	97	ARG
1	aE	108	THR
1	aE	184	TRP
1	bE	99	PRO
1	bE	108	THR
1	cE	48	THR
1	cE	108	THR
1	cE	147	PRO
1	cE	184	TRP
1	cE	195	ASN
1	cE	227	LYS
1	dE	1	PRO
1	dE	10	MET
1	dE	99	PRO
1	dE	108	THR
1	dE	121	ASN
1	dE	175	GLU
1	dE	179	GLN
1	dE	184	TRP
1	dE	196	PRO
1	eE	72	THR
1	eE	184	TRP

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Mol	Chain	Res	Type
1	eE	197	ASP
1	eE	227	LYS
1	eE	229	ARG
1	fE	72	THR
1	fE	121	ASN
1	fE	123	PRO
1	fE	184	TRP
1	fE	195	ASN
1	gE	2	ILE
1	gE	108	THR
1	gE	110	THR
1	gE	184	TRP
1	gE	189	LEU
1	gE	195	ASN
1	hE	34	PRO
1	hE	58	THR
1	hE	148	THR
1	hE	184	TRP
1	hE	211	LEU
1	iE	108	THR
1	iE	113	GLU
1	iE	175	GLU
1	iE	195	ASN
1	iE	203	LYS
1	iE	230	VAL
1	iE	231	LEU
1	jE	85	PRO
1	jE	121	ASN
1	jE	227	LYS
1	kE	10	MET
1	kE	18	ARG
1	kE	84	HIS
1	kE	110	THR
1	lE	72	THR
1	lE	121	ASN
1	mE	15	ILE
1	mE	87	HIS
1	mE	96	MET
1	mE	175	GLU
1	mE	184	TRP
1	mE	202	LEU
1	nE	96	MET

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Mol	Chain	Res	Type
1	nE	122	PRO
1	nE	171	THR
1	nE	179	GLN
1	nE	184	TRP
1	oE	48	THR
1	oE	50	GLN
1	oE	96	MET
1	oE	108	THR
1	oE	147	PRO
1	oE	184	TRP
1	pE	1	PRO
1	pE	48	THR
1	pE	72	THR
1	pE	96	MET
1	pE	99	PRO
1	pE	108	THR
1	pE	121	ASN
1	pE	148	THR
1	pE	195	ASN
1	pE	226	HIS
1	pE	229	ARG
1	qE	30	LYS
1	qE	107	THR
1	qE	148	THR
1	qE	184	TRP
1	rE	97	ARG
1	rE	98	GLU
1	rE	108	THR
1	rE	121	ASN
1	rE	148	THR
1	sE	107	THR
1	sE	122	PRO
1	sE	184	TRP
1	tE	48	THR
1	tE	54	THR
1	tE	96	MET
1	tE	139	ASN
1	tE	165	VAL
1	uE	15	ILE
1	uE	96	MET
1	uE	108	THR
1	uE	147	PRO

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Mol	Chain	Res	Type
1	uE	184	TRP
1	uE	195	ASN
1	vE	96	MET
1	vE	99	PRO
1	vE	148	THR
1	vE	175	GLU
1	wE	2	ILE
1	wE	18	ARG
1	wE	110	THR
1	wE	148	THR
1	wE	188	THR
1	wE	205	LEU
1	xE	10	MET
1	xE	54	THR
1	xE	97	ARG
1	xE	121	ASN
1	xE	122	PRO
1	xE	226	HIS
1	yE	10	MET
1	yE	69	LEU
1	yE	108	THR
1	zE	2	ILE
1	zE	67	GLN
1	zE	108	THR
1	zE	110	THR
1	zE	139	ASN
1	zE	148	THR
1	zE	165	VAL
1	zE	172	LEU
1	0E	53	ASN
1	0E	96	MET
1	0E	99	PRO
1	0E	107	THR
1	0E	108	THR
1	0E	147	PRO
1	0E	230	VAL
1	1E	10	MET
1	1E	58	THR
1	1E	69	LEU
1	1E	110	THR
1	1E	148	THR
1	2E	30	LYS

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Mol	Chain	Res	Type
1	2E	72	THR
1	2E	107	THR
1	2E	148	THR
1	2E	231	LEU
1	3E	184	TRP
1	4E	96	MET
1	4E	108	THR
1	4E	121	ASN
1	4E	122	PRO
1	4E	139	ASN
1	5E	25	LYS
1	5E	97	ARG
1	5E	110	THR
1	5E	113	GLU
1	5E	195	ASN
1	6E	15	ILE
1	6E	21	ASN
1	6E	108	THR
1	6E	139	ASN
1	6E	147	PRO
1	7E	10	MET
1	7E	15	ILE
1	7E	72	THR
1	7E	85	PRO
1	7E	107	THR
1	7E	172	LEU
1	8E	2	ILE
1	8E	96	MET
1	8E	107	THR
1	8E	148	THR
1	9E	54	THR
1	9E	96	MET
1	9E	108	THR
1	9E	121	ASN
1	9E	184	TRP
1	9E	210	THR
1	AF	9	GLN
1	AF	107	THR
1	AF	122	PRO
1	AF	184	TRP
1	AF	200	THR
1	BF	2	ILE

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Mol	Chain	Res	Type
1	BF	108	THR
1	BF	171	THR
1	CF	7	GLN
1	CF	48	THR
1	CF	66	MET
1	CF	96	MET
1	CF	107	THR
1	CF	147	PRO
1	CF	188	THR
1	CF	189	LEU
1	CF	195	ASN
1	DF	10	MET
1	DF	13	GLN
1	DF	50	GLN
1	DF	85	PRO
1	DF	99	PRO
1	DF	107	THR
1	DF	171	THR
1	DF	219	GLN
1	DF	230	VAL
1	FF	4	GLN
1	FF	48	THR
1	FF	58	THR
1	FF	96	MET
1	FF	97	ARG
1	FF	107	THR
1	FF	205	LEU

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1126
Number of shifts mapped to atoms	1126
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	223	-0.48 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	205	0.46 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	190	-0.48 ± 0.12	None needed (< 0.5 ppm)
^{15}N	209	0.39 ± 0.14	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 1095 atoms were assigned a chemical shift out of a possible 1185408. 0 out of 12474 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	612/429786 (0%)	0/174636 (0%)	413/174636 (0%)	199/80514 (0%)
Sidechain	440/688338 (0%)	0/449442 (0%)	440/212814 (0%)	0/26082 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	43/67284 (0%)	0/34020 (0%)	43/29106 (0%)	0/4158 (0%)
Overall	1095/1185408 (0%)	0/658098 (0%)	896/416556 (0%)	199/110754 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 1095 atoms were assigned a chemical shift out of a possible 1185408. 0 out of 12474 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	612/429786 (0%)	0/174636 (0%)	413/174636 (0%)	199/80514 (0%)
Sidechain	440/688338 (0%)	0/449442 (0%)	440/212814 (0%)	0/26082 (0%)
Aromatic	43/67284 (0%)	0/34020 (0%)	43/29106 (0%)	0/4158 (0%)
Overall	1095/1185408 (0%)	0/658098 (0%)	896/416556 (0%)	199/110754 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

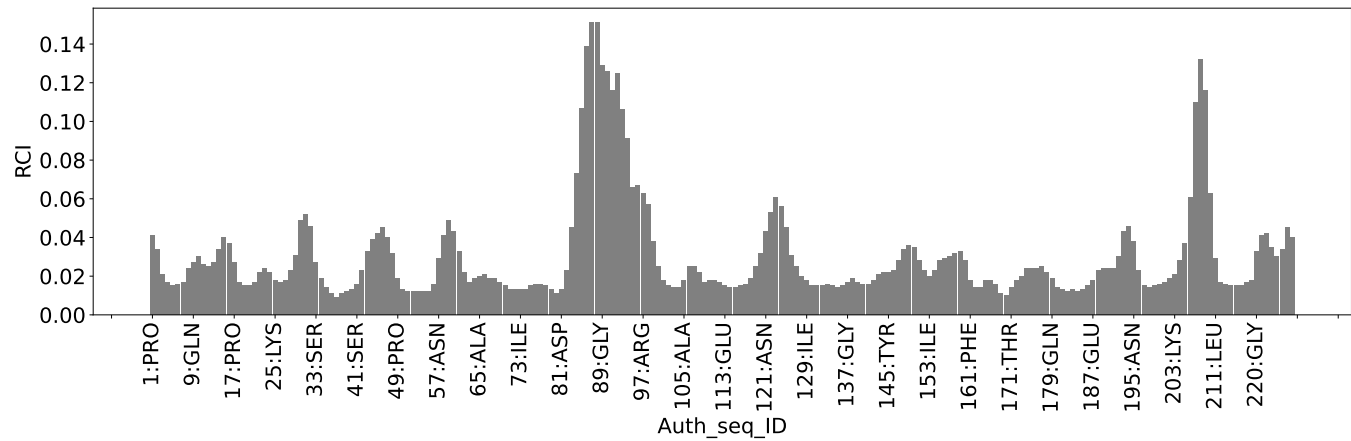
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1121
Intra-residue ($ i-j =0$)	488
Sequential ($ i-j =1$)	220
Medium range ($ i-j >1$ and $ i-j <5$)	204
Long range ($ i-j \geq 5$)	209
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	388
Number of unmapped restraints	0
Number of restraints per residue	0.0
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.0	0.2
0.2-0.5 (Medium)	15.0	0.45
>0.5 (Large)	35.0	3.5

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	17.0	9.1
10.0-20.0 (Medium)	10.0	19.39
>20.0 (Large)	24.0	147.78

9 Distance violation analysis ⓘ

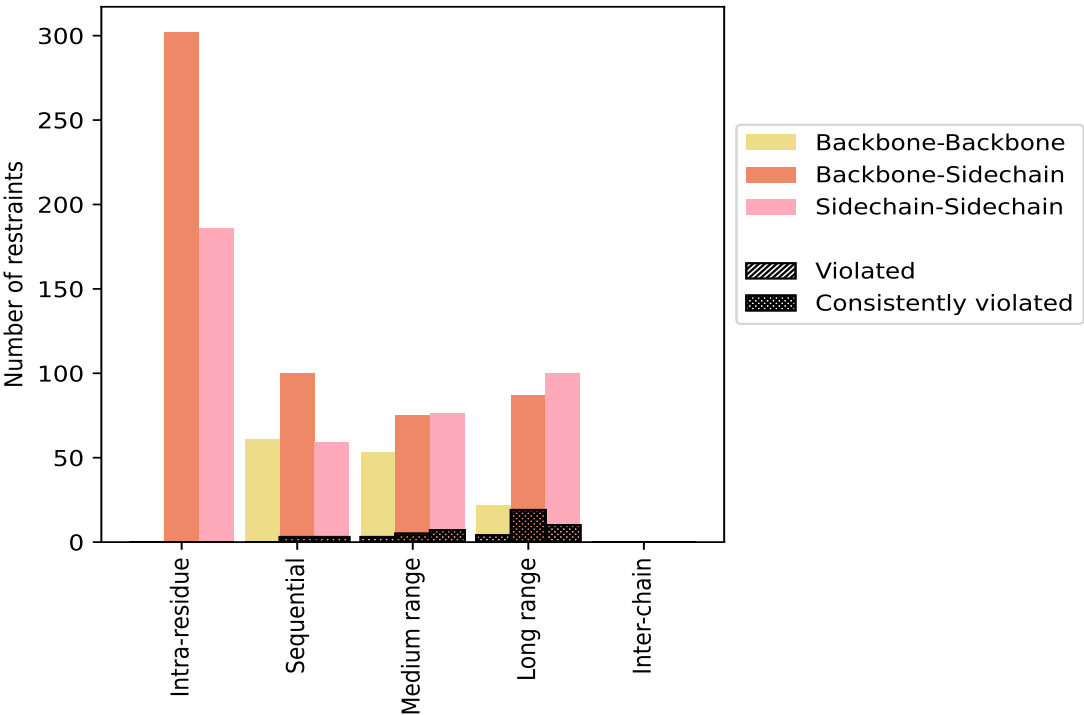
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	488	43.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	302	26.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	186	16.6	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	220	19.6	6	2.7	0.5	6	2.7	0.5
Backbone-Backbone	61	5.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	100	8.9	3	3.0	0.3	3	3.0	0.3
Sidechain-Sidechain	59	5.3	3	5.1	0.3	3	5.1	0.3
Medium range ($i-j >1$ & $i-j <5$)	204	18.2	15	7.4	1.3	15	7.4	1.3
Backbone-Backbone	53	4.7	3	5.7	0.3	3	5.7	0.3
Backbone-Sidechain	75	6.7	5	6.7	0.4	5	6.7	0.4
Sidechain-Sidechain	76	6.8	7	9.2	0.6	7	9.2	0.6
Long range ($i-j \geq 5$)	209	18.6	33	15.8	2.9	33	15.8	2.9
Backbone-Backbone	22	2.0	4	18.2	0.4	4	18.2	0.4
Backbone-Sidechain	87	7.8	19	21.8	1.7	19	21.8	1.7
Sidechain-Sidechain	100	8.9	10	10.0	0.9	10	10.0	0.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1121	100.0	54	4.8	4.8	54	4.8	4.8
Backbone-Backbone	136	12.1	7	5.1	0.6	7	5.1	0.6
Backbone-Sidechain	564	50.3	27	4.8	2.4	27	4.8	2.4
Sidechain-Sidechain	421	37.6	20	4.8	1.8	20	4.8	1.8

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

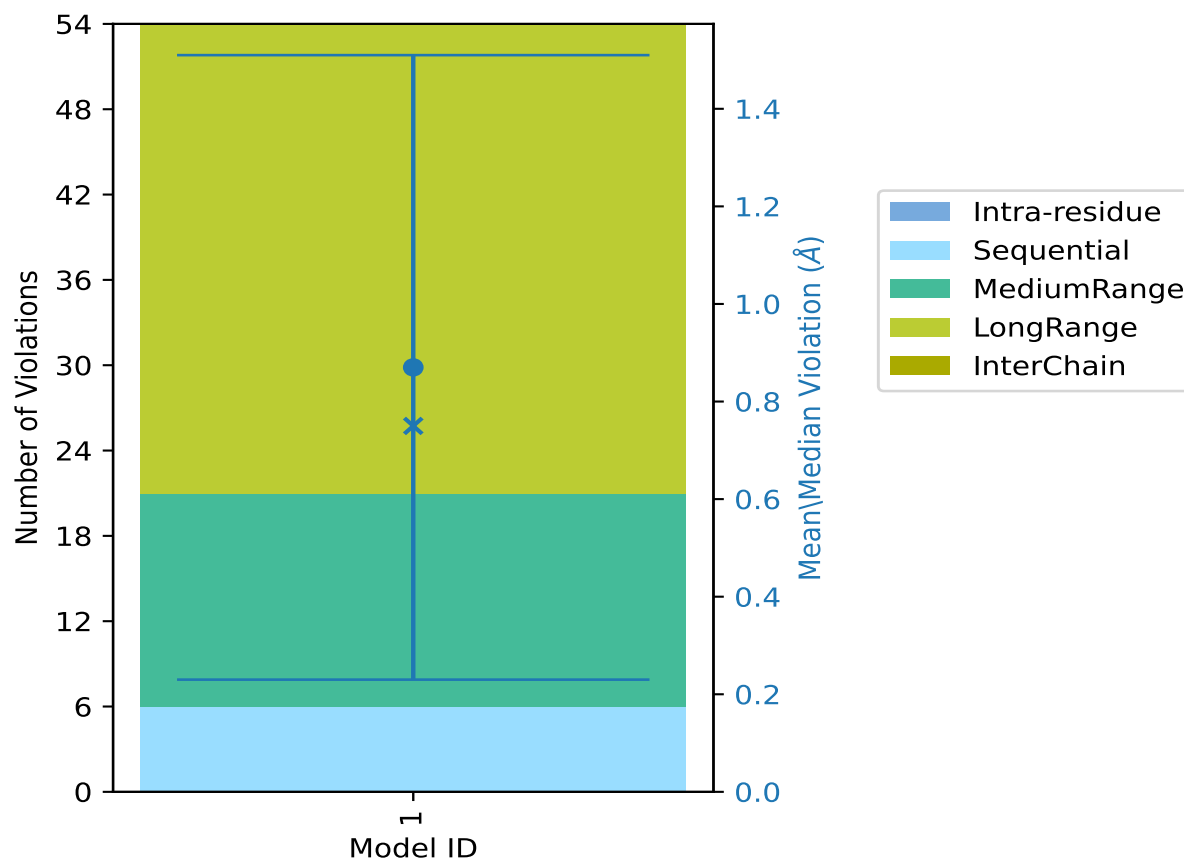
9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	6	15	33	0	54	0.87	3.5	0.64	0.75

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

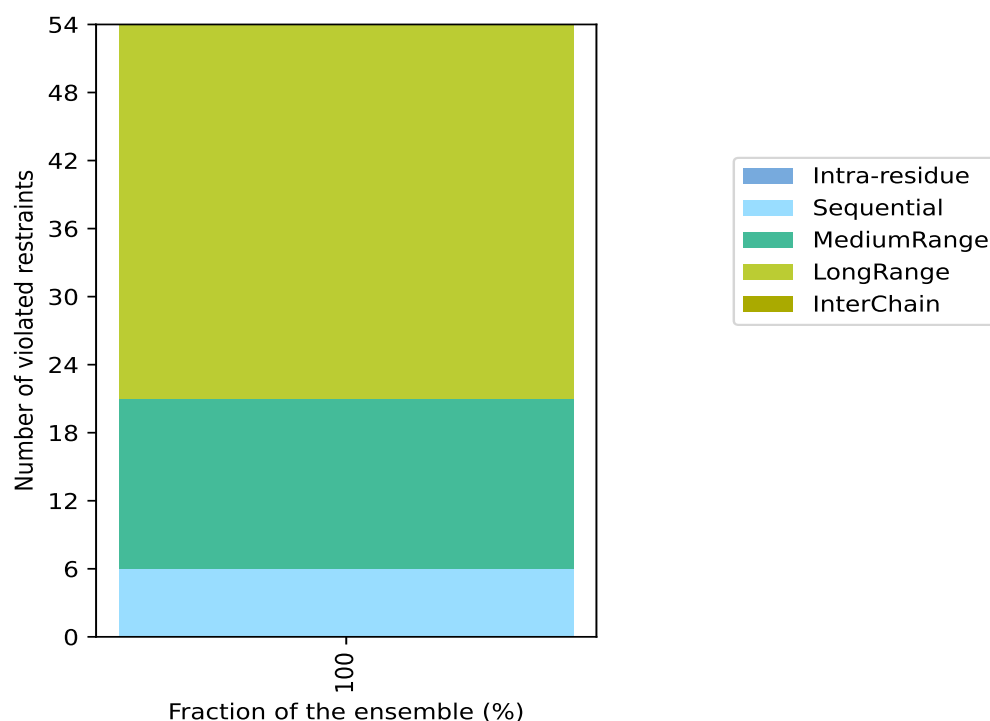
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1067(IR:488, SQ:214, MR:189, LR:176, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	6	15	33	0	54	1	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



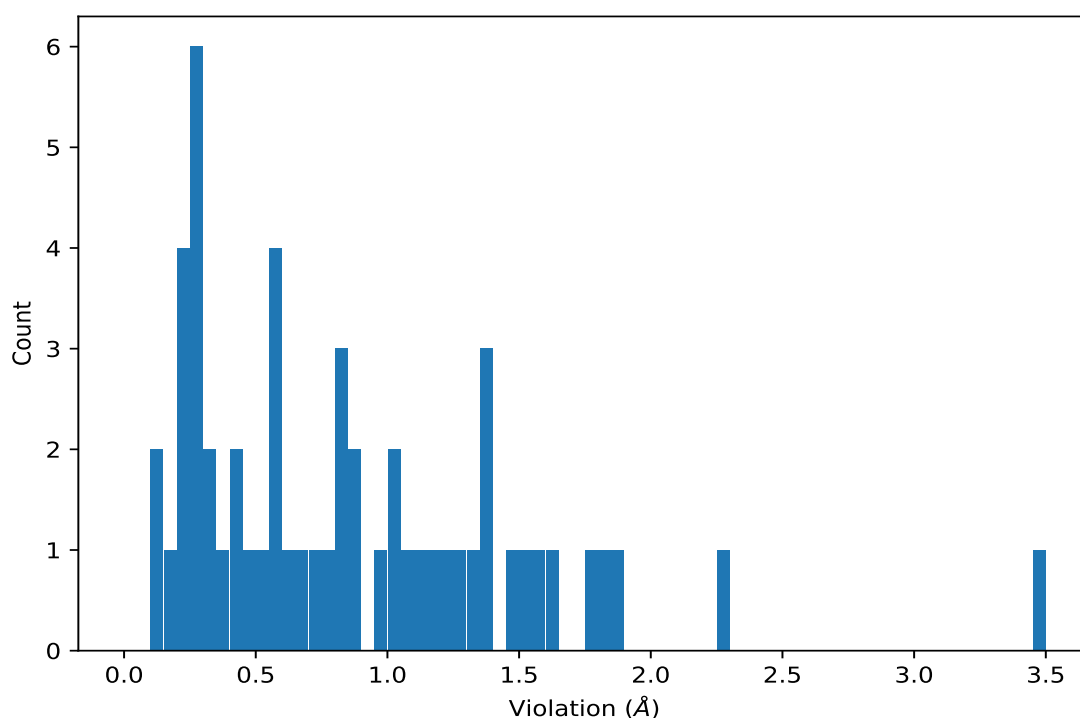
9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:79:A:GLU:CD	1:82:A:ARG:CD	1	3.5
(1,817)	1:52:A:LEU:CD1	1:54:A:THR:CB	1	2.3
(1,171)	1:150:A:ILE:CB	1:185:A:MET:CA	1	1.85
(1,858)	1:45:A:GLU:CG	1:42:A:ALA:CB	1	1.81
(1,203)	1:198:A:CYS:CA	1:218:A:CYS:CA	1	1.78
(1,197)	1:165:A:VAL:CB	1:215:A:MET:CA	1	1.65
(1,59)	1:37:A:ILE:CB	1:142:A:VAL:CA	1	1.56
(1,62)	1:40:A:PHE:CB	1:55:A:MET:CE	1	1.51
(1,169)	1:150:A:ILE:CD1	1:169:A:TYR:CA	1	1.48
(1,116)	1:80:A:TRP:CD1	1:133:A:TRP:CD1	1	1.4
(1,996)	1:87:A:HIS:CG	1:91:A:ILE:CB	1	1.38
(1,51)	1:32:A:PHE:CD1	1:141:A:ILE:CD1	1	1.38
(1,193)	1:161:A:PHE:CB	1:215:A:MET:CA	1	1.31
(1,74)	1:48:A:THR:CB	1:111:A:LEU:CA	1	1.29
(1,926)	1:1:A:PRO:CG	1:3:A:VAL:CG2	1	1.22
(1,1119)	1:43:A:LEU:C	1:47:A:ALA:CA	1	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:23:A:TRP:CZ2	1:36:A:VAL:CA	1	1.11
(1,885)	1:159:A:GLU:CG	1:158:A:LYS:CG	1	1.06
(1,1121)	1:153:A:ILE:CB	1:151:A:LEU:CG	1	1.04
(1,985)	1:131:A:LYS:CE	1:127:A:GLY:CA	1	1.01
(1,766)	1:103:A:ASP:CA	1:107:A:THR:CA	1	0.98
(1,131)	1:102:A:SER:CB	1:107:A:THR:CB	1	0.87
(1,130)	1:102:A:SER:CB	1:107:A:THR:CA	1	0.87
(1,1004)	1:80:A:TRP:CG	1:83:A:LEU:CB	1	0.83
(1,163)	1:118:A:MET:CA	1:125:A:PRO:CD	1	0.83
(1,1078)	1:153:A:ILE:CB	1:154:A:ARG:CD	1	0.81
(1,82)	1:49:A:PRO:CA	1:126:A:VAL:CG1	1	0.77
(1,206)	1:202:A:LEU:CD2	1:214:A:MET:CA	1	0.73
(1,1017)	1:47:A:ALA:CA	1:51:A:ASP:CA	1	0.7
(1,1118)	1:80:A:TRP:CE3	1:76:A:GLU:CA	1	0.62
(1,192)	1:161:A:PHE:CD1	1:202:A:LEU:CA	1	0.6
(1,106)	1:80:A:TRP:CZ2	1:101:A:GLY:CA	1	0.6
(1,179)	1:154:A:ARG:CA	1:194:A:ALA:CB	1	0.59
(1,880)	1:117:A:TRP:CE3	1:118:A:MET:CB	1	0.58
(1,715)	1:84:A:HIS:C	1:81:A:ASP:CB	1	0.52
(1,164)	1:118:A:MET:CA	1:126:A:VAL:CA	1	0.45
(1,175)	1:153:A:ILE:CA	1:171:A:THR:CB	1	0.44
(1,45)	1:24:A:VAL:CG1	1:58:A:THR:CA	1	0.44
(1,14)	1:15:A:ILE:CA	1:51:A:ASP:CA	1	0.36
(1,190)	1:161:A:PHE:CB	1:194:A:ALA:CB	1	0.31
(1,2)	1:1:A:PRO:CB	1:47:A:ALA:CB	1	0.31
(1,702)	1:121:A:ASN:CA	1:123:A:PRO:CG	1	0.3
(1,41)	1:23:A:TRP:CD1	1:59:A:VAL:CG1	1	0.3
(1,207)	1:202:A:LEU:CD2	1:214:A:MET:CB	1	0.29
(1,138)	1:103:A:ASP:CB	1:108:A:THR:CG2	1	0.29
(1,1072)	1:139:A:ASN:CA	1:140:A:LYS:CE	1	0.28
(1,884)	1:117:A:TRP:CE3	1:118:A:MET:CA	1	0.26
(1,29)	1:23:A:TRP:CA	1:40:A:PHE:CA	1	0.24
(1,128)	1:99:A:PRO:CA	1:126:A:VAL:CB	1	0.22
(1,24)	1:20:A:LEU:CG	1:55:A:MET:CA	1	0.22
(1,974)	1:184:A:TRP:CG	1:182:A:LYS:CA	1	0.2
(1,64)	1:40:A:PHE:CD1	1:131:A:LYS:CG	1	0.16
(1,740)	1:80:A:TRP:CD1	1:79:A:GLU:CA	1	0.11
(1,172)	1:153:A:ILE:CB	1:164:A:TYR:CA	1	0.11

10 Dihedral-angle violation analysis [i](#)

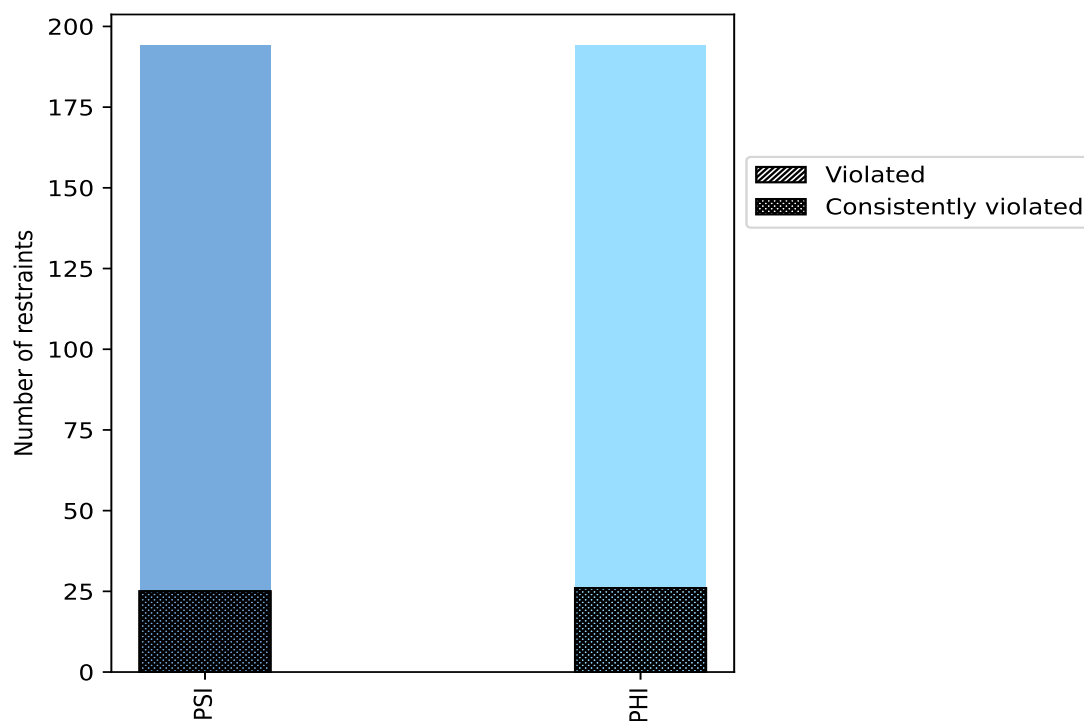
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	194	50.0	25	12.9	6.4	25	12.9	6.4
PHI	194	50.0	26	13.4	6.7	26	13.4	6.7
Total	388	100.0	51	13.1	13.1	51	13.1	13.1

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



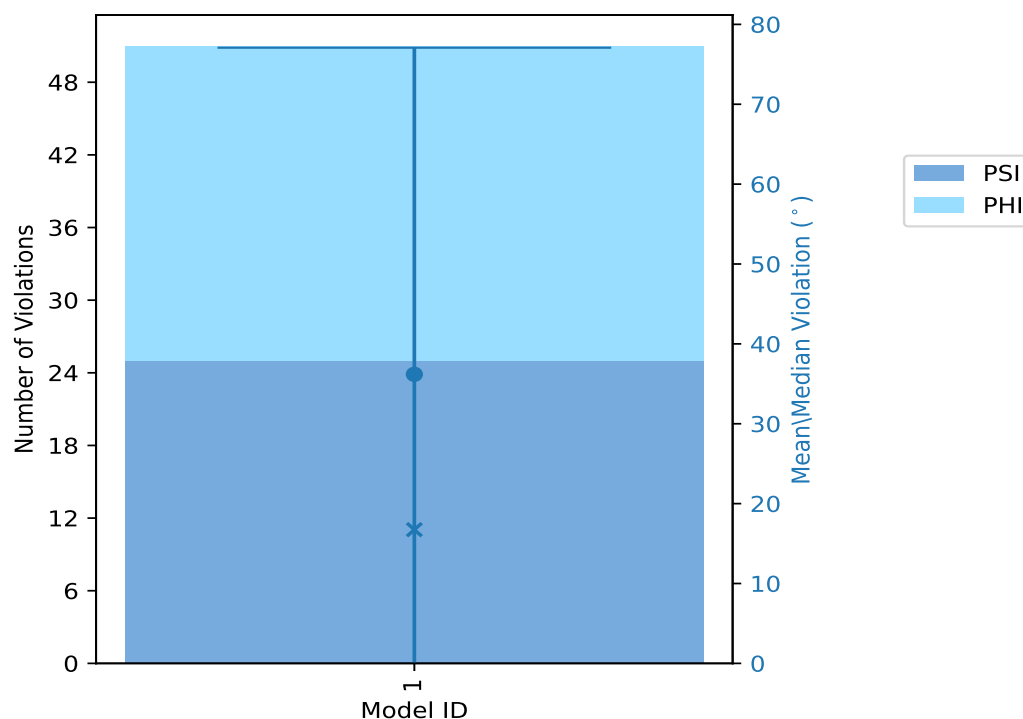
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	25	26	51	36.19	147.78	40.89	16.74

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

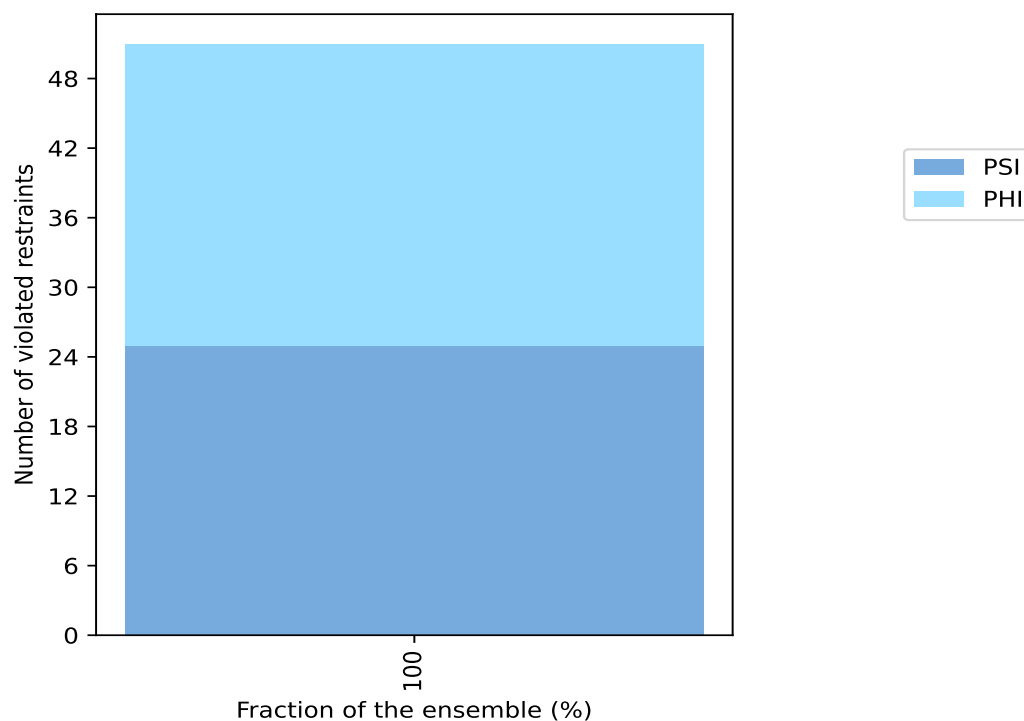
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
25	26	51	1	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



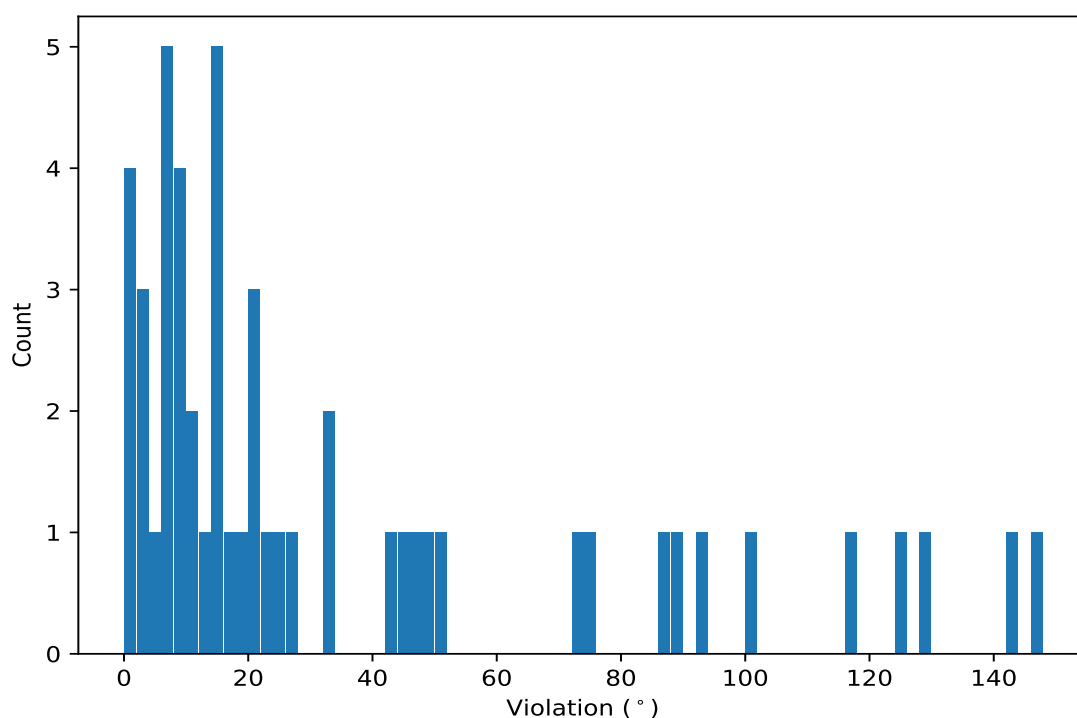
10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

No violations found

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	1:9:A:GLN:N	1	147.78
(1,5)	1:3:A:VAL:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1	142.39
(1,153)	1:96:A:MET:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1	128.32
(1,152)	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	1:97:A:ARG:N	1	125.76
(1,166)	1:105:A:ALA:N	1:105:A:ALA:CA	1:105:A:ALA:C	1:106:A:GLY:N	1	116.2
(1,8)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:LEU:N	1	100.09
(1,377)	1:60:A:GLY:C	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1	93.93
(1,382)	1:176:A:GLN:N	1:176:A:GLN:CA	1:176:A:GLN:C	1:177:A:ALA:N	1	88.06
(1,380)	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1:176:A:GLN:N	1	86.9
(1,104)	1:62:A:HIS:N	1:62:A:HIS:CA	1:62:A:HIS:C	1:63:A:GLN:N	1	74.28
(1,378)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:HIS:N	1	72.48
(1,369)	1:145:A:TYR:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1	51.75
(1,7)	1:4:A:GLN:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1	48.27
(1,11)	1:7:A:GLN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	1	47.24
(1,373)	1:176:A:GLN:C	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	1	45.6
(1,364)	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1:45:A:GLU:N	1	42.54
(1,80)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ALA:N	1	33.13
(1,381)	1:175:A:GLU:C	1:176:A:GLN:N	1:176:A:GLN:CA	1:176:A:GLN:C	1	32.84
(1,81)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1	27.91
(1,13)	1:9:A:GLN:C	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1	25.42
(1,56)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:SER:N	1	22.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,321)	1:197:A:ASP:C	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1	21.65
(1,188)	1:117:A:TRP:N	1:117:A:TRP:CA	1:117:A:TRP:C	1:118:A:MET:N	1	21.0
(1,143)	1:81:A:ASP:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	1	20.44
(1,82)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:PRO:N	1	19.39
(1,191)	1:118:A:MET:C	1:119:A:THR:N	1:119:A:THR:CA	1:119:A:THR:C	1	16.74
(1,240)	1:149:A:SER:N	1:149:A:SER:CA	1:149:A:SER:C	1:150:A:ILE:N	1	15.32
(1,189)	1:117:A:TRP:C	1:118:A:MET:N	1:118:A:MET:CA	1:118:A:MET:C	1	15.17
(1,79)	1:45:A:GLU:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1	15.07
(1,103)	1:61:A:GLY:C	1:62:A:HIS:N	1:62:A:HIS:CA	1:62:A:HIS:C	1	14.08
(1,283)	1:173:A:ARG:C	1:174:A:ALA:N	1:174:A:ALA:CA	1:174:A:ALA:C	1	14.01
(1,361)	1:30:A:LYS:C	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	1	12.34
(1,370)	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1:147:A:PRO:N	1	11.53
(1,358)	1:220:A:GLY:N	1:220:A:GLY:CA	1:220:A:GLY:C	1:221:A:VAL:N	1	10.54
(1,77)	1:44:A:SER:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	1	9.1
(1,51)	1:28:A:GLU:C	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1	8.55
(1,60)	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	1:36:A:VAL:N	1	8.18
(1,154)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:GLU:N	1	8.05
(1,383)	1:8:A:GLY:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	1	6.82
(1,78)	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	1:46:A:GLY:N	1	6.72
(1,354)	1:218:A:CYS:N	1:218:A:CYS:CA	1:218:A:CYS:C	1:219:A:GLN:N	1	6.52
(1,387)	1:205:A:LEU:C	1:206:A:GLY:N	1:206:A:GLY:CA	1:206:A:GLY:C	1	6.16
(1,58)	1:34:A:PRO:N	1:34:A:PRO:CA	1:34:A:PRO:C	1:35:A:GLU:N	1	6.15
(1,196)	1:122:A:PRO:N	1:122:A:PRO:CA	1:122:A:PRO:C	1:123:A:PRO:N	1	5.74
(1,55)	1:31:A:ALA:C	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1	2.88
(1,357)	1:219:A:GLN:C	1:220:A:GLY:N	1:220:A:GLY:CA	1:220:A:GLY:C	1	2.23
(1,158)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:GLY:N	1	2.22
(1,285)	1:177:A:ALA:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1	1.74
(1,362)	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	1:32:A:PHE:N	1	1.58
(1,187)	1:116:A:GLY:C	1:117:A:TRP:N	1:117:A:TRP:CA	1:117:A:TRP:C	1	1.39
(1,322)	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1:199:A:LYS:N	1	1.15