Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 03:14 AM EDT

PDB ID	:	6X63
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.; Schwieters, C.D.; Perilla, J.R.; Gronenborn, A.M.; Polenova, T.
Deposited on	:	2020-05-27

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

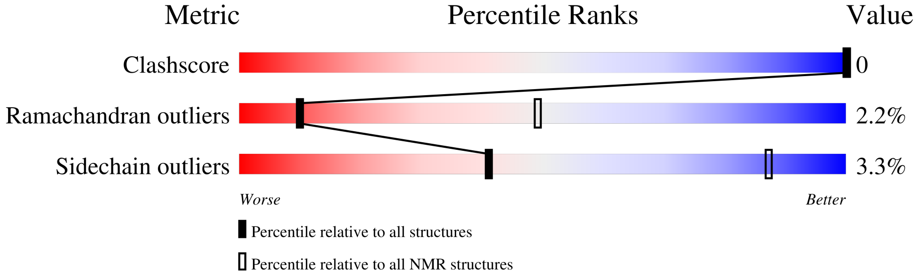
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

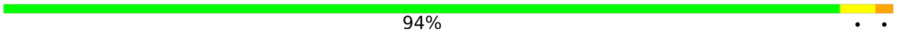
The overall completeness of chemical shifts assignment is 0%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	0	231	
1	0A	231	
1	0B	231	
1	0C	231	
1	0D	231	
1	0E	231	
1	1	231	
1	1A	231	

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

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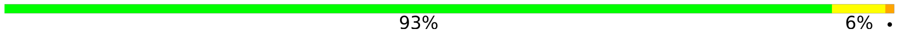
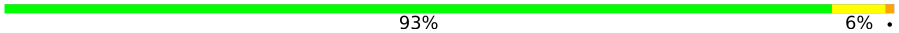
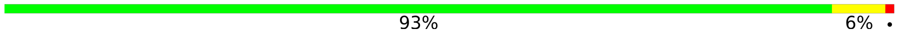
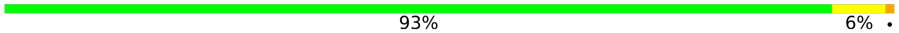
Mol	Chain	Length	Quality of chain
1	5C	231	
1	5D	231	
1	5E	231	
1	6	231	
1	6A	231	
1	6B	231	
1	6C	231	
1	6D	231	
1	6E	231	
1	7	231	
1	7A	231	
1	7B	231	
1	7C	231	
1	7D	231	
1	7E	231	
1	8	231	
1	8A	231	
1	8B	231	
1	8C	231	
1	8D	231	
1	8E	231	
1	9	231	
1	9A	231	
1	9B	231	
1	9C	231	

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Mol	Chain	Length	Quality of chain
1	9D	231	91% 7% •
1	9E	231	91% 8% •
1	A	231	90% 7% •
1	AA	231	93% 6% •
1	AB	231	90% 9% •
1	AC	231	92% 6% •
1	AD	231	91% 7% •
1	AE	231	90% 10%
1	AF	231	91% 8% •
1	B	231	94% 6%
1	BA	231	91% 8%
1	BB	231	92% 7% •
1	BC	231	91% 7% •
1	BD	231	92% 6% •
1	BE	231	92% 7% •
1	BF	231	91% 9%
1	C	231	91% 8% •
1	CA	231	92% 8%
1	CB	231	94% 5% •
1	CC	231	90% 7% •
1	CD	231	92% 6% •
1	CE	231	91% 9%
1	CF	231	91% 7% ••
1	D	231	91% 7% •
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	91% 7% ••
1	DE	231	92% 7% •
1	DF	231	88% 11% •
1	E	231	90% 10%
1	EA	231	92% 6% •
1	EB	231	92% 7%
1	EC	231	91% 7% •
1	ED	231	90% 7% •
1	EE	231	91% 7% •
1	EF	231	92% 7%
1	F	231	89% 10%
1	FA	231	90% 9% •
1	FB	231	90% 8% •
1	FC	231	90% 8% •
1	FD	231	93% 7%
1	FE	231	90% 8% •
1	FF	231	89% 9% •
1	G	231	92% 6% •
1	GA	231	93% • •
1	GB	231	92% 7%
1	GC	231	91% 8%
1	GD	231	90% 7% •
1	GE	231	92% 7%

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

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Mol	Chain	Length	Quality of chain
1	LA	231	93% 6% •
1	LB	231	90% 9% •
1	LC	231	90% 9% •
1	LD	231	93% 6% •
1	LE	231	91% 8% •
1	M	231	92% 6% •
1	MA	231	91% 7% •
1	MB	231	92% 6% •
1	MC	231	93% 6% •
1	MD	231	92% 7% •
1	ME	231	90% 9% •
1	N	231	91% 8% •
1	NA	231	91% 8% •
1	NB	231	89% 10% •
1	NC	231	90% 10%
1	ND	231	93% 6% •
1	NE	231	93% 7%
1	O	231	90% 7% •
1	OA	231	90% 8% •
1	OB	231	90% 10%
1	OC	231	90% 8% •
1	OD	231	92% 8%
1	OE	231	93% 5% •
1	P	231	92% 6% •
1	PA	231	92% 6% •

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Mol	Chain	Length	Quality of chain
1	PB	231	90% 8% •
1	PC	231	90% 9% •
1	PD	231	91% 8% •
1	PE	231	93% 6% •
1	Q	231	91% 7% •
1	QA	231	92% 8%
1	QB	231	93% 6% •
1	QC	231	91% 8% •
1	QD	231	91% 8% •
1	QE	231	90% 9%
1	R	231	90% 8% •
1	RA	231	92% 6% •
1	RB	231	91% 8% •
1	RC	231	91% 8% •
1	RD	231	92% 8%
1	RE	231	91% 7% •
1	S	231	90% 9%
1	SA	231	92% 6% • •
1	SB	231	90% 10%
1	SC	231	92% 7% •
1	SD	231	91% 6% •
1	SE	231	92% 7% •
1	T	231	92% 6% •
1	TA	231	93% 6% •
1	TB	231	91% 7% •

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Mol	Chain	Length	Quality of chain
1	TC	231	93% 7%
1	TD	231	91% 8% •
1	TE	231	92% 6% •
1	U	231	93% 6% •
1	UA	231	93% 7%
1	UB	231	93% 6% •
1	UC	231	91% 6% •
1	UD	231	89% 9% •
1	UE	231	93% 6% •
1	V	231	89% 10%
1	VA	231	87% 12% •
1	VB	231	93% 6% •
1	VC	231	90% 9% •
1	VD	231	90% 8% •
1	VE	231	92% 6% •
1	W	231	94% 6%
1	WA	231	92% 7%
1	WB	231	92% 6% •
1	WC	231	93% 7%
1	WD	231	92% 7%
1	WE	231	91% 7% •
1	X	231	92% 6% •
1	XA	231	91% 7% •
1	XB	231	92% 7% •
1	XC	231	90% 9% •

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Mol	Chain	Length	Quality of chain
1	XD	231	91% 8% •
1	XE	231	91% 9%
1	Y	231	91% 8%
1	YA	231	93% 5% ••
1	YB	231	90% 10%
1	YC	231	90% 10%
1	YD	231	90% 7% •
1	YE	231	91% 7% •
1	Z	231	89% 10%
1	ZA	231	93% 6% •
1	ZB	231	92% 6% •
1	ZC	231	93% 5% •
1	ZD	231	91% 8% •
1	ZE	231	90% 10%
1	a	231	92% 5% •
1	aA	231	93% 7%
1	aB	231	94% 5% •
1	aC	231	90% 6% •
1	aD	231	88% 12%
1	aE	231	91% 8% •
1	b	231	88% 9% •
1	bA	231	92% 6% •
1	bB	231	92% 7%
1	bC	231	90% 9% •
1	bD	231	92% 6% •

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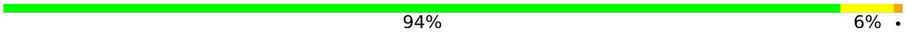
Mol	Chain	Length	Quality of chain
1	bE	231	 94% 6% •
1	c	231	 92% 8%
1	cA	231	 93% 5% •
1	cB	231	 92% 6% •
1	cC	231	 91% 8% •
1	cD	231	 92% 6% •
1	cE	231	 91% 7% •
1	d	231	 91% 8% •
1	dA	231	 91% 9%
1	dB	231	 91% 8% •
1	dC	231	 92% 6% •
1	dD	231	 90% 9% •
1	dE	231	 91% 8% •
1	e	231	 91% 7% •
1	eA	231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

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Mol	Chain	Length	Quality of chain
1	g	231	91% 8% •
1	gA	231	90% 10%
1	gB	231	92% 6% •
1	gC	231	92% 6% •
1	gD	231	90% 9% •
1	gE	231	91% 7% •
1	h	231	91% 8% •
1	hA	231	90% 9% •
1	hB	231	92% 6% •
1	hC	231	94% 6%
1	hD	231	92% 5% •
1	hE	231	92% 7% •
1	i	231	94% 6%
1	iA	231	92% 6% •
1	iB	231	90% 7% ••
1	iC	231	92% 6% •
1	iD	231	91% 6% •
1	iE	231	90% 8% •
1	j	231	92% 7% •
1	jA	231	90% 9% •
1	jB	231	90% 8% •
1	jC	231	93% 5% •
1	jD	231	93% 7%
1	jE	231	92% 7% •
1	k	231	91% 8% •

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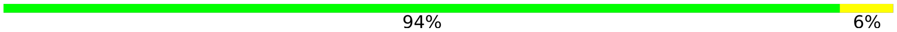
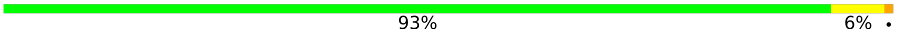
Mol	Chain	Length	Quality of chain
1	kA	231	 90% 8% •
1	kB	231	 91% 7% •
1	kC	231	 92% 7% •
1	kD	231	 91% 7% ••
1	kE	231	 90% 7% •
1	l	231	 89% 10% •
1	lA	231	 92% 7%
1	lB	231	 90% 9% •
1	lC	231	 92% 6% •
1	lD	231	 90% 10%
1	lE	231	 91% 6% •
1	m	231	 90% 9% •
1	mA	231	 92% 8%
1	mB	231	 91% 8% •
1	mC	231	 91% 7% •
1	mD	231	 92% 8%
1	mE	231	 91% 7% •
1	n	231	 91% 8% •
1	nA	231	 91% 8% •
1	nB	231	 94% 6%
1	nC	231	 91% 6% •
1	nD	231	 91% 7% •
1	nE	231	 91% 8%
1	o	231	 92% 7% •
1	oA	231	 93% 6% •

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Mol	Chain	Length	Quality of chain
1	oB	231	90% 8% ••
1	oC	231	91% 7% •
1	oD	231	92% 6% •
1	oE	231	91% 7% •
1	p	231	91% 6% •
1	pA	231	92% 6% •
1	pB	231	91% 8% •
1	pC	231	90% 8% •
1	pD	231	92% 7%
1	pE	231	90% 8% •
1	q	231	90% 8% •
1	qA	231	91% 7% •
1	qB	231	90% 9% •
1	qC	231	92% 8%
1	qD	231	89% 10% •
1	qE	231	90% 8% •
1	r	231	92% 6% •
1	rA	231	90% 9% •
1	rB	231	91% 8% •
1	rC	231	92% 6% •
1	rD	231	90% 9% •
1	rE	231	91% 7% •
1	s	231	92% 6% •
1	sA	231	89% 11%
1	sB	231	92% 6% •

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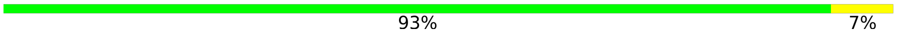
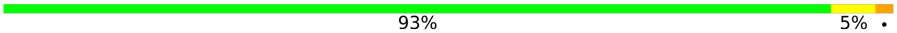
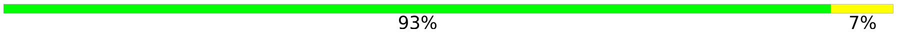
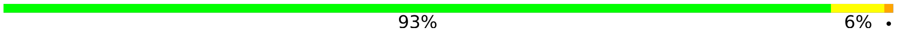
Mol	Chain	Length	Quality of chain
1	sC	231	 92% 6% •
1	sD	231	 92% 7%
1	sE	231	 91% 7% •
1	t	231	 92% 7% •
1	tA	231	 90% 9% •
1	tB	231	 91% 7% •
1	tC	231	 90% 10%
1	tD	231	 90% 8% •
1	tE	231	 93% 7%
1	u	231	 91% 8% •
1	uA	231	 91% 8% •
1	uB	231	 90% 7% •
1	uC	231	 93% 5% •
1	uD	231	 90% 9% •
1	uE	231	 91% 7% •
1	v	231	 90% 8% •
1	vA	231	 92% 7%
1	vB	231	 93% 7%
1	vC	231	 90% 8% •
1	vD	231	 90% 8% •
1	vE	231	 91% 7% •
1	w	231	 93% 6% •
1	wA	231	 91% 8% •
1	wB	231	 91% 7% •
1	wC	231	 90% 8% •

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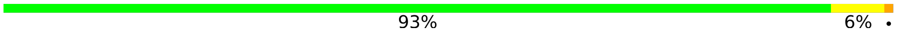
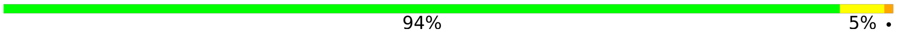
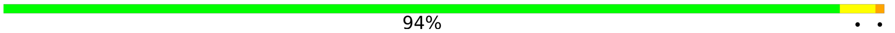
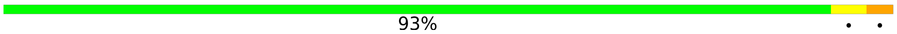
Mol	Chain	Length	Quality of chain
1	wD	231	 90% 8% •
1	wE	231	 91% 8% •
1	x	231	 93% 6% •
1	xA	231	 91% 9%
1	xB	231	 90% 9%
1	xC	231	 94% 5% •
1	xD	231	 91% 9%
1	xE	231	 92% 6% •
1	y	231	 90% 8% •
1	yA	231	 91% 8% •
1	yB	231	 90% 7% •
1	yC	231	 91% 7% •
1	yD	231	 94% • •
1	yE	231	 92% 7% •
1	z	231	 92% 7% •
1	zA	231	 92% 6% •
1	zB	231	 93% • •
1	zC	231	 90% 9% •
1	zD	231	 92% 7%
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
			Total	C	H	N	O	S	
1	A	231	3596	1131	1801	317	334	13	0
1	B	231	3596	1131	1801	317	334	13	0
1	C	231	3596	1131	1801	317	334	13	0
1	D	231	3596	1131	1801	317	334	13	0
1	E	231	3596	1131	1801	317	334	13	0
1	F	231	3596	1131	1801	317	334	13	0
1	G	231	3596	1131	1801	317	334	13	0
1	H	231	3596	1131	1801	317	334	13	0
1	I	231	3596	1131	1801	317	334	13	0
1	J	231	3596	1131	1801	317	334	13	0
1	K	231	3596	1131	1801	317	334	13	0
1	L	231	3596	1131	1801	317	334	13	0
1	M	231	3596	1131	1801	317	334	13	0
1	N	231	3596	1131	1801	317	334	13	0
1	O	231	3596	1131	1801	317	334	13	0
1	P	231	3596	1131	1801	317	334	13	0
1	Q	231	3596	1131	1801	317	334	13	0
1	R	231	3596	1131	1801	317	334	13	0
1	S	231	3596	1131	1801	317	334	13	0

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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 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
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

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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	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	
1	QB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	RB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	SB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	TB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	UB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
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	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

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

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

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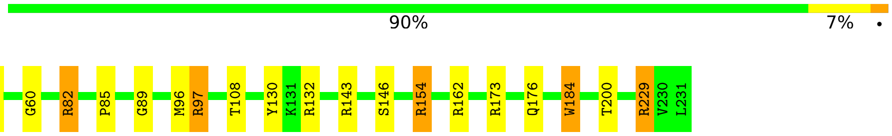
Mol	Chain	Residues	Atoms						Trace
1	EF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

4 Residue-property plots ⓘ

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.

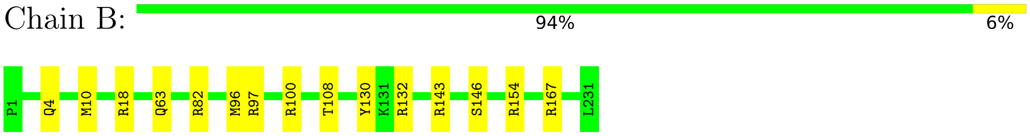
- Molecule 1: HIV-1 capsid protein

Chain A:



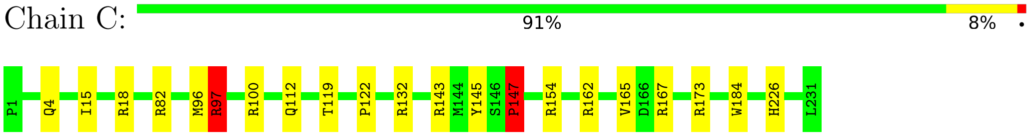
- Molecule 1: HIV-1 capsid protein

Chain B:



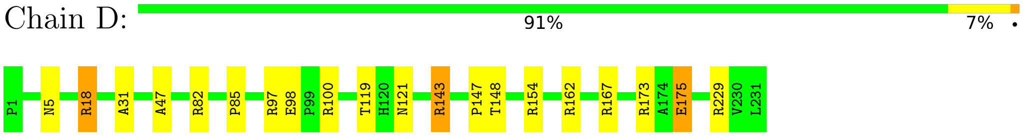
- Molecule 1: HIV-1 capsid protein

Chain C:



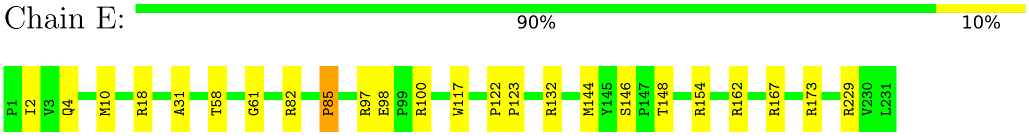
- Molecule 1: HIV-1 capsid protein

Chain D:



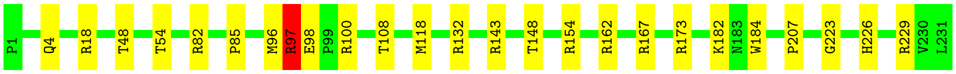
- Molecule 1: HIV-1 capsid protein

Chain E:



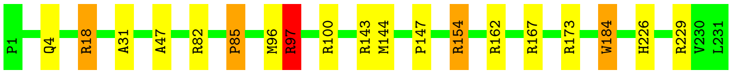
- Molecule 1: HIV-1 capsid protein

Chain F:



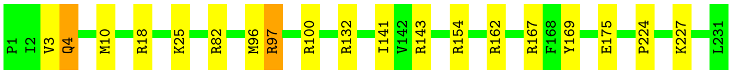
- Molecule 1: HIV-1 capsid protein

Chain G:



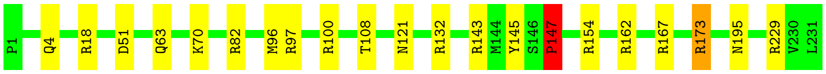
- Molecule 1: HIV-1 capsid protein

Chain H:



- Molecule 1: HIV-1 capsid protein

Chain I:



- Molecule 1: HIV-1 capsid protein

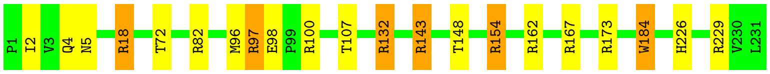
Chain J:

- Molecule 1: HIV-1 capsid protein

Chain K:

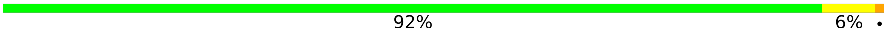
- Molecule 1: HIV-1 capsid protein

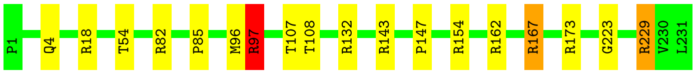
Chain L:



- Molecule 1: HIV-1 capsid protein

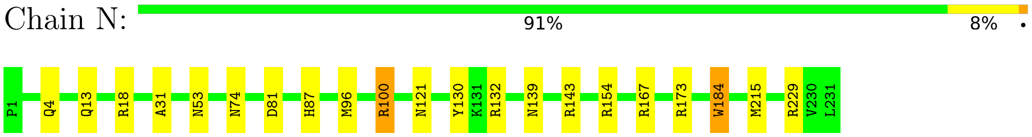
Chain M:





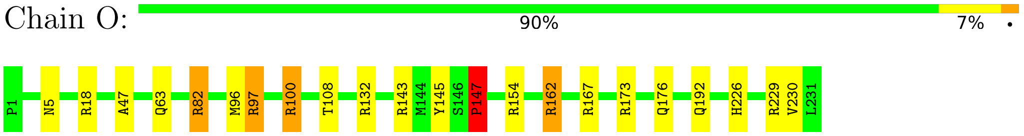
- Molecule 1: HIV-1 capsid protein

Chain N:



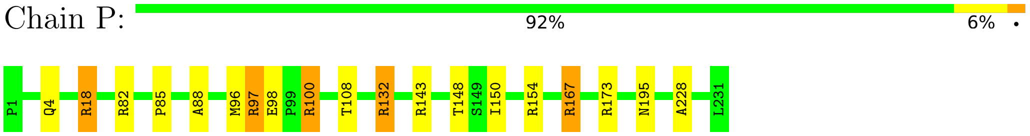
- Molecule 1: HIV-1 capsid protein

Chain O:



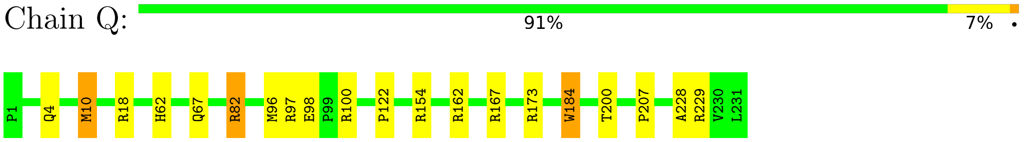
- Molecule 1: HIV-1 capsid protein

Chain P:



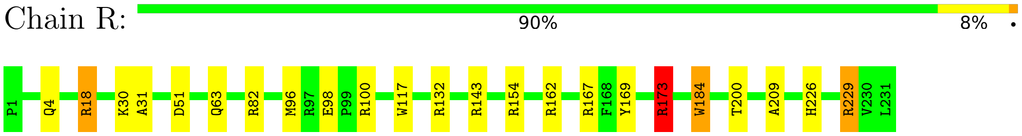
- Molecule 1: HIV-1 capsid protein

Chain Q:



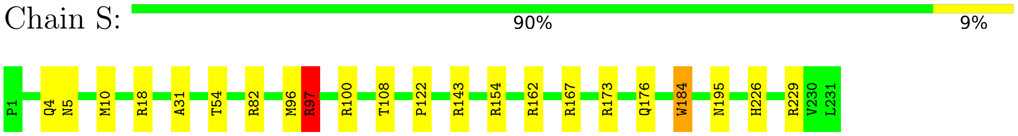
- Molecule 1: HIV-1 capsid protein

Chain R:



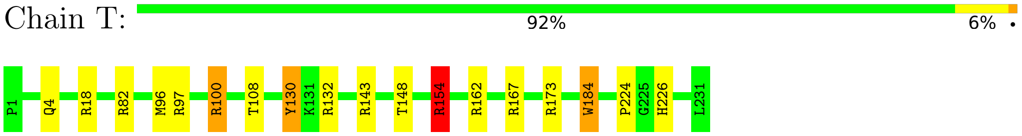
- Molecule 1: HIV-1 capsid protein

Chain S:



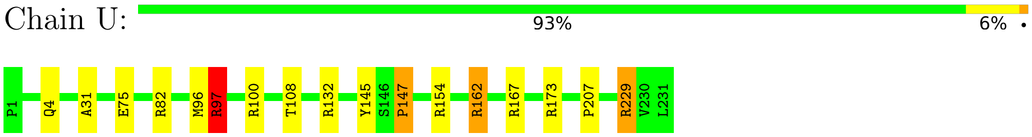
- Molecule 1: HIV-1 capsid protein

Chain T:



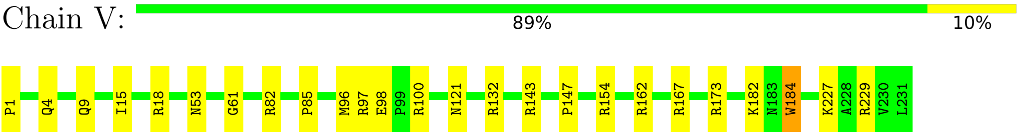
- Molecule 1: HIV-1 capsid protein

Chain U:



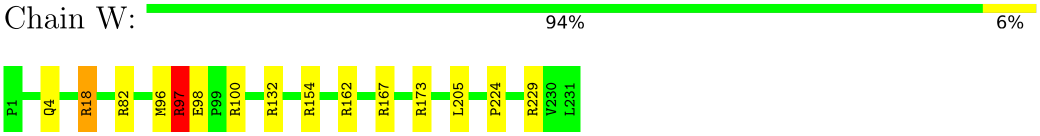
- Molecule 1: HIV-1 capsid protein

Chain V:



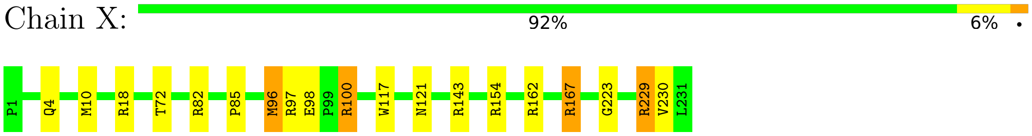
- Molecule 1: HIV-1 capsid protein

Chain W:



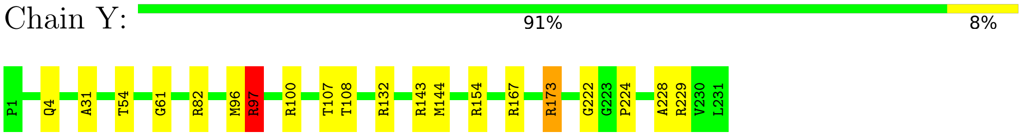
- Molecule 1: HIV-1 capsid protein

Chain X:



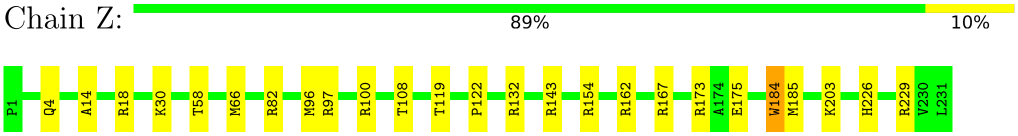
- Molecule 1: HIV-1 capsid protein

Chain Y:



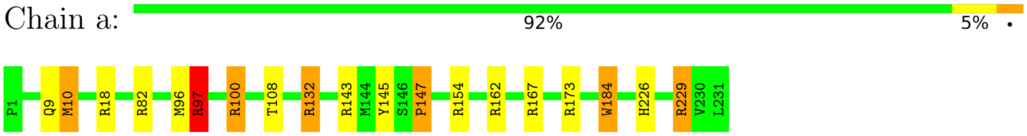
- Molecule 1: HIV-1 capsid protein

Chain Z:



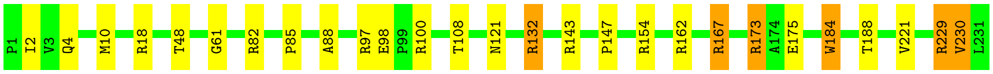
- Molecule 1: HIV-1 capsid protein

Chain a:



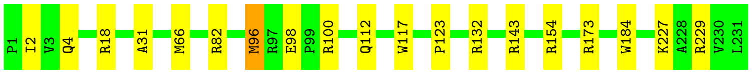
- Molecule 1: HIV-1 capsid protein

Chain b:



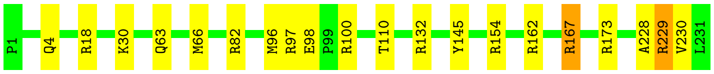
- Molecule 1: HIV-1 capsid protein

Chain c:



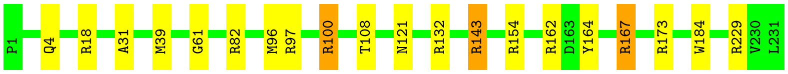
- Molecule 1: HIV-1 capsid protein

Chain d:



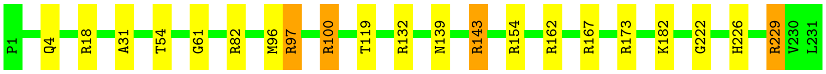
- Molecule 1: HIV-1 capsid protein

Chain e:



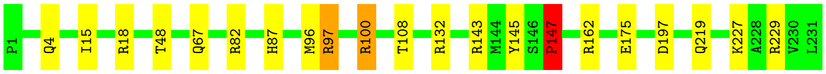
- Molecule 1: HIV-1 capsid protein

Chain f:



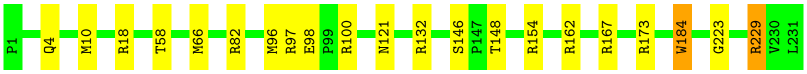
- Molecule 1: HIV-1 capsid protein

Chain g:



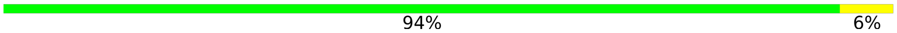
- Molecule 1: HIV-1 capsid protein

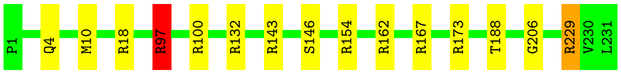
Chain h:



- Molecule 1: HIV-1 capsid protein

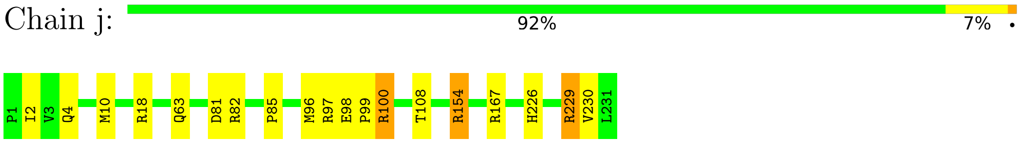
Chain i:





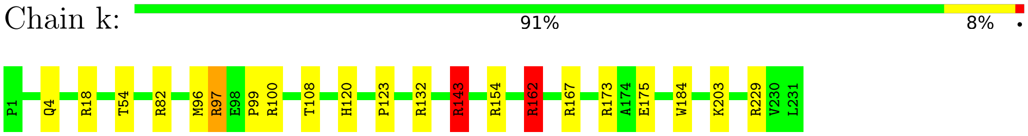
- Molecule 1: HIV-1 capsid protein

Chain j:



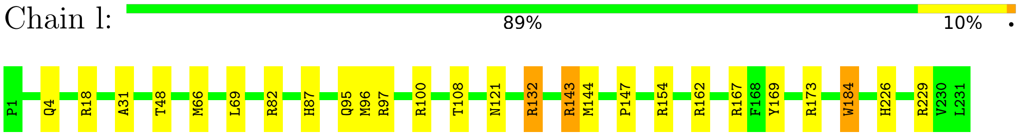
- Molecule 1: HIV-1 capsid protein

Chain k:



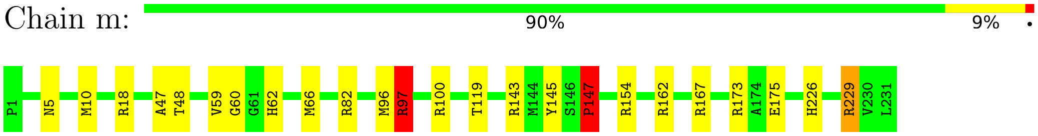
- Molecule 1: HIV-1 capsid protein

Chain l:



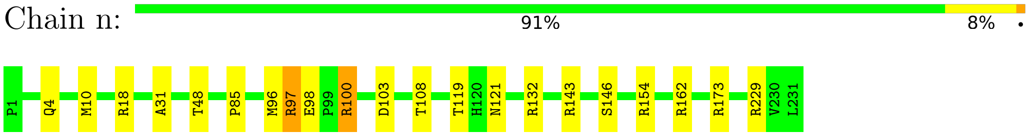
- Molecule 1: HIV-1 capsid protein

Chain m:



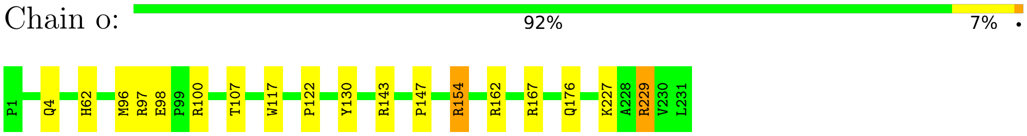
- Molecule 1: HIV-1 capsid protein

Chain n:



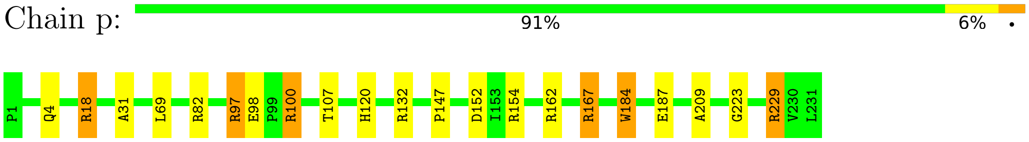
- Molecule 1: HIV-1 capsid protein

Chain o:



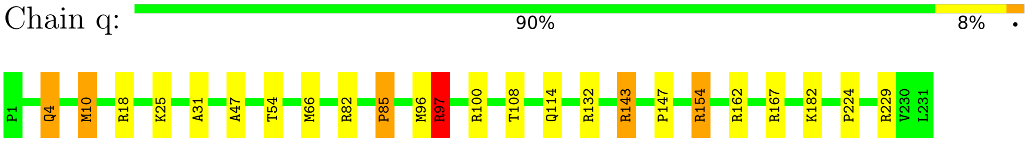
- Molecule 1: HIV-1 capsid protein

Chain p:



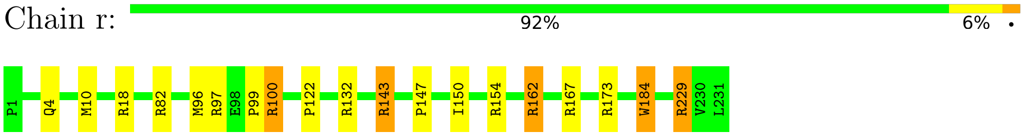
- Molecule 1: HIV-1 capsid protein

Chain q:



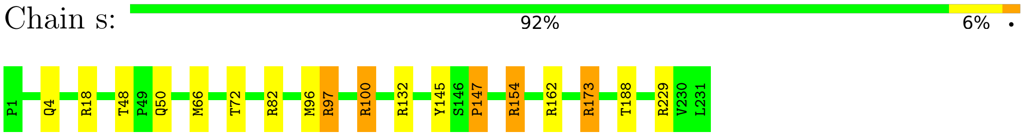
- Molecule 1: HIV-1 capsid protein

Chain r:



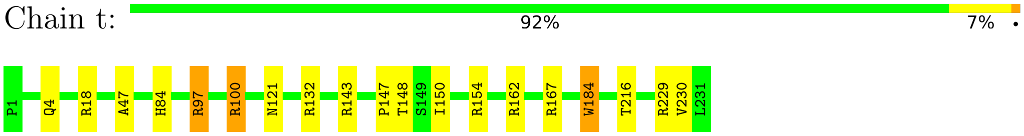
- Molecule 1: HIV-1 capsid protein

Chain s:



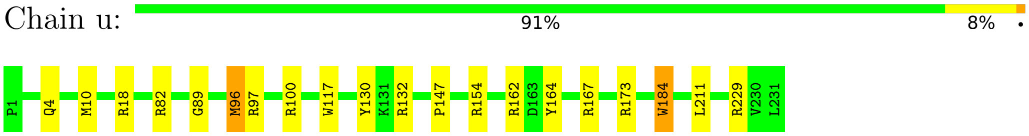
- Molecule 1: HIV-1 capsid protein

Chain t:



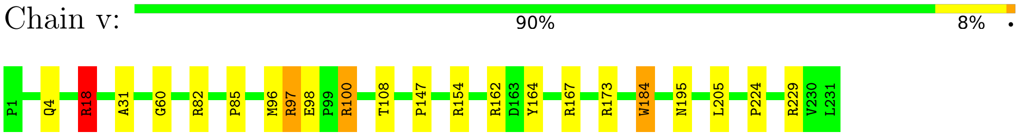
- Molecule 1: HIV-1 capsid protein

Chain u:



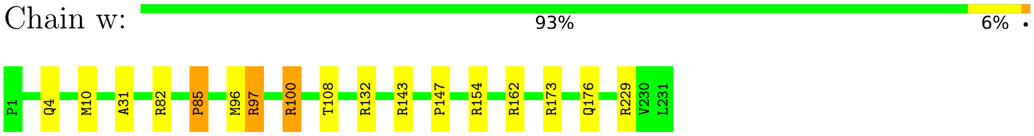
- Molecule 1: HIV-1 capsid protein

Chain v:



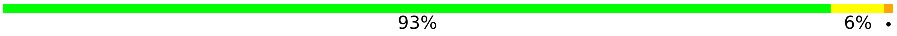
- Molecule 1: HIV-1 capsid protein

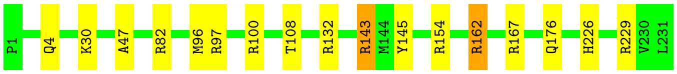
Chain w:



- Molecule 1: HIV-1 capsid protein

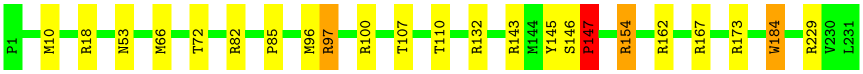
Chain x:





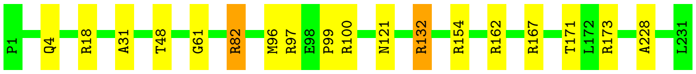
- Molecule 1: HIV-1 capsid protein

Chain y:



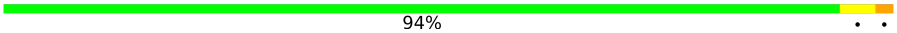
- Molecule 1: HIV-1 capsid protein

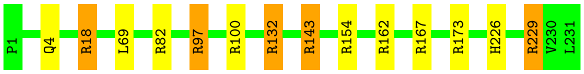
Chain z:



- Molecule 1: HIV-1 capsid protein

Chain 0:



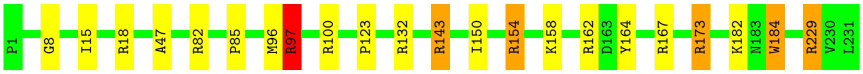


- Molecule 1: HIV-1 capsid protein

Chain 1:

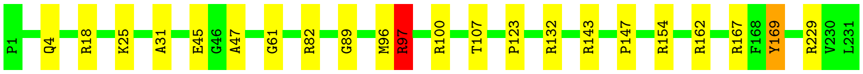
- Molecule 1: HIV-1 capsid protein

Chain 2:



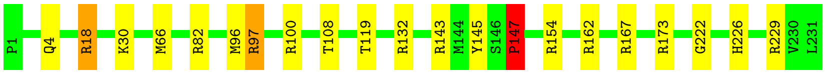
- Molecule 1: HIV-1 capsid protein

Chain 3:



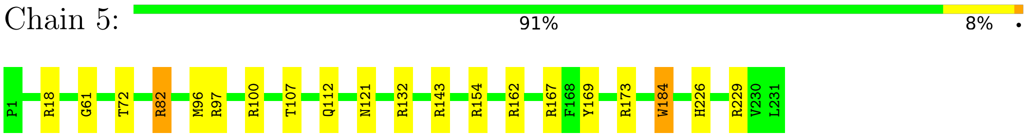
- Molecule 1: HIV-1 capsid protein

Chain 4:



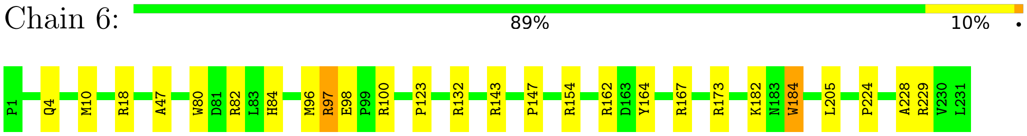
- Molecule 1: HIV-1 capsid protein

Chain 5:



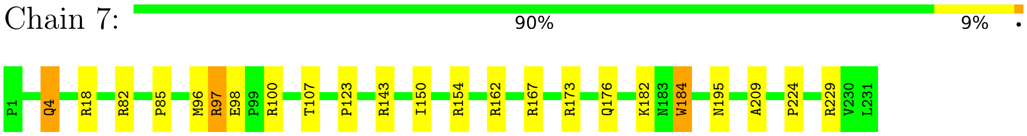
- Molecule 1: HIV-1 capsid protein

Chain 6:



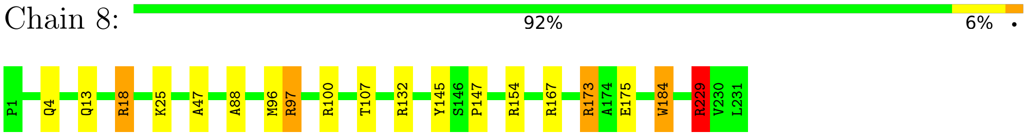
- Molecule 1: HIV-1 capsid protein

Chain 7:



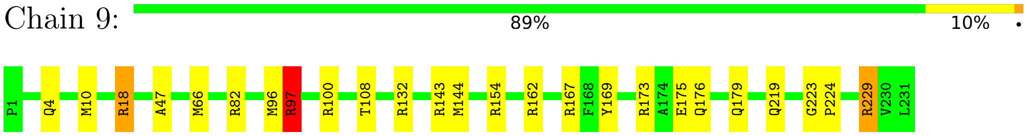
- Molecule 1: HIV-1 capsid protein

Chain 8:



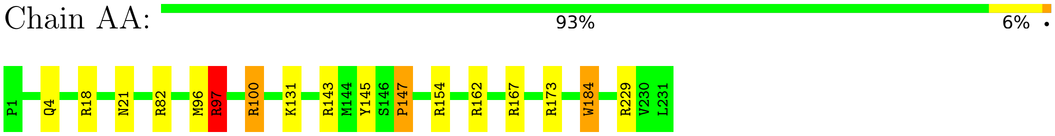
- Molecule 1: HIV-1 capsid protein

Chain 9:



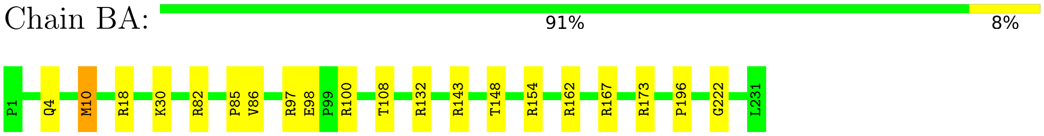
- Molecule 1: HIV-1 capsid protein

Chain AA:



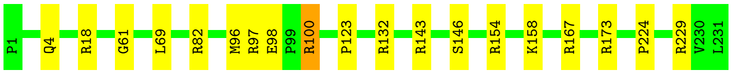
- Molecule 1: HIV-1 capsid protein

Chain BA:



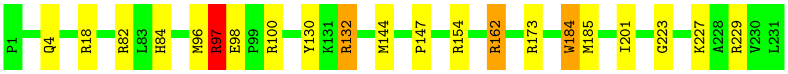
- Molecule 1: HIV-1 capsid protein

Chain CA:



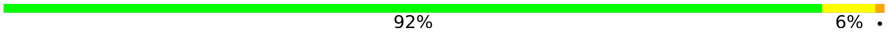
- Molecule 1: HIV-1 capsid protein

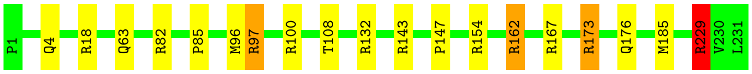
Chain DA:



- Molecule 1: HIV-1 capsid protein

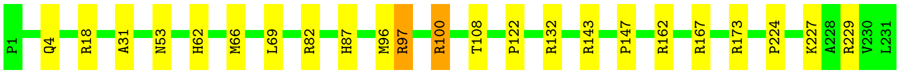
Chain EA:





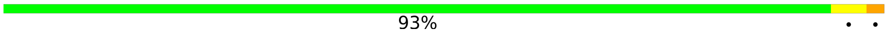
- Molecule 1: HIV-1 capsid protein

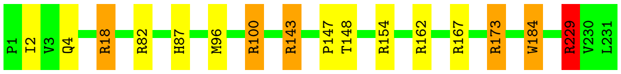
Chain FA:



- Molecule 1: HIV-1 capsid protein

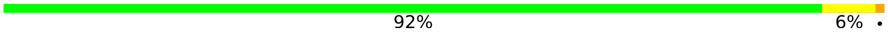
Chain GA:





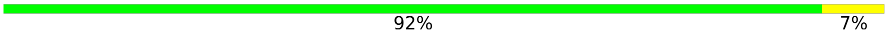
- Molecule 1: HIV-1 capsid protein

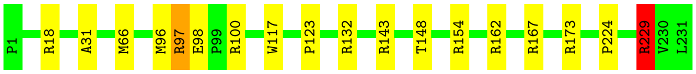
Chain HA:



- Molecule 1: HIV-1 capsid protein

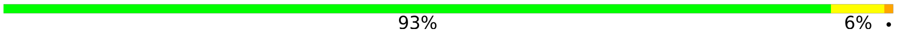
Chain IA:

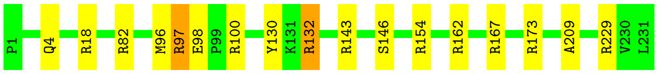




- Molecule 1: HIV-1 capsid protein

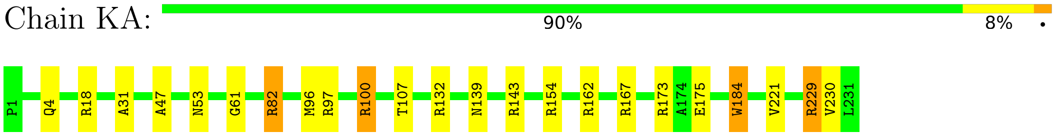
Chain JA:





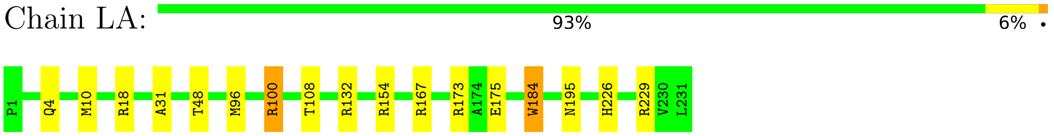
- Molecule 1: HIV-1 capsid protein

Chain KA:



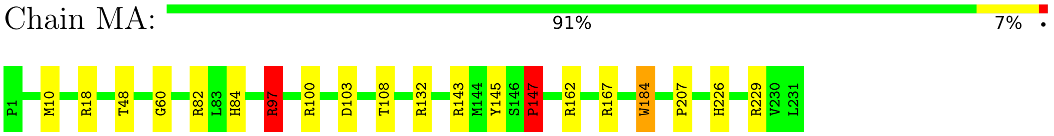
- Molecule 1: HIV-1 capsid protein

Chain LA:



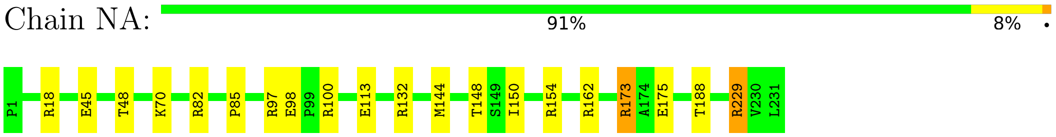
- Molecule 1: HIV-1 capsid protein

Chain MA:



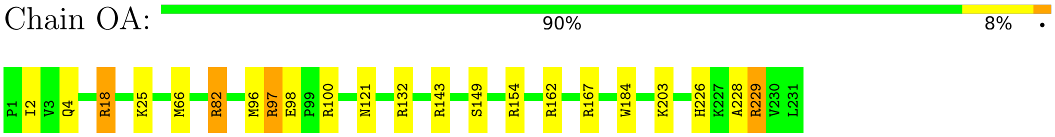
- Molecule 1: HIV-1 capsid protein

Chain NA:



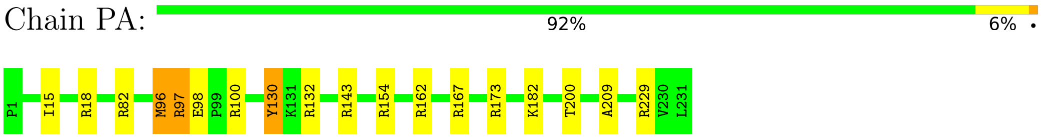
- Molecule 1: HIV-1 capsid protein

Chain OA:



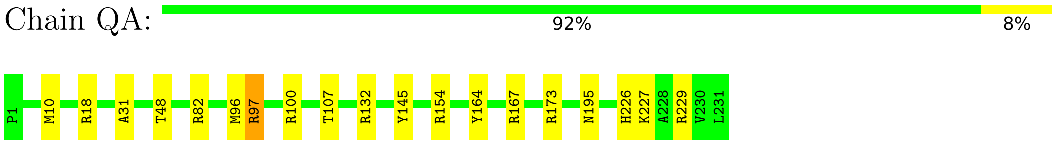
- Molecule 1: HIV-1 capsid protein

Chain PA:



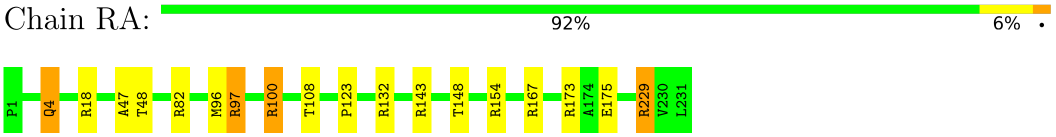
- Molecule 1: HIV-1 capsid protein

Chain QA:



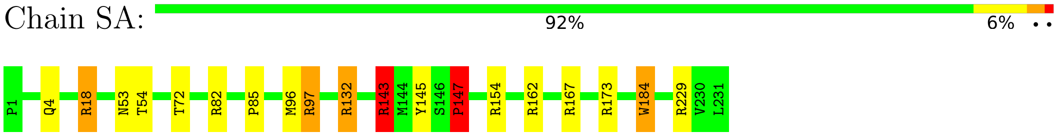
- Molecule 1: HIV-1 capsid protein

Chain RA:



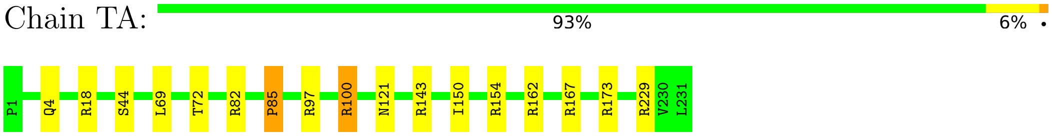
- Molecule 1: HIV-1 capsid protein

Chain SA:



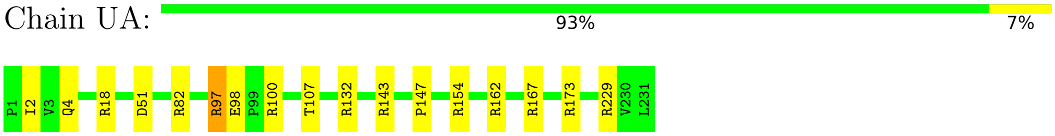
- Molecule 1: HIV-1 capsid protein

Chain TA:



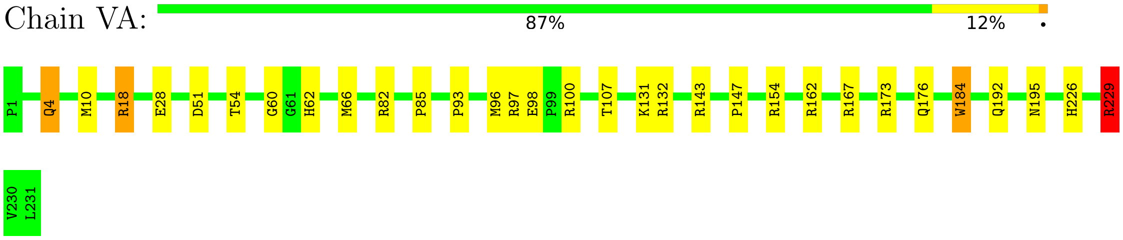
- Molecule 1: HIV-1 capsid protein

Chain UA:



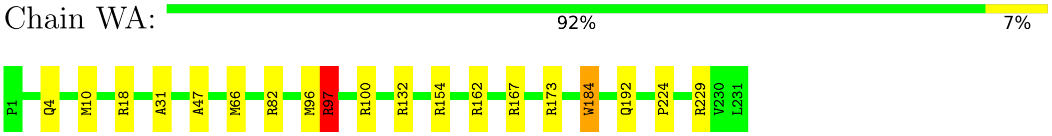
- Molecule 1: HIV-1 capsid protein

Chain VA:



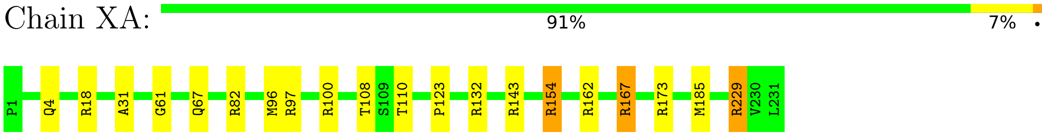
- Molecule 1: HIV-1 capsid protein

Chain WA:



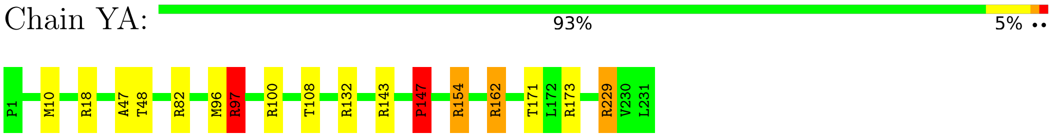
- Molecule 1: HIV-1 capsid protein

Chain XA:



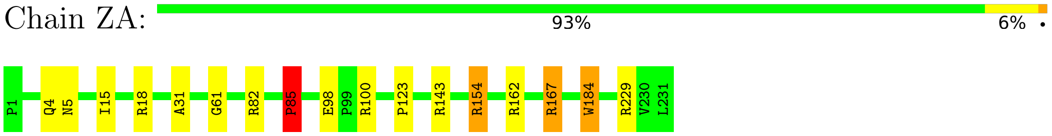
- Molecule 1: HIV-1 capsid protein

Chain YA:



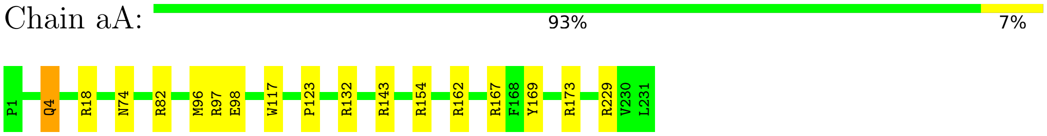
- Molecule 1: HIV-1 capsid protein

Chain ZA:



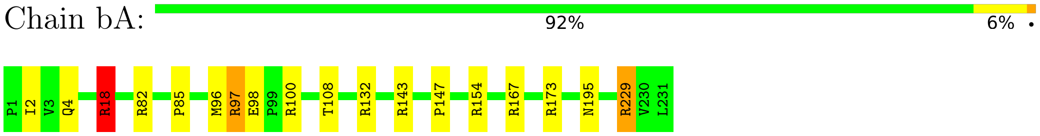
- Molecule 1: HIV-1 capsid protein

Chain aA:



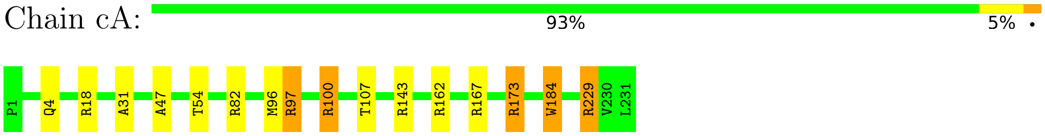
- Molecule 1: HIV-1 capsid protein

Chain bA:



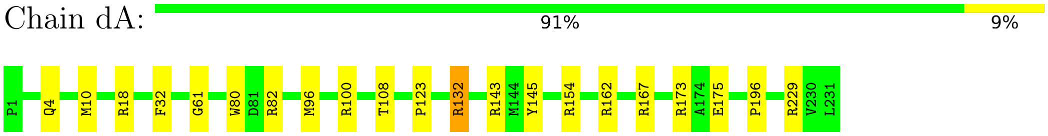
- Molecule 1: HIV-1 capsid protein

Chain cA:



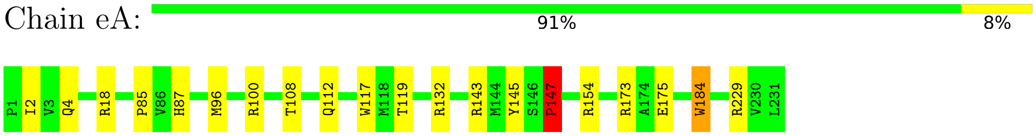
- Molecule 1: HIV-1 capsid protein

Chain dA:



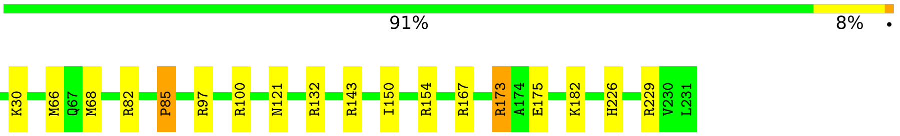
- Molecule 1: HIV-1 capsid protein

Chain eA:



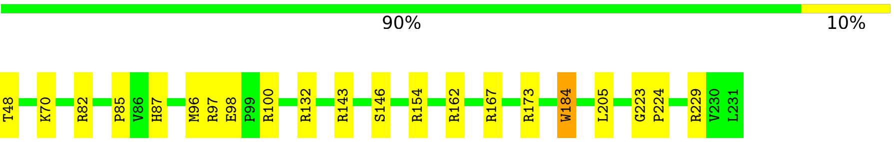
- Molecule 1: HIV-1 capsid protein

Chain fA:



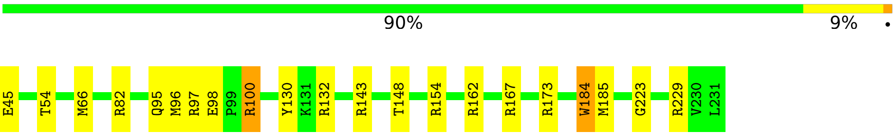
- Molecule 1: HIV-1 capsid protein

Chain gA:



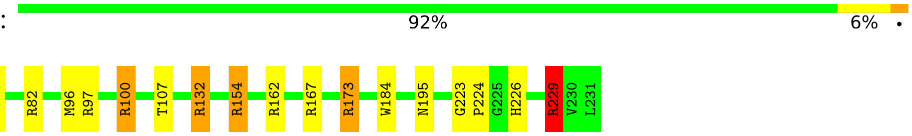
- Molecule 1: HIV-1 capsid protein

Chain hA:



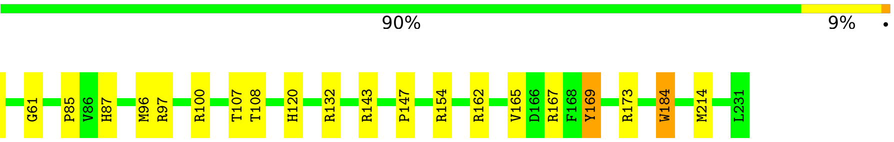
- Molecule 1: HIV-1 capsid protein

Chain iA:



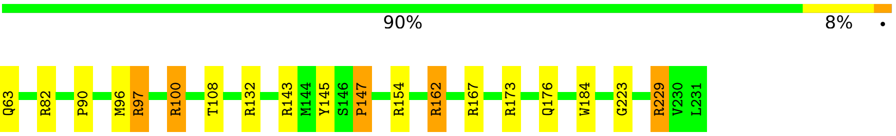
- Molecule 1: HIV-1 capsid protein

Chain jA:



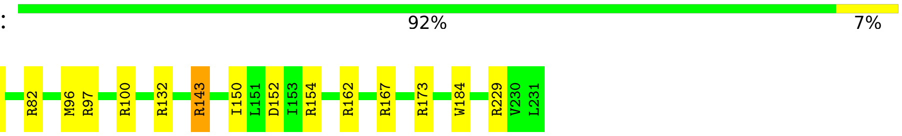
- Molecule 1: HIV-1 capsid protein

Chain kA:



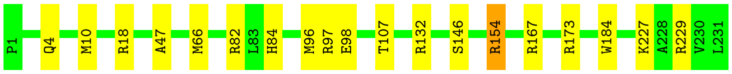
- Molecule 1: HIV-1 capsid protein

Chain lA:



- Molecule 1: HIV-1 capsid protein

Chain mA:

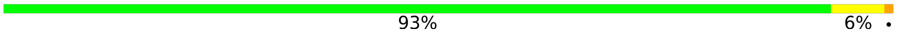


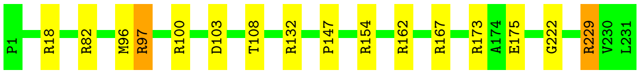
- Molecule 1: HIV-1 capsid protein

Chain nA:

- Molecule 1: HIV-1 capsid protein

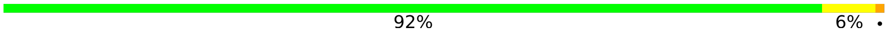
Chain oA:

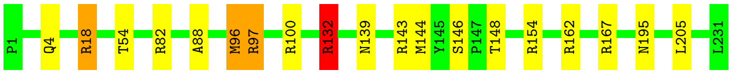




- Molecule 1: HIV-1 capsid protein

Chain pA:



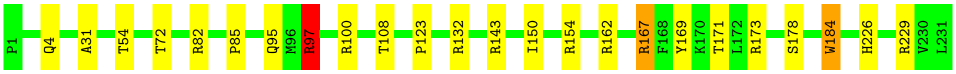


- Molecule 1: HIV-1 capsid protein

Chain qA:

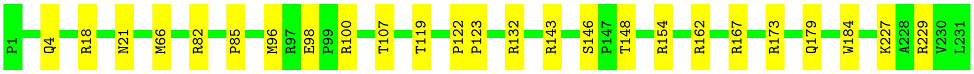
- Molecule 1: HIV-1 capsid protein

Chain rA:



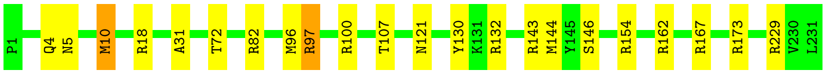
- Molecule 1: HIV-1 capsid protein

Chain sA:



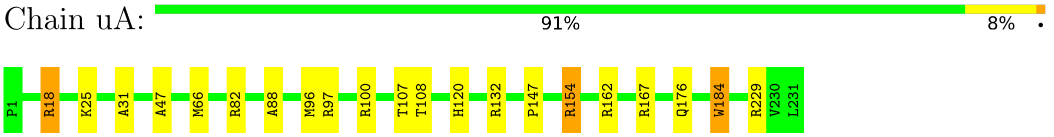
- Molecule 1: HIV-1 capsid protein

Chain tA:



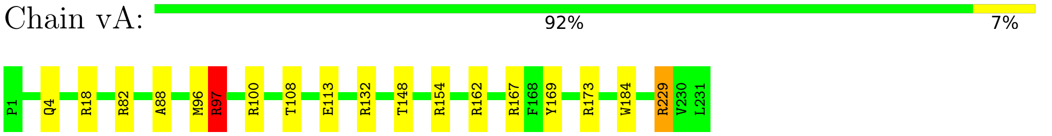
- Molecule 1: HIV-1 capsid protein

Chain uA:



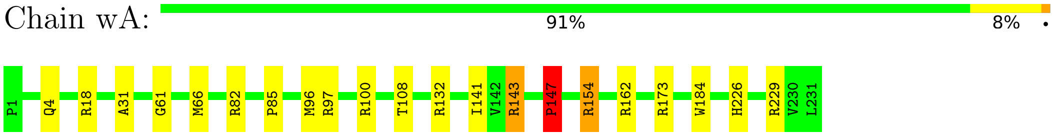
- Molecule 1: HIV-1 capsid protein

Chain vA:



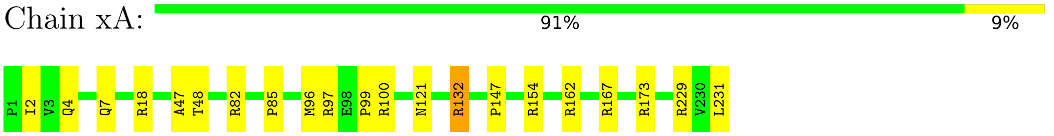
- Molecule 1: HIV-1 capsid protein

Chain wA:



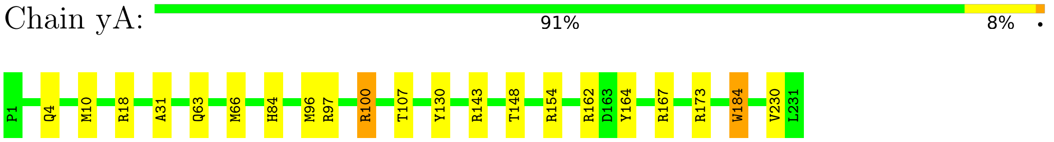
- Molecule 1: HIV-1 capsid protein

Chain xA:



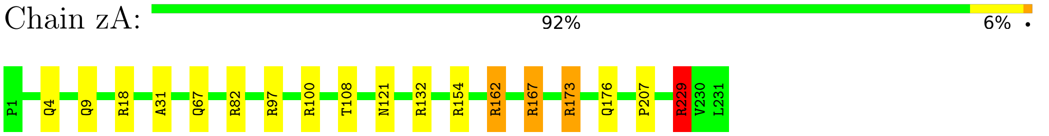
- Molecule 1: HIV-1 capsid protein

Chain yA:



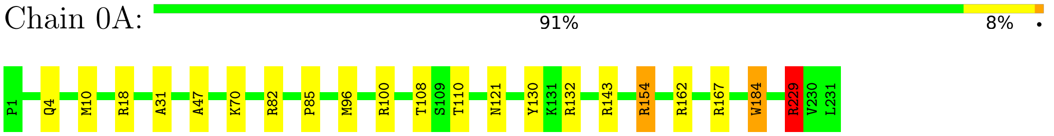
- Molecule 1: HIV-1 capsid protein

Chain zA:



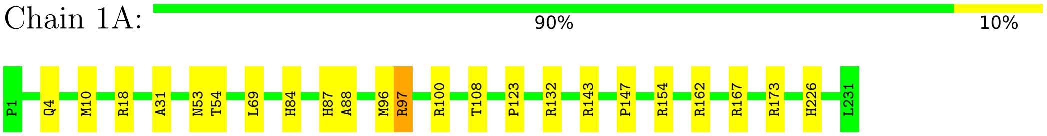
- Molecule 1: HIV-1 capsid protein

Chain 0A:



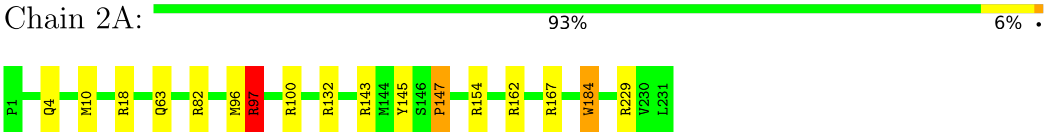
- Molecule 1: HIV-1 capsid protein

Chain 1A:



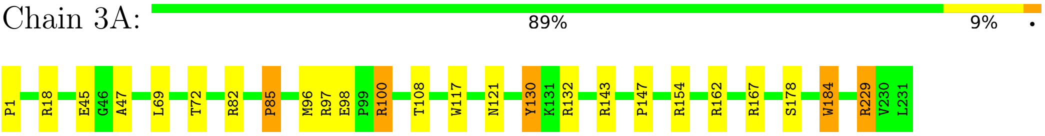
- Molecule 1: HIV-1 capsid protein

Chain 2A:



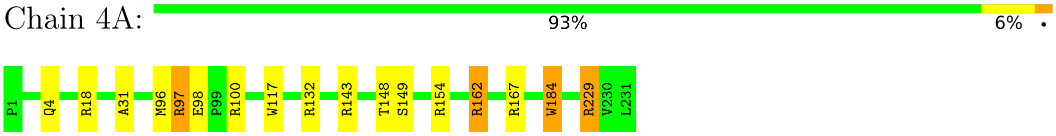
- Molecule 1: HIV-1 capsid protein

Chain 3A:



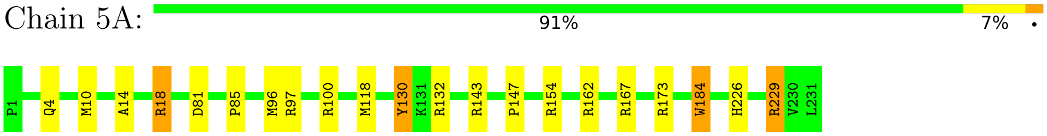
- Molecule 1: HIV-1 capsid protein

Chain 4A:



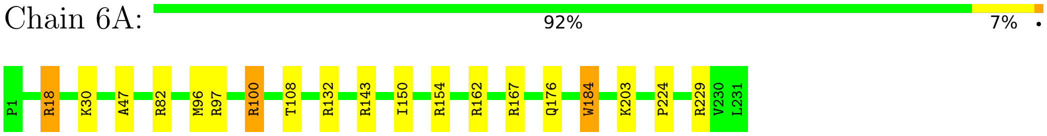
- Molecule 1: HIV-1 capsid protein

Chain 5A:



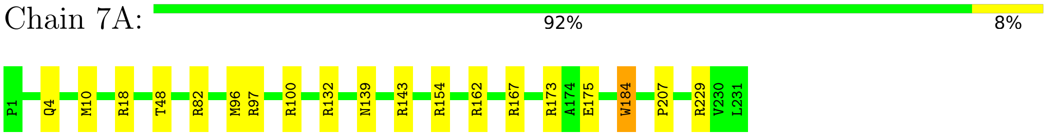
- Molecule 1: HIV-1 capsid protein

Chain 6A:



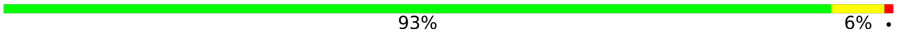
- Molecule 1: HIV-1 capsid protein

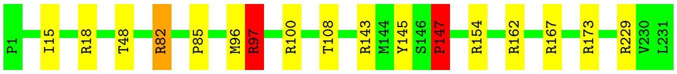
Chain 7A:



- Molecule 1: HIV-1 capsid protein

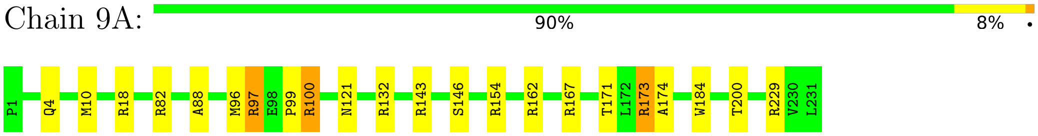
Chain 8A:





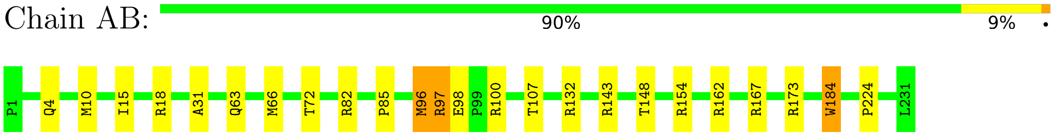
- Molecule 1: HIV-1 capsid protein

Chain 9A:



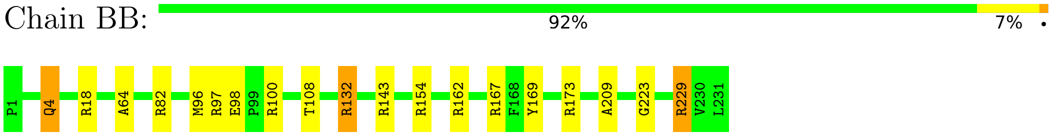
- Molecule 1: HIV-1 capsid protein

Chain AB:



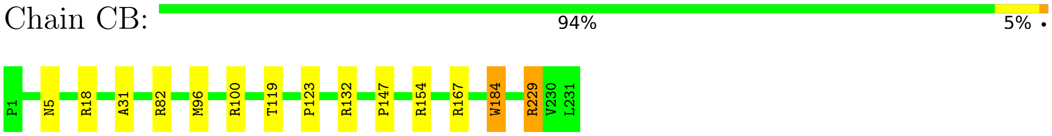
- Molecule 1: HIV-1 capsid protein

Chain BB:



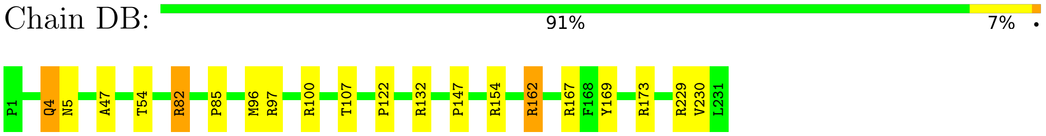
- Molecule 1: HIV-1 capsid protein

Chain CB:



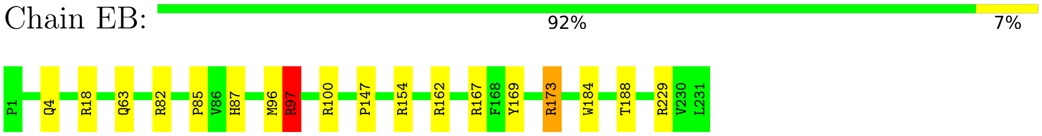
- Molecule 1: HIV-1 capsid protein

Chain DB:



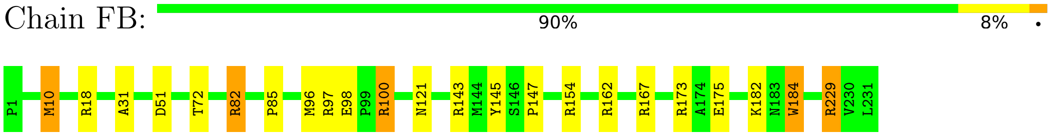
- Molecule 1: HIV-1 capsid protein

Chain EB:



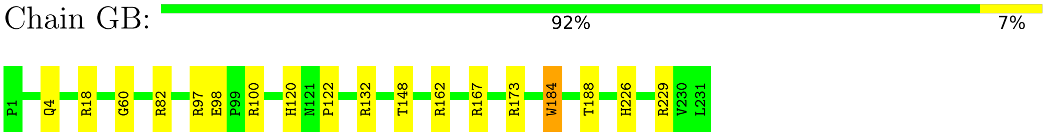
- Molecule 1: HIV-1 capsid protein

Chain FB:



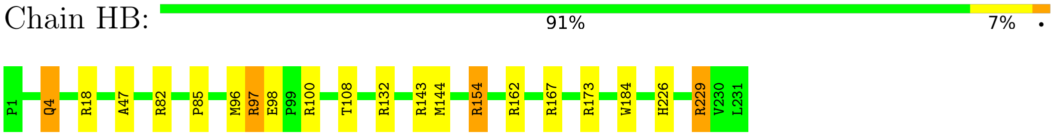
- Molecule 1: HIV-1 capsid protein

Chain GB:



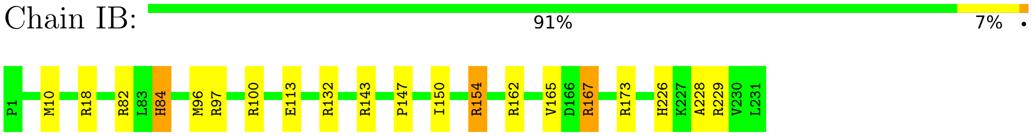
- Molecule 1: HIV-1 capsid protein

Chain HB:



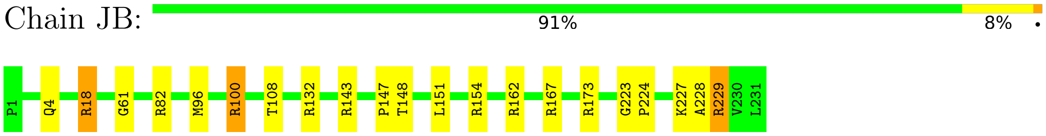
- Molecule 1: HIV-1 capsid protein

Chain IB:



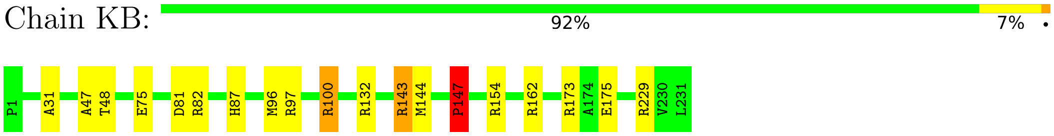
- Molecule 1: HIV-1 capsid protein

Chain JB:



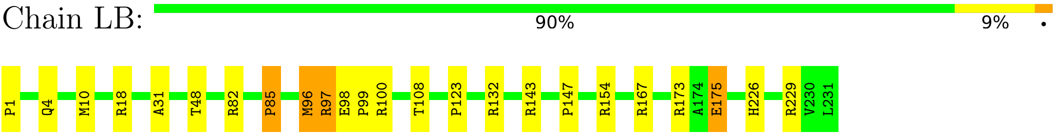
- Molecule 1: HIV-1 capsid protein

Chain KB:



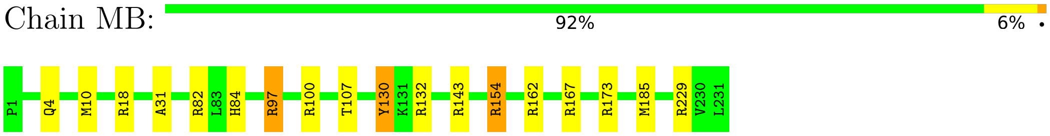
- Molecule 1: HIV-1 capsid protein

Chain LB:

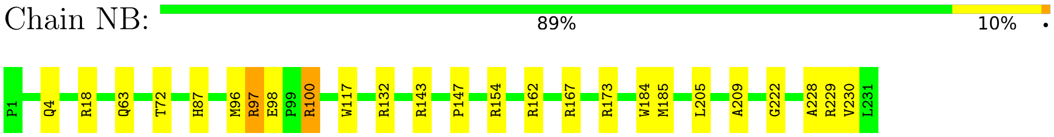


- Molecule 1: HIV-1 capsid protein

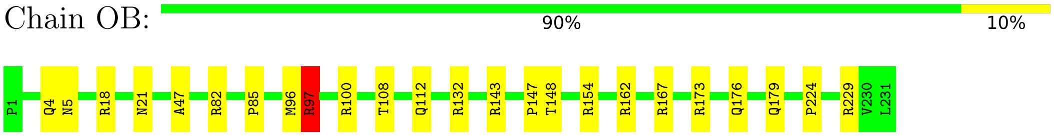
Chain MB:



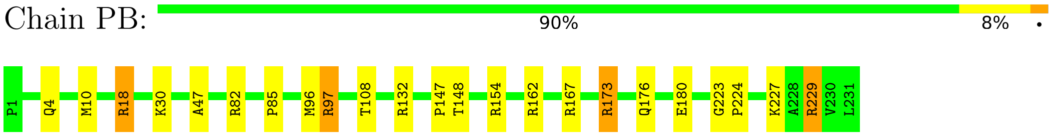
- Molecule 1: HIV-1 capsid protein



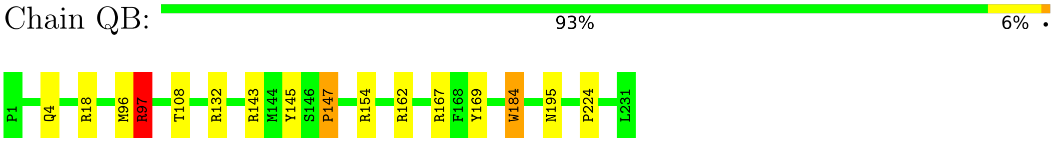
• Molecule 1: HIV-1 capsid protein



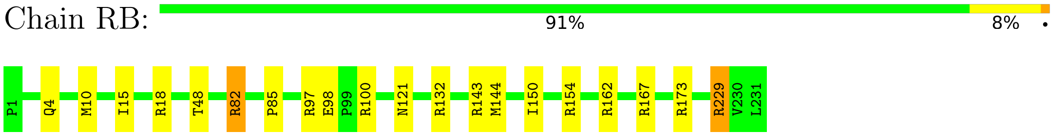
• Molecule 1: HIV-1 capsid protein



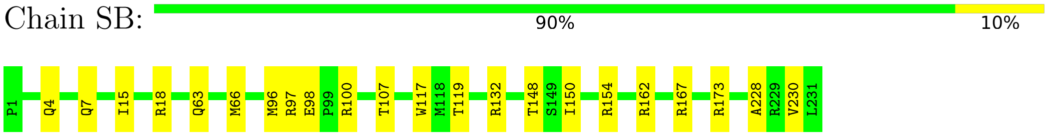
• Molecule 1: HIV-1 capsid protein



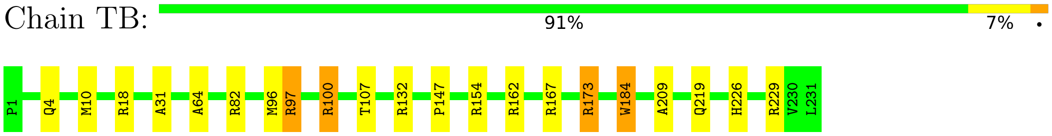
• Molecule 1: HIV-1 capsid protein



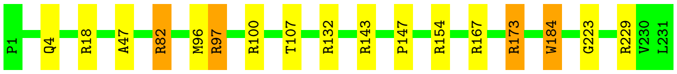
• Molecule 1: HIV-1 capsid protein



• Molecule 1: HIV-1 capsid protein

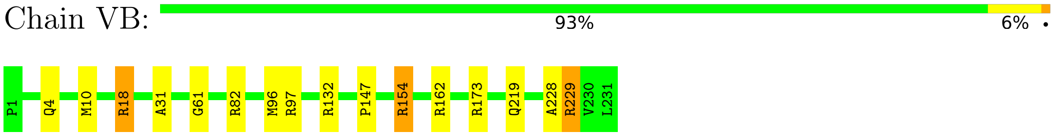


• Molecule 1: HIV-1 capsid protein



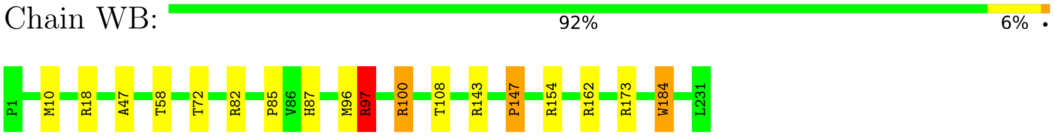
- Molecule 1: HIV-1 capsid protein

Chain VB:



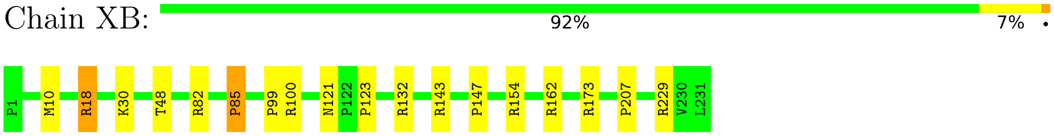
- Molecule 1: HIV-1 capsid protein

Chain WB:



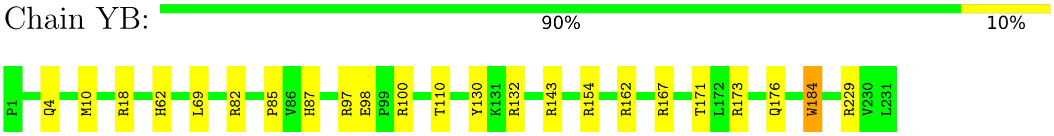
- Molecule 1: HIV-1 capsid protein

Chain XB:



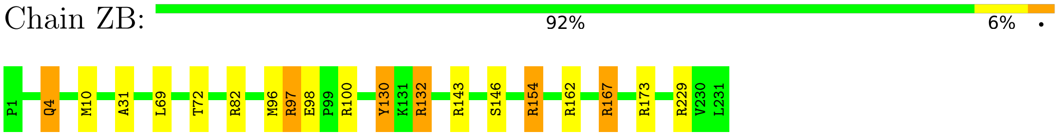
- Molecule 1: HIV-1 capsid protein

Chain YB:



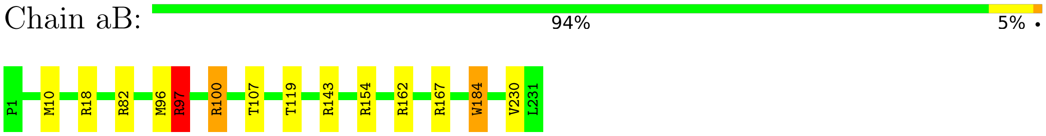
- Molecule 1: HIV-1 capsid protein

Chain ZB:



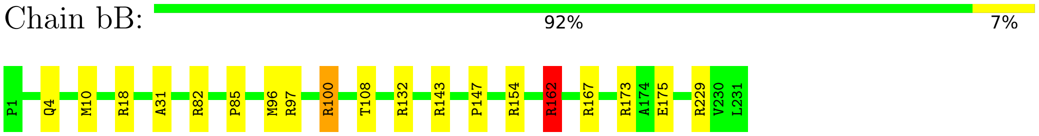
- Molecule 1: HIV-1 capsid protein

Chain aB:



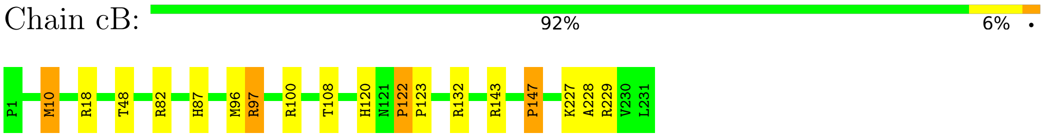
- Molecule 1: HIV-1 capsid protein

Chain bB:



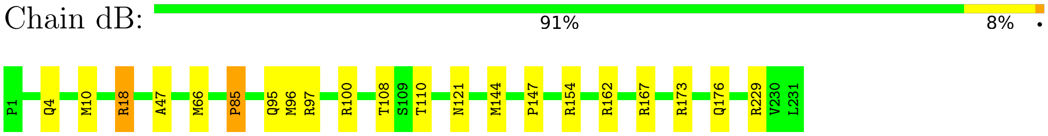
- Molecule 1: HIV-1 capsid protein

Chain cB:



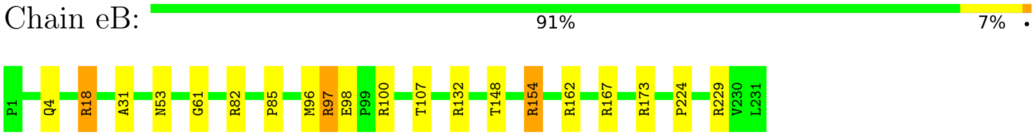
- Molecule 1: HIV-1 capsid protein

Chain dB:



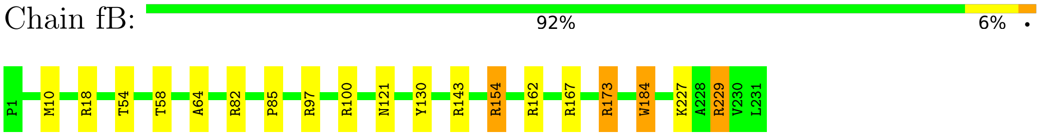
- Molecule 1: HIV-1 capsid protein

Chain eB:



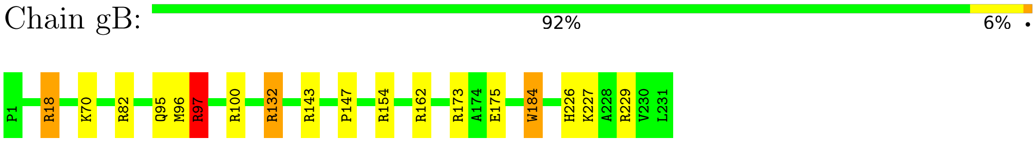
- Molecule 1: HIV-1 capsid protein

Chain fB:



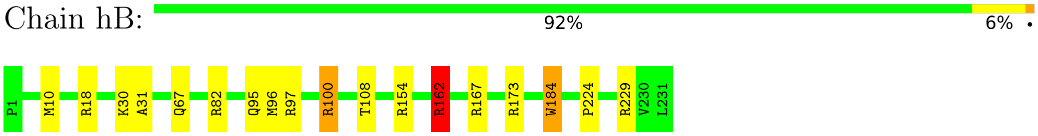
- Molecule 1: HIV-1 capsid protein

Chain gB:



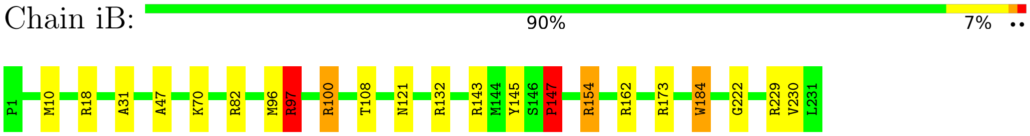
- Molecule 1: HIV-1 capsid protein

Chain hB:



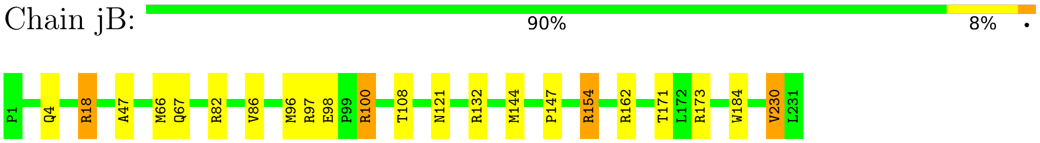
- Molecule 1: HIV-1 capsid protein

Chain iB:



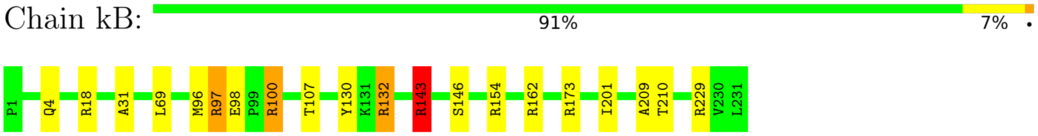
- Molecule 1: HIV-1 capsid protein

Chain jB:



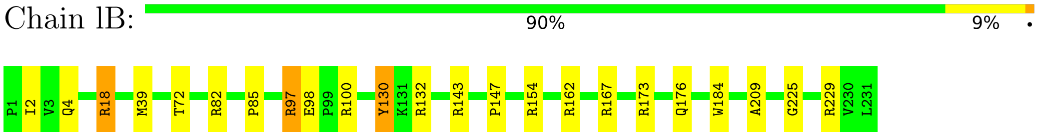
- Molecule 1: HIV-1 capsid protein

Chain kB:



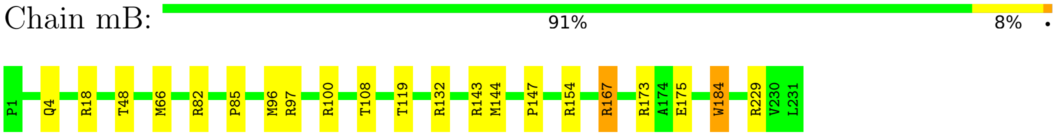
- Molecule 1: HIV-1 capsid protein

Chain lB:



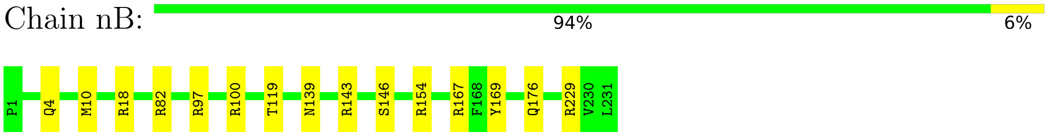
- Molecule 1: HIV-1 capsid protein

Chain mB:



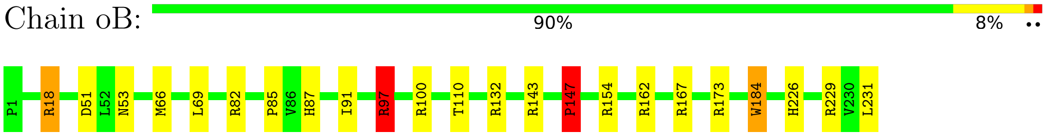
- Molecule 1: HIV-1 capsid protein

Chain nB:



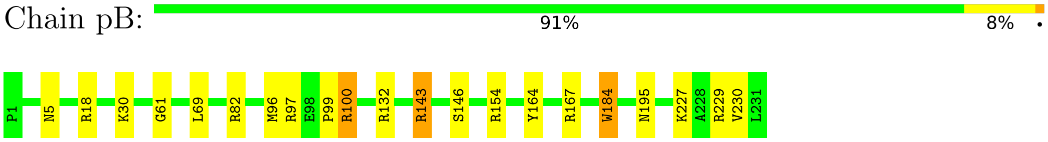
- Molecule 1: HIV-1 capsid protein

Chain oB:



- Molecule 1: HIV-1 capsid protein

Chain pB:

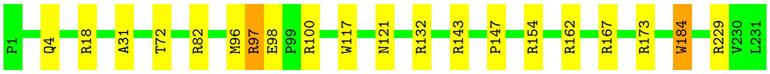


- Molecule 1: HIV-1 capsid protein

Chain qB:

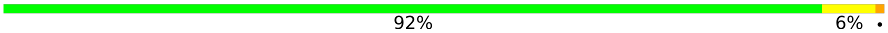
- Molecule 1: HIV-1 capsid protein

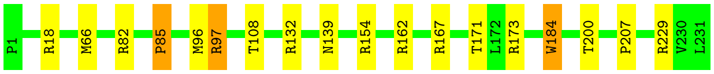
Chain rB:



- Molecule 1: HIV-1 capsid protein

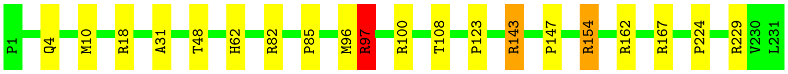
Chain sB:





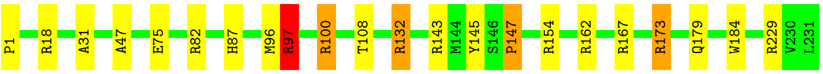
- Molecule 1: HIV-1 capsid protein

Chain tB:



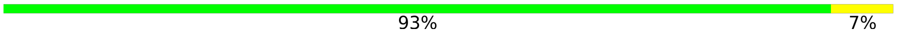
- Molecule 1: HIV-1 capsid protein

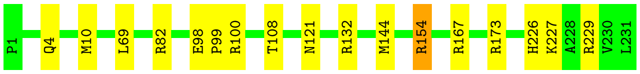
Chain uB:



- Molecule 1: HIV-1 capsid protein

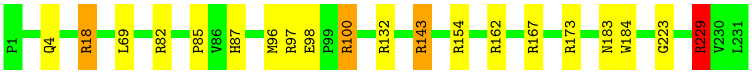
Chain vB:





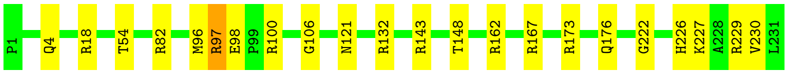
- Molecule 1: HIV-1 capsid protein

Chain wB:

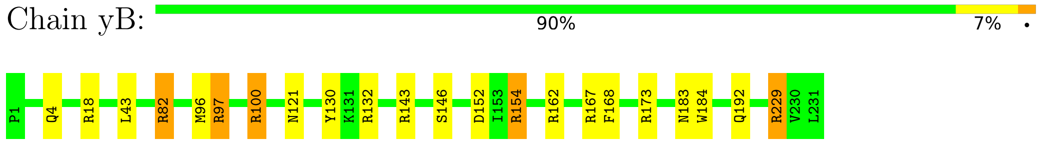


- Molecule 1: HIV-1 capsid protein

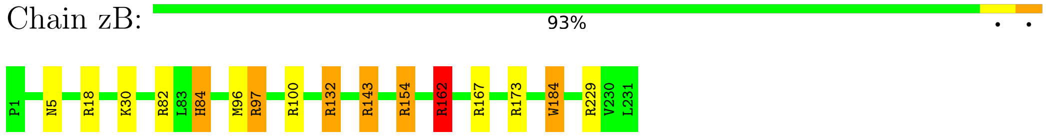
Chain xB:



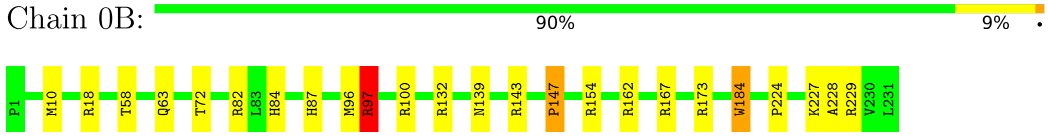
- Molecule 1: HIV-1 capsid protein



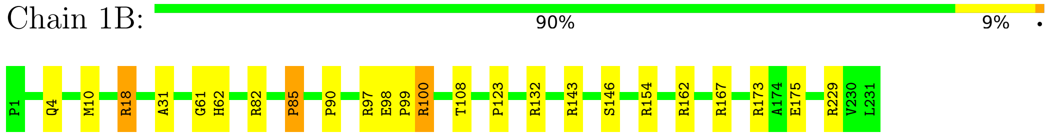
- Molecule 1: HIV-1 capsid protein



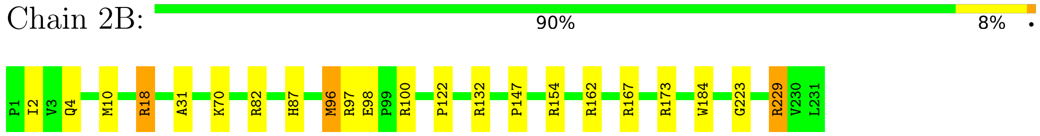
- Molecule 1: HIV-1 capsid protein



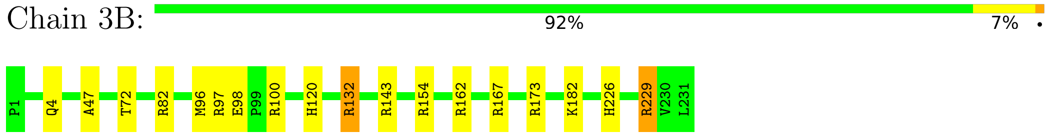
- Molecule 1: HIV-1 capsid protein



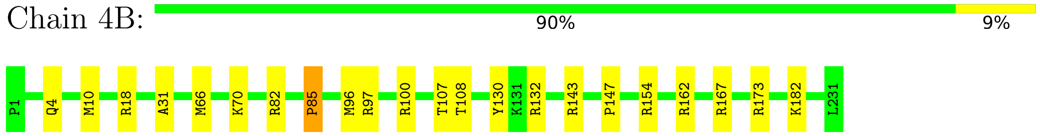
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

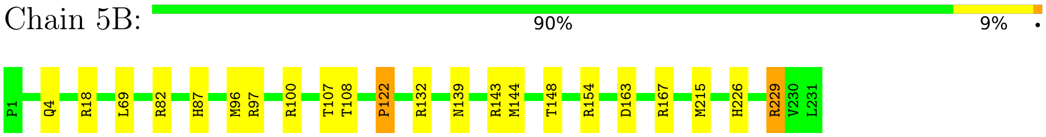


- Molecule 1: HIV-1 capsid protein



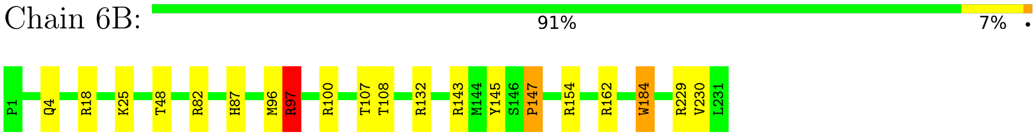
- Molecule 1: HIV-1 capsid protein

Chain 5B:



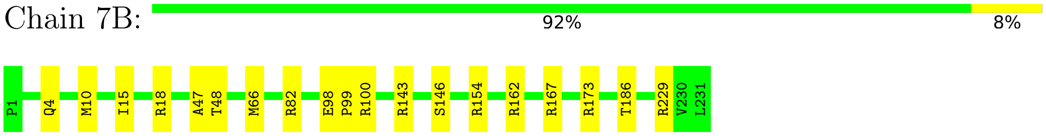
- Molecule 1: HIV-1 capsid protein

Chain 6B:



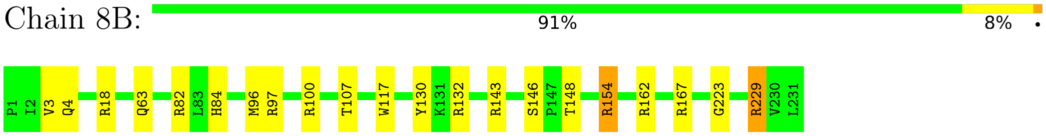
- Molecule 1: HIV-1 capsid protein

Chain 7B:



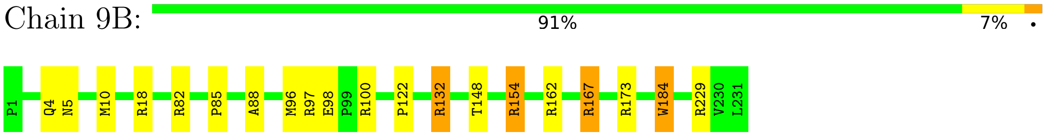
- Molecule 1: HIV-1 capsid protein

Chain 8B:



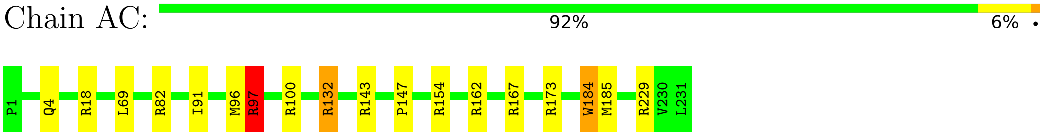
- Molecule 1: HIV-1 capsid protein

Chain 9B:



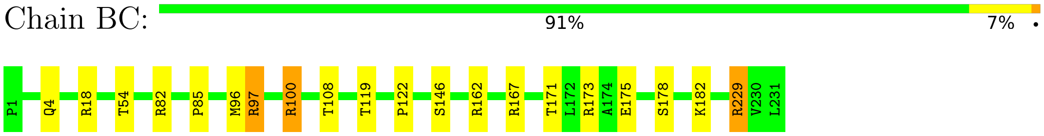
- Molecule 1: HIV-1 capsid protein

Chain AC:



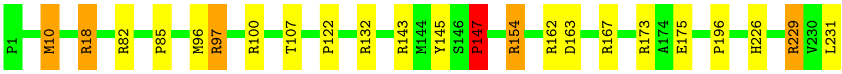
- Molecule 1: HIV-1 capsid protein

Chain BC:



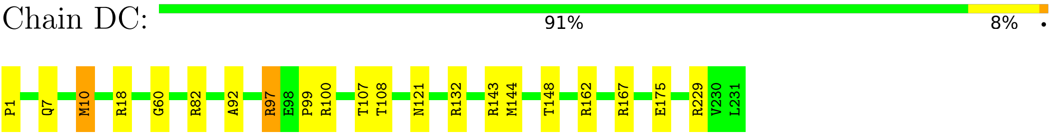
- Molecule 1: HIV-1 capsid protein

Chain CC:



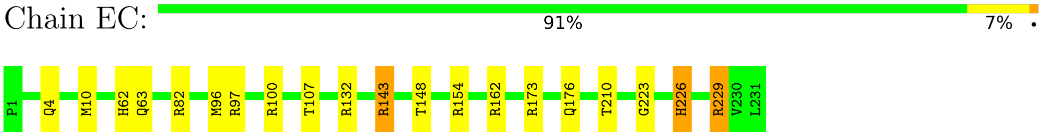
- Molecule 1: HIV-1 capsid protein

Chain DC:



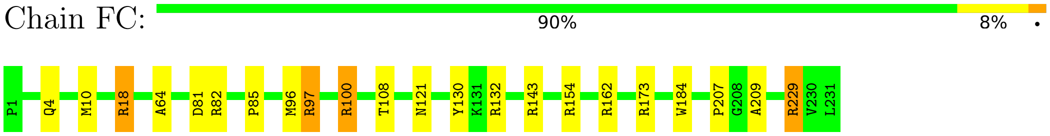
- Molecule 1: HIV-1 capsid protein

Chain EC:



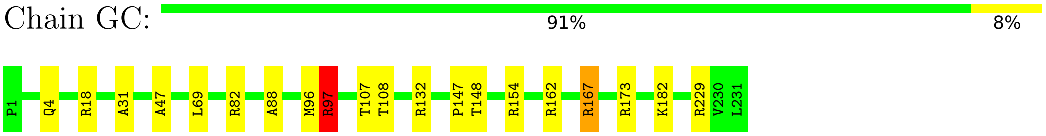
- Molecule 1: HIV-1 capsid protein

Chain FC:



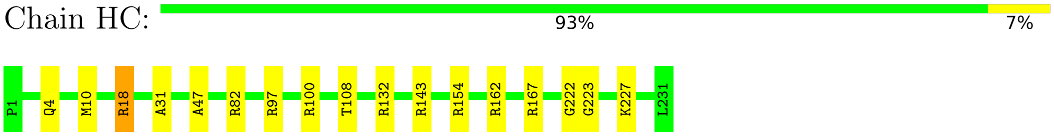
- Molecule 1: HIV-1 capsid protein

Chain GC:



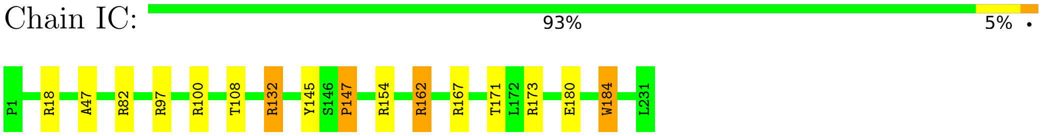
- Molecule 1: HIV-1 capsid protein

Chain HC:



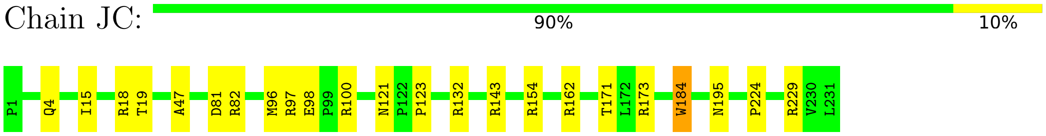
- Molecule 1: HIV-1 capsid protein

Chain IC:



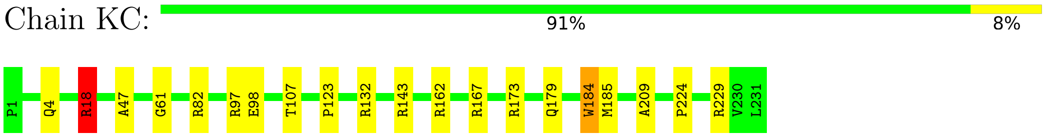
- Molecule 1: HIV-1 capsid protein

Chain JC:



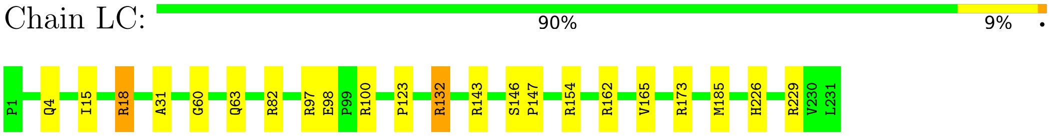
- Molecule 1: HIV-1 capsid protein

Chain KC:



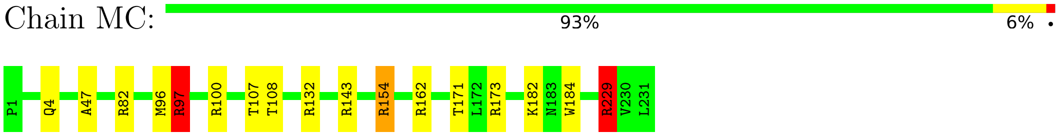
- Molecule 1: HIV-1 capsid protein

Chain LC:



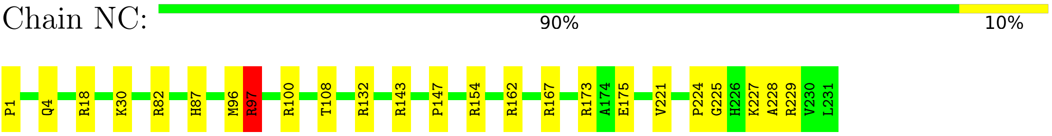
- Molecule 1: HIV-1 capsid protein

Chain MC:



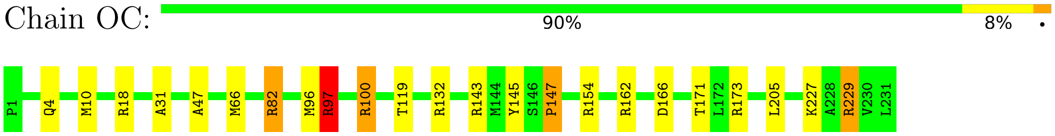
- Molecule 1: HIV-1 capsid protein

Chain NC:



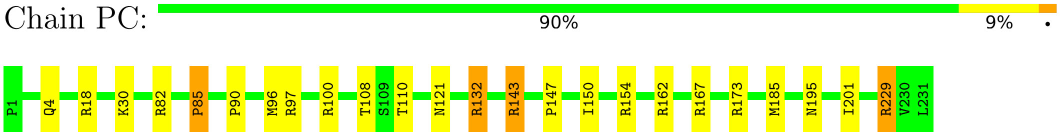
- Molecule 1: HIV-1 capsid protein

Chain OC:



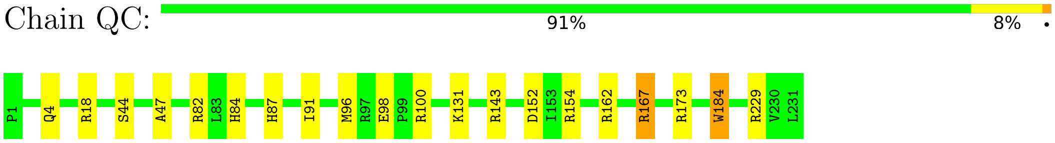
- Molecule 1: HIV-1 capsid protein

Chain PC:



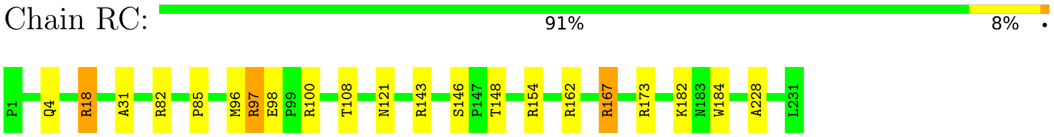
- Molecule 1: HIV-1 capsid protein

Chain QC:



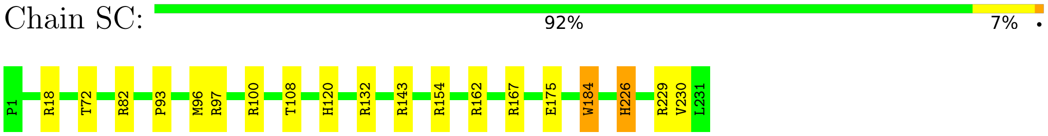
- Molecule 1: HIV-1 capsid protein

Chain RC:



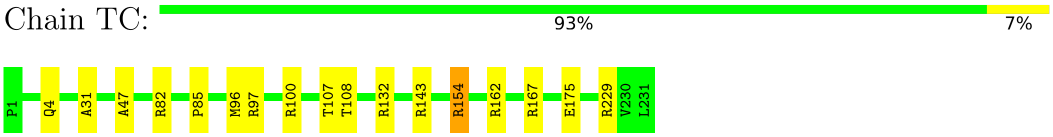
- Molecule 1: HIV-1 capsid protein

Chain SC:



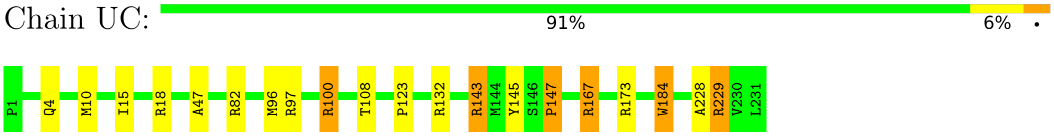
- Molecule 1: HIV-1 capsid protein

Chain TC:



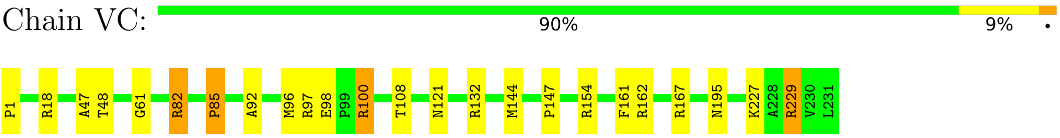
- Molecule 1: HIV-1 capsid protein

Chain UC:



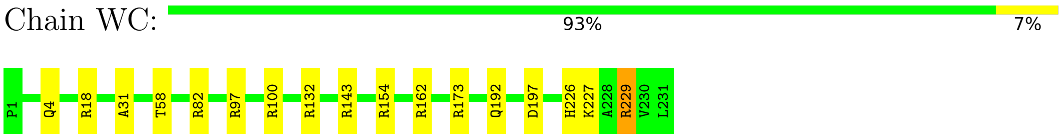
- Molecule 1: HIV-1 capsid protein

Chain VC:



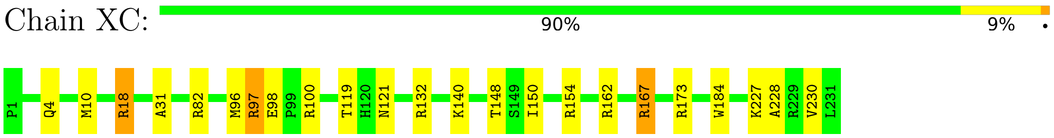
- Molecule 1: HIV-1 capsid protein

Chain WC:



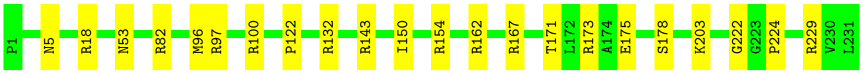
- Molecule 1: HIV-1 capsid protein

Chain XC:



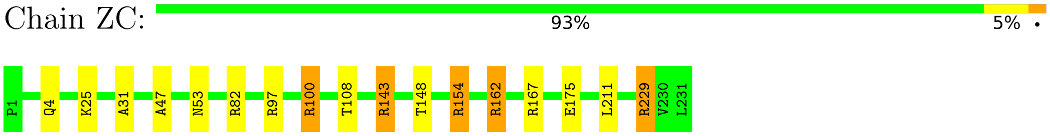
- Molecule 1: HIV-1 capsid protein

Chain YC:



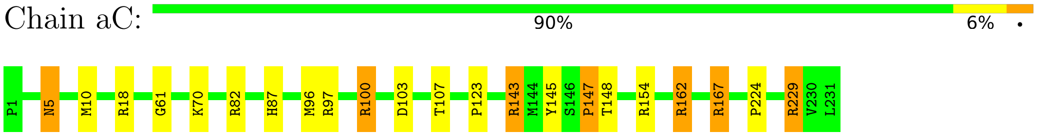
- Molecule 1: HIV-1 capsid protein

Chain ZC:



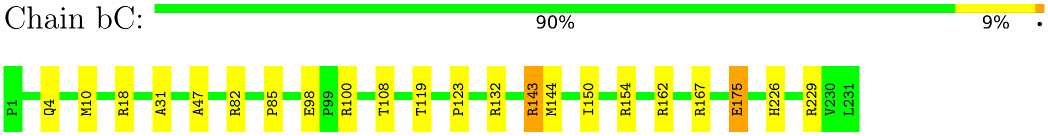
- Molecule 1: HIV-1 capsid protein

Chain aC:



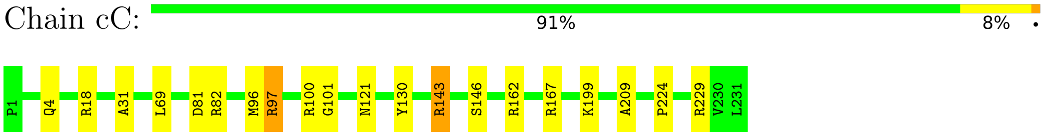
- Molecule 1: HIV-1 capsid protein

Chain bC:



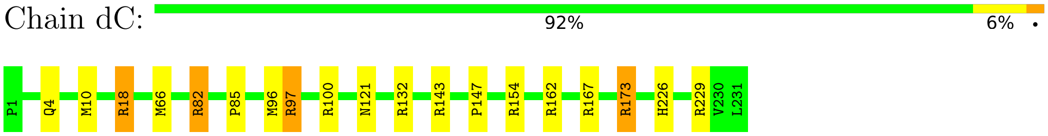
- Molecule 1: HIV-1 capsid protein

Chain cC:



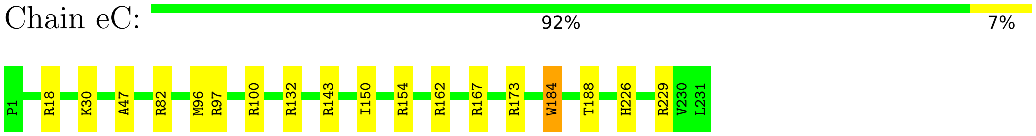
- Molecule 1: HIV-1 capsid protein

Chain dC:



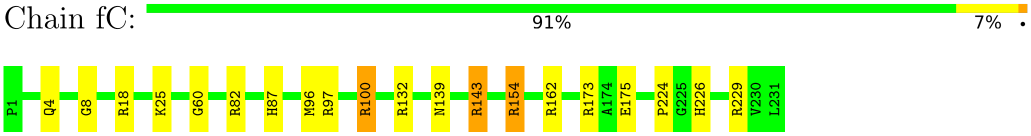
- Molecule 1: HIV-1 capsid protein

Chain eC:



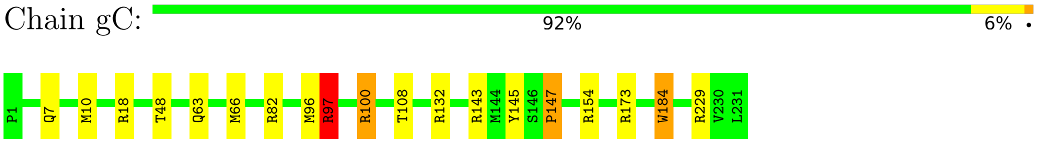
- Molecule 1: HIV-1 capsid protein

Chain fC:



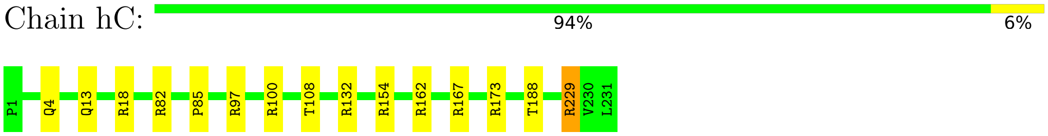
- Molecule 1: HIV-1 capsid protein

Chain gC:



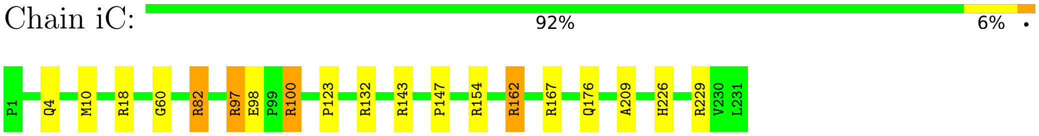
- Molecule 1: HIV-1 capsid protein

Chain hC:



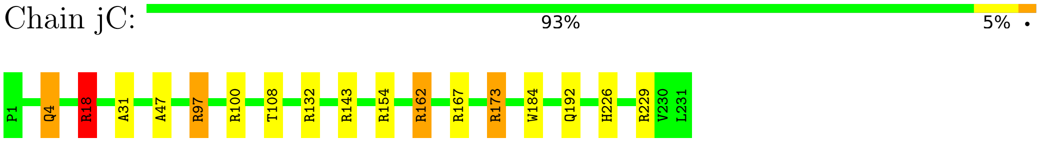
- Molecule 1: HIV-1 capsid protein

Chain iC:



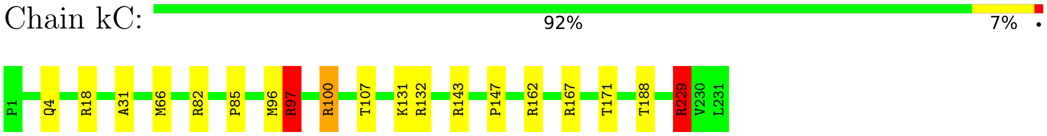
- Molecule 1: HIV-1 capsid protein

Chain jC:



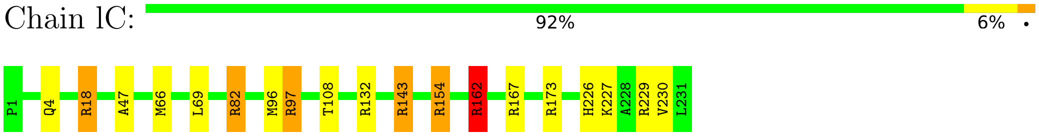
- Molecule 1: HIV-1 capsid protein

Chain kC:



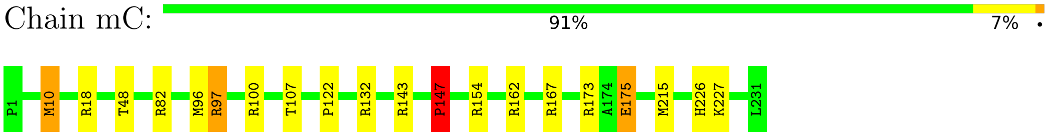
- Molecule 1: HIV-1 capsid protein

Chain lC:



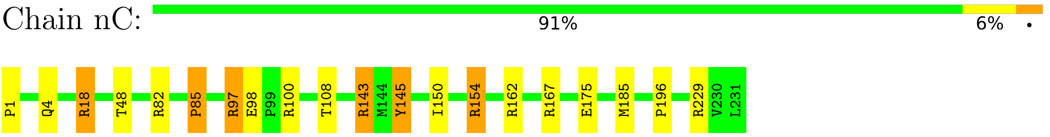
- Molecule 1: HIV-1 capsid protein

Chain mC:



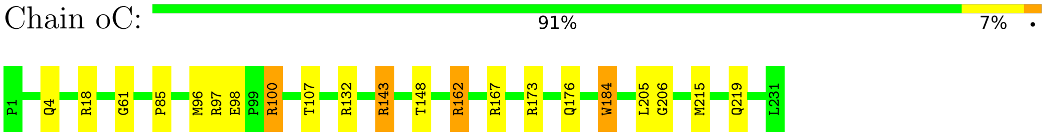
- Molecule 1: HIV-1 capsid protein

Chain nC:



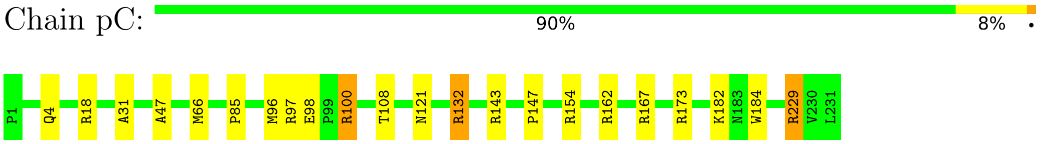
- Molecule 1: HIV-1 capsid protein

Chain oC:



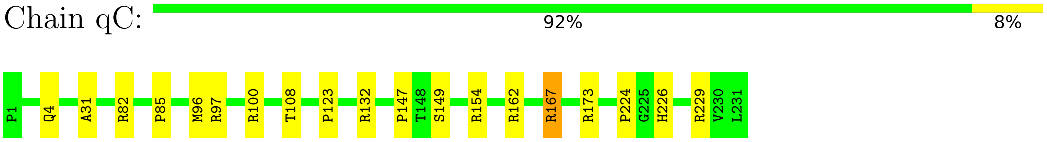
- Molecule 1: HIV-1 capsid protein

Chain pC:



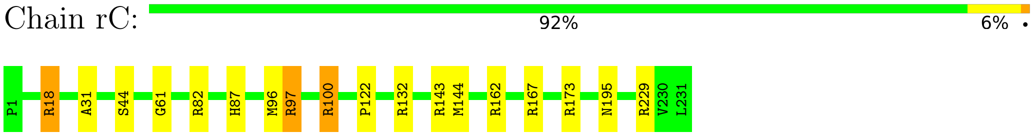
- Molecule 1: HIV-1 capsid protein

Chain qC:



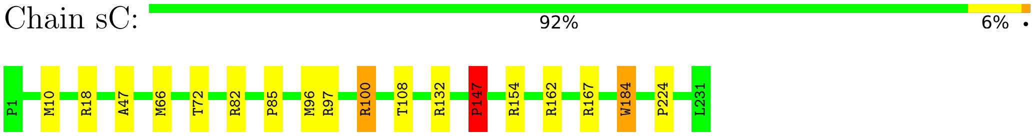
- Molecule 1: HIV-1 capsid protein

Chain rC:



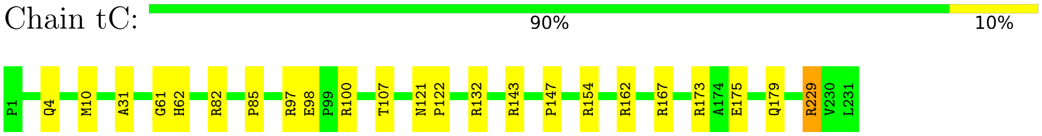
- Molecule 1: HIV-1 capsid protein

Chain sC:



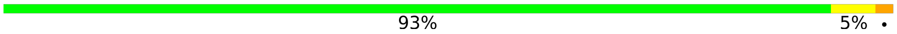
- Molecule 1: HIV-1 capsid protein

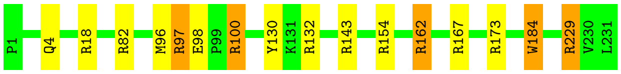
Chain tC:



- Molecule 1: HIV-1 capsid protein

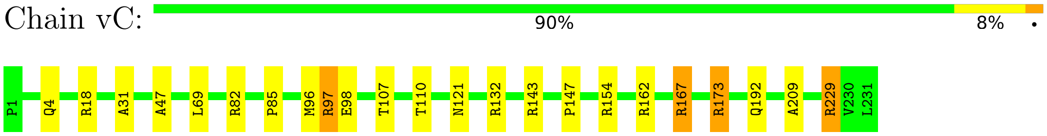
Chain uC:





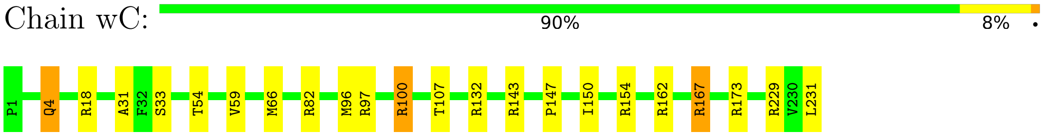
- Molecule 1: HIV-1 capsid protein

Chain vC:



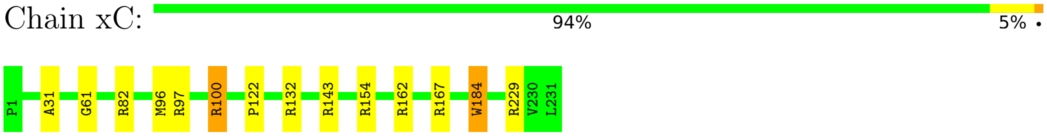
- Molecule 1: HIV-1 capsid protein

Chain wC:



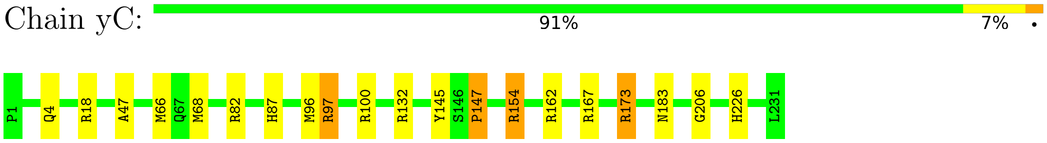
- Molecule 1: HIV-1 capsid protein

Chain xC:



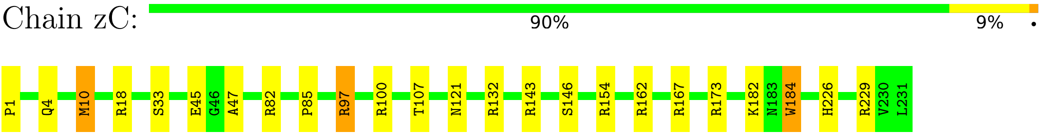
- Molecule 1: HIV-1 capsid protein

Chain yC:



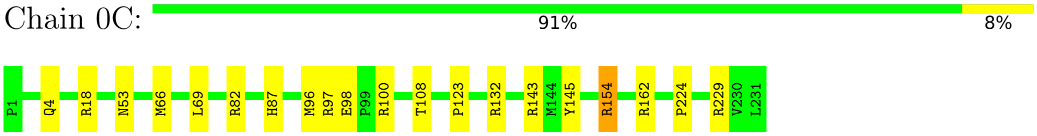
- Molecule 1: HIV-1 capsid protein

Chain zC:



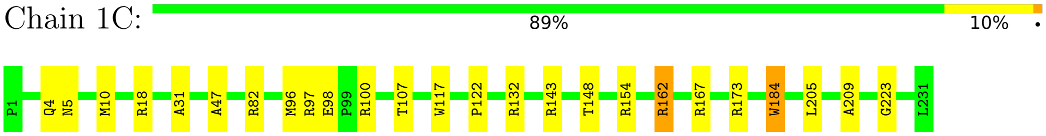
- Molecule 1: HIV-1 capsid protein

Chain 0C:



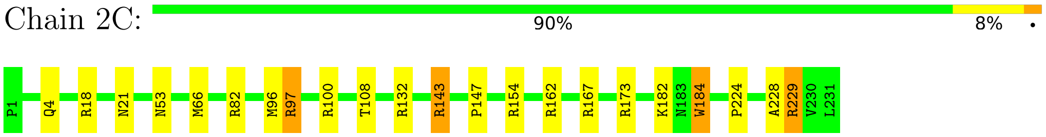
- Molecule 1: HIV-1 capsid protein

Chain 1C:



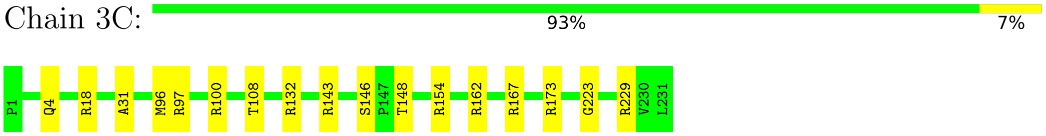
- Molecule 1: HIV-1 capsid protein

Chain 2C:



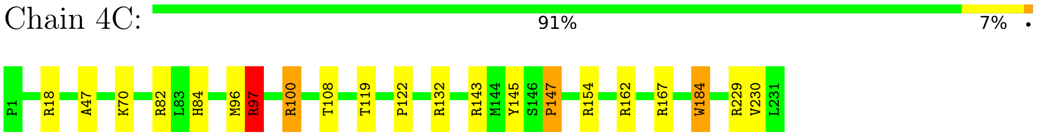
- Molecule 1: HIV-1 capsid protein

Chain 3C:



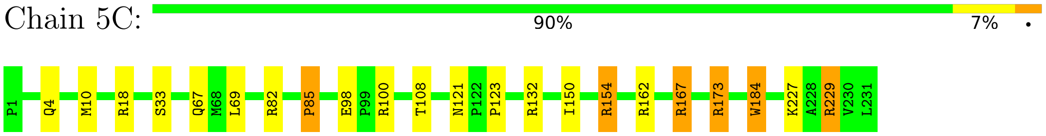
- Molecule 1: HIV-1 capsid protein

Chain 4C:



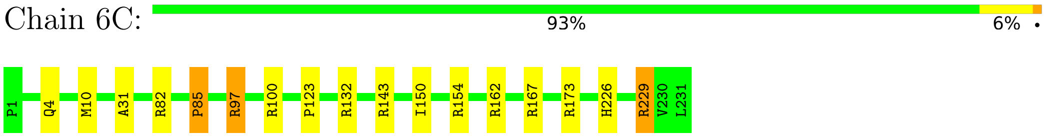
- Molecule 1: HIV-1 capsid protein

Chain 5C:



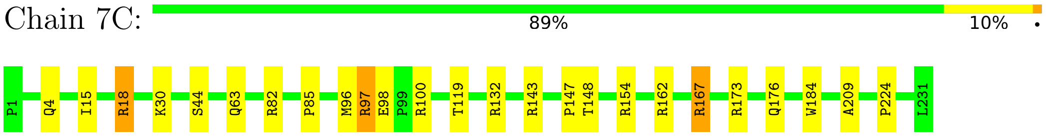
- Molecule 1: HIV-1 capsid protein

Chain 6C:



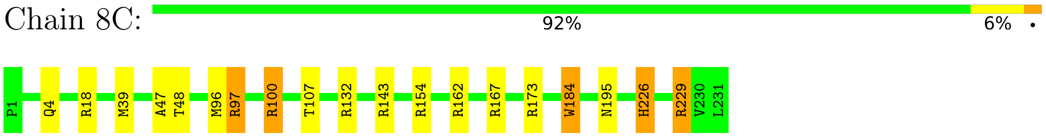
- Molecule 1: HIV-1 capsid protein

Chain 7C:



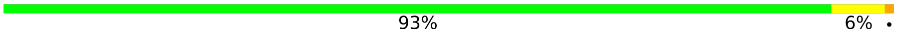
- Molecule 1: HIV-1 capsid protein

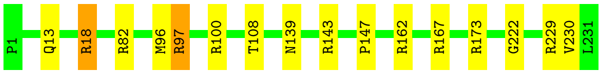
Chain 8C:



- Molecule 1: HIV-1 capsid protein

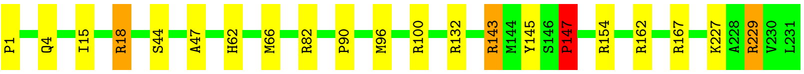
Chain 9C:





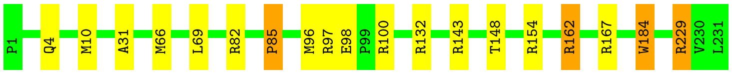
- Molecule 1: HIV-1 capsid protein

Chain AD:



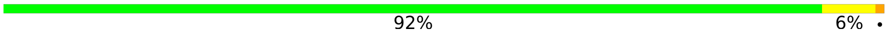
- Molecule 1: HIV-1 capsid protein

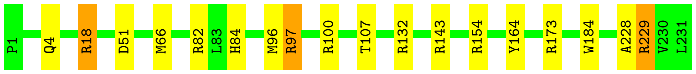
Chain BD:



- Molecule 1: HIV-1 capsid protein

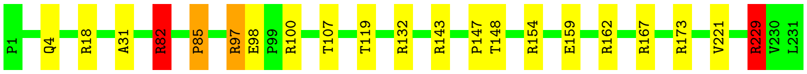
Chain CD:





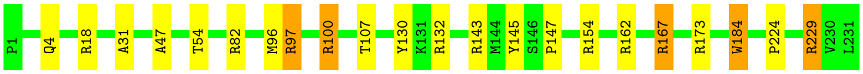
- Molecule 1: HIV-1 capsid protein

Chain DD:



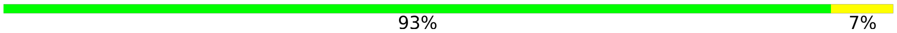
- Molecule 1: HIV-1 capsid protein

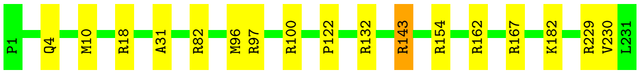
Chain ED:



- Molecule 1: HIV-1 capsid protein

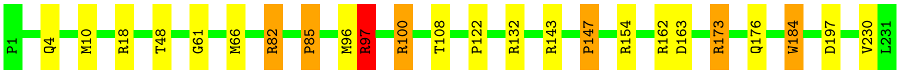
Chain FD:





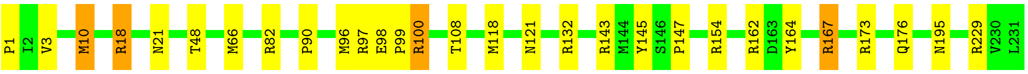
- Molecule 1: HIV-1 capsid protein

Chain GD:



- Molecule 1: HIV-1 capsid protein

Chain HD:



- Molecule 1: HIV-1 capsid protein

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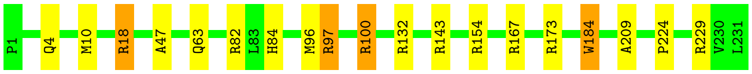
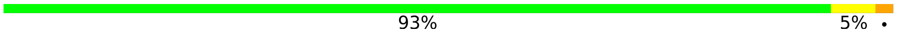
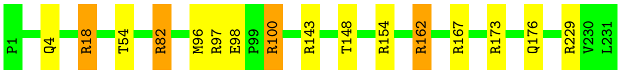


- Molecule 1: HIV-1 capsid protein

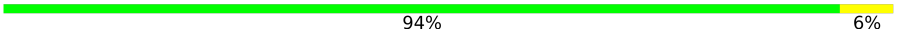
Chain JD:

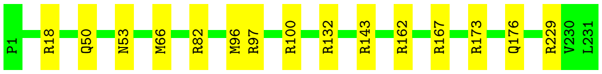




- Molecule 1: HIV-1 capsid protein

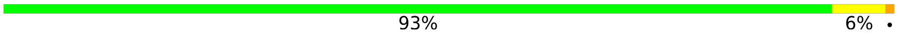
Chain KD:

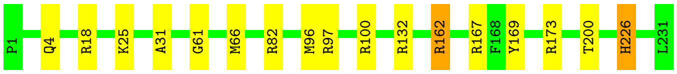




- Molecule 1: HIV-1 capsid protein

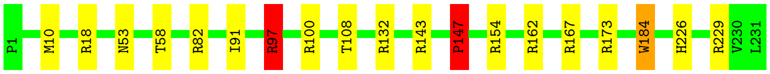
Chain LD:





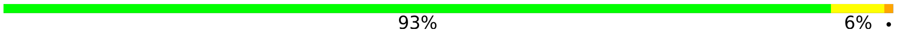
- Molecule 1: HIV-1 capsid protein

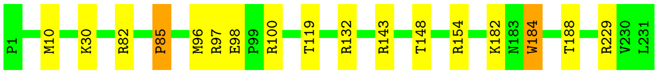
Chain MD:



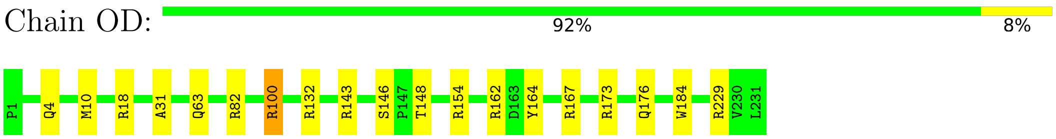
- Molecule 1: HIV-1 capsid protein

Chain ND:

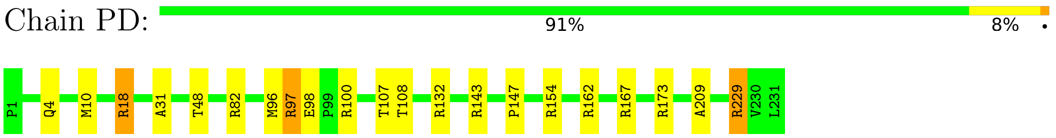




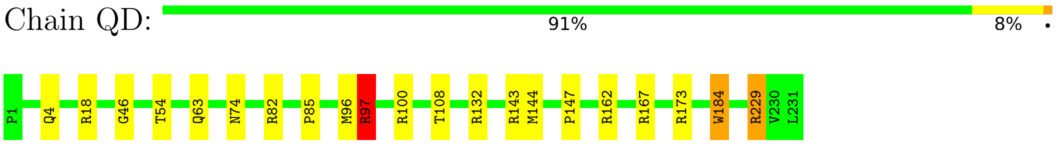
- Molecule 1: HIV-1 capsid protein



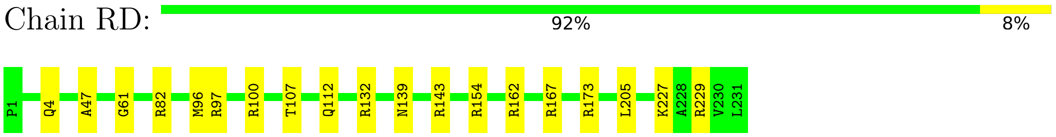
- Molecule 1: HIV-1 capsid protein



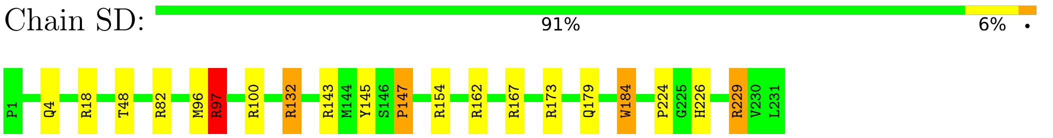
- Molecule 1: HIV-1 capsid protein



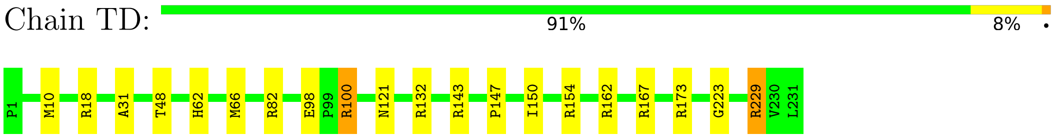
- Molecule 1: HIV-1 capsid protein



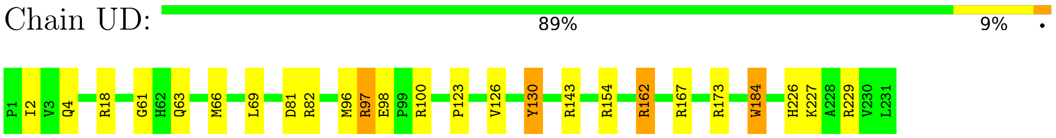
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

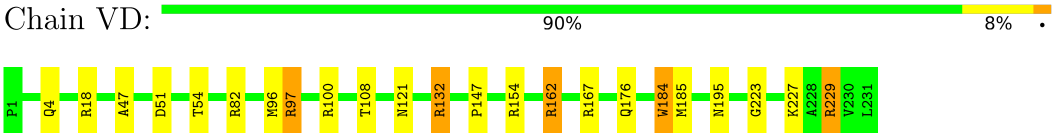


- Molecule 1: HIV-1 capsid protein



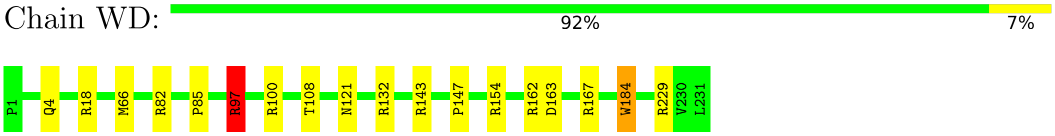
- Molecule 1: HIV-1 capsid protein

Chain VD:



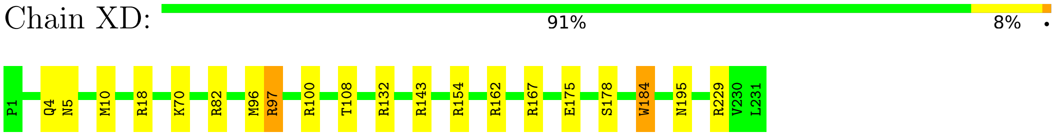
- Molecule 1: HIV-1 capsid protein

Chain WD:



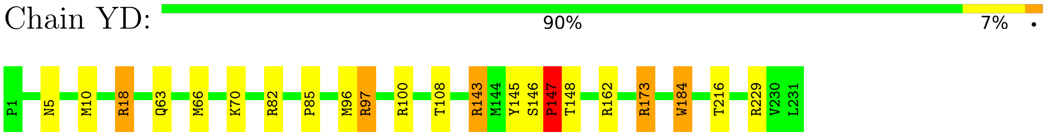
- Molecule 1: HIV-1 capsid protein

Chain XD:



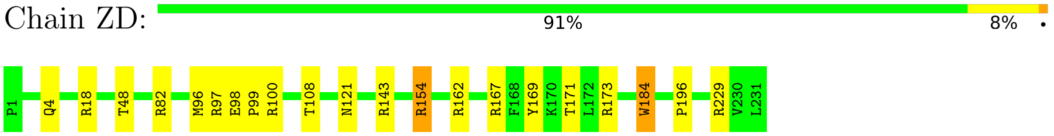
- Molecule 1: HIV-1 capsid protein

Chain YD:



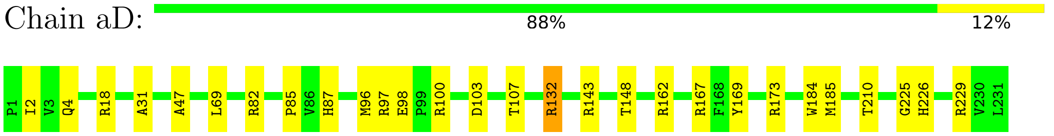
- Molecule 1: HIV-1 capsid protein

Chain ZD:



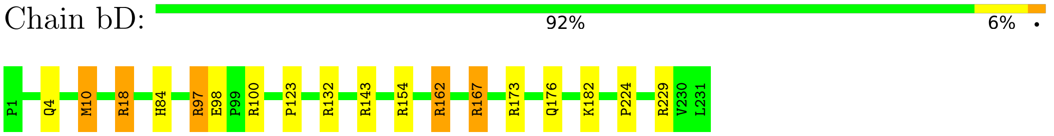
- Molecule 1: HIV-1 capsid protein

Chain aD:



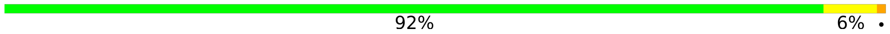
- Molecule 1: HIV-1 capsid protein

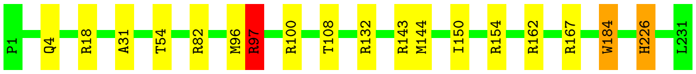
Chain bD:



- Molecule 1: HIV-1 capsid protein

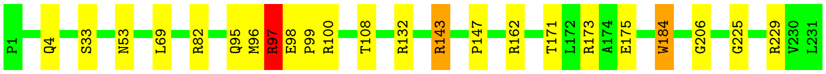
Chain cD:





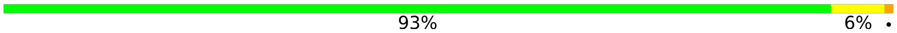
• Molecule 1: HIV-1 capsid protein

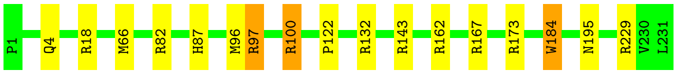
Chain dD:



• Molecule 1: HIV-1 capsid protein

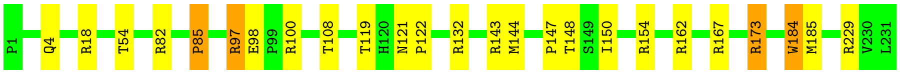
Chain eD:





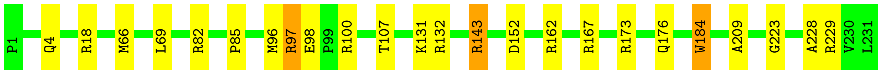
• Molecule 1: HIV-1 capsid protein

Chain fD:



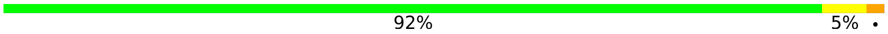
• Molecule 1: HIV-1 capsid protein

Chain gD:



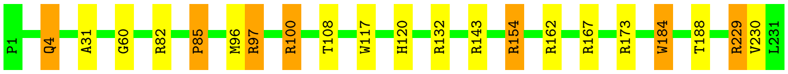
• Molecule 1: HIV-1 capsid protein

Chain hD:



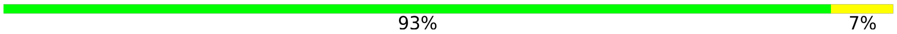
• Molecule 1: HIV-1 capsid protein

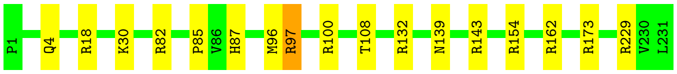
Chain iD:



• Molecule 1: HIV-1 capsid protein

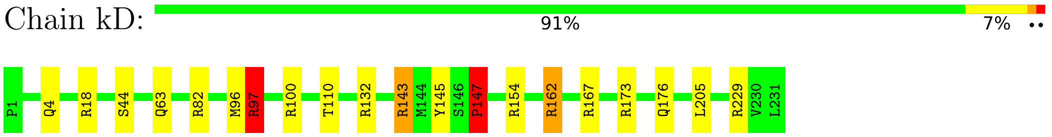
Chain jD:





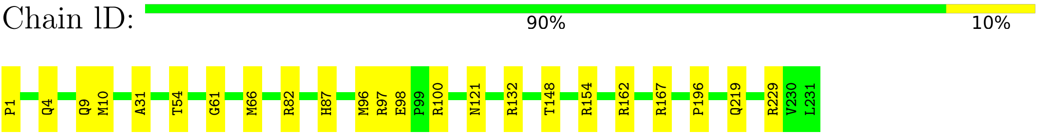
- Molecule 1: HIV-1 capsid protein

Chain kD:



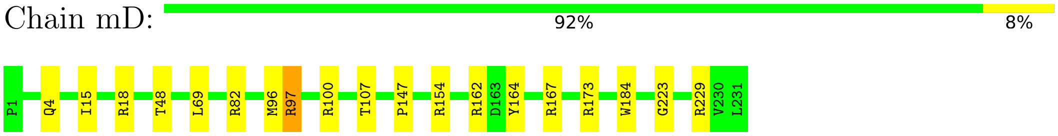
- Molecule 1: HIV-1 capsid protein

Chain lD:



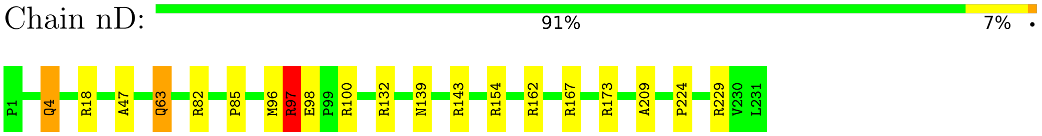
- Molecule 1: HIV-1 capsid protein

Chain mD:



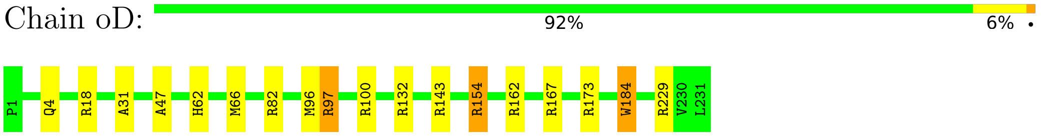
- Molecule 1: HIV-1 capsid protein

Chain nD:



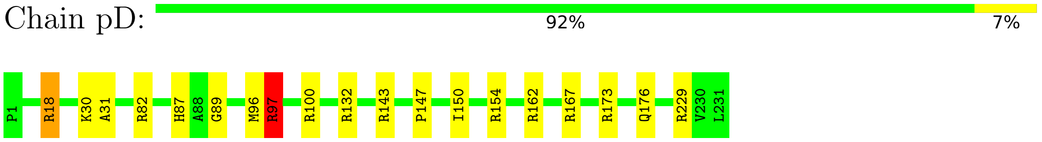
- Molecule 1: HIV-1 capsid protein

Chain oD:



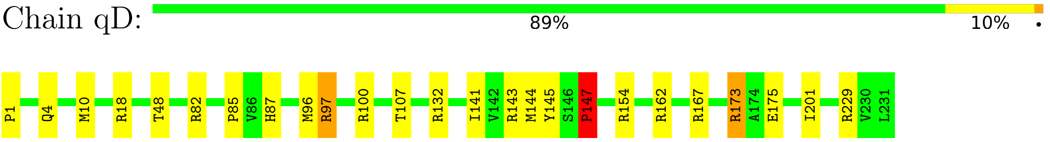
- Molecule 1: HIV-1 capsid protein

Chain pD:



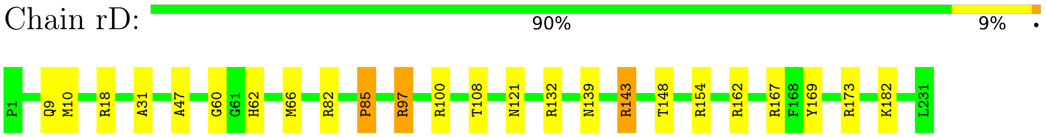
- Molecule 1: HIV-1 capsid protein

Chain qD:



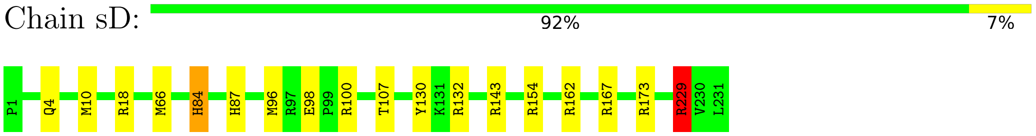
- Molecule 1: HIV-1 capsid protein

Chain rD:



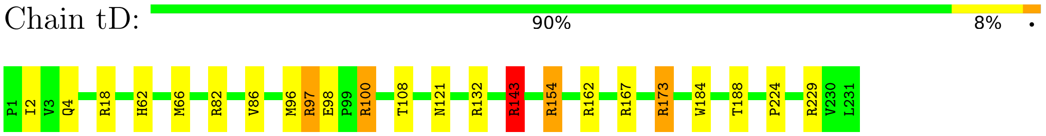
- Molecule 1: HIV-1 capsid protein

Chain sD:



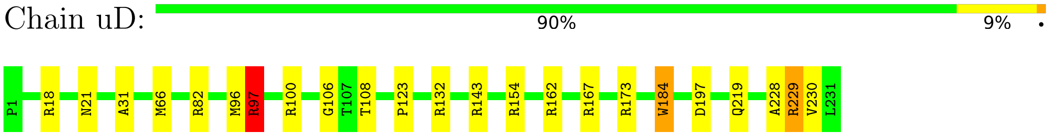
- Molecule 1: HIV-1 capsid protein

Chain tD:



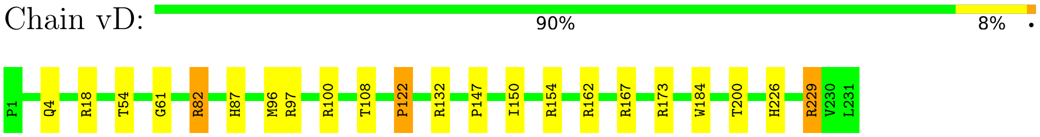
- Molecule 1: HIV-1 capsid protein

Chain uD:



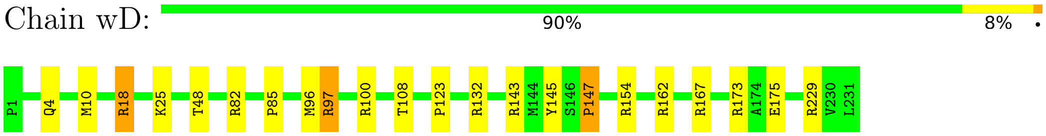
- Molecule 1: HIV-1 capsid protein

Chain vD:



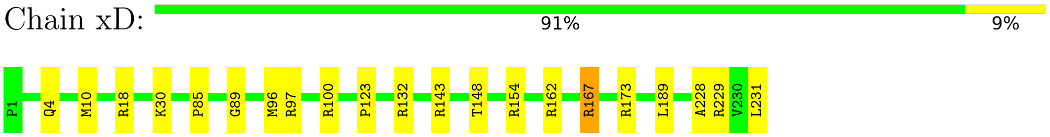
- Molecule 1: HIV-1 capsid protein

Chain wD:



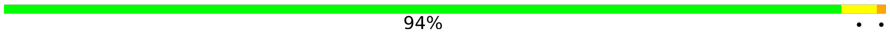
- Molecule 1: HIV-1 capsid protein

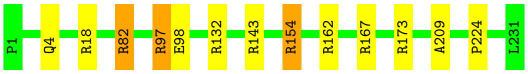
Chain xD:



- Molecule 1: HIV-1 capsid protein

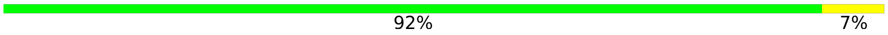
Chain yD:

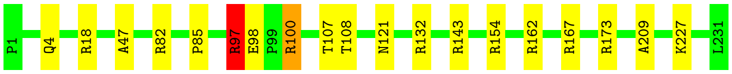




- Molecule 1: HIV-1 capsid protein

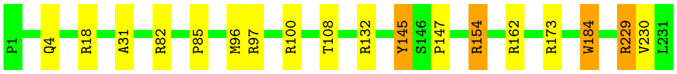
Chain zD:





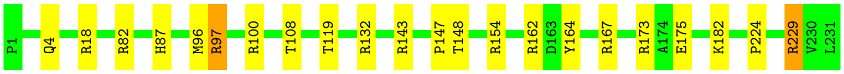
- Molecule 1: HIV-1 capsid protein

Chain 0D:



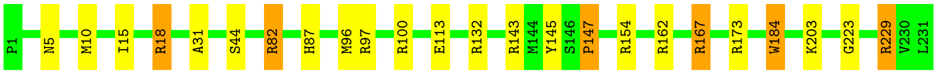
- Molecule 1: HIV-1 capsid protein

Chain 1D:



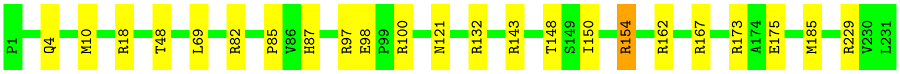
- Molecule 1: HIV-1 capsid protein

Chain 2D:



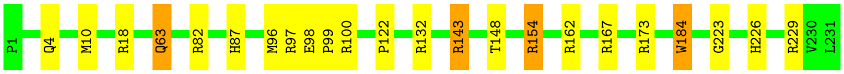
- Molecule 1: HIV-1 capsid protein

Chain 3D:



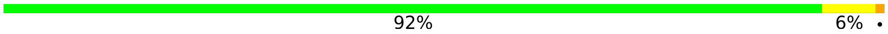
- Molecule 1: HIV-1 capsid protein

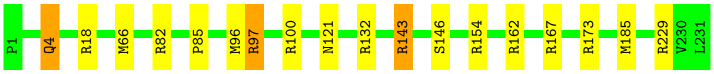
Chain 4D:



- Molecule 1: HIV-1 capsid protein

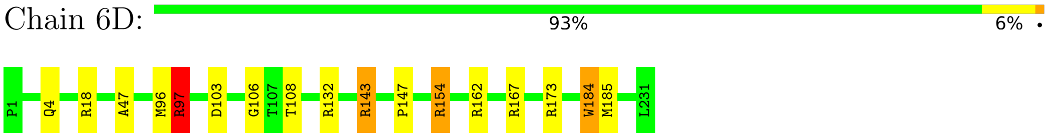
Chain 5D:





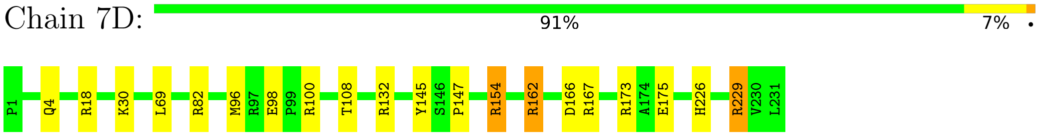
- Molecule 1: HIV-1 capsid protein

Chain 6D:



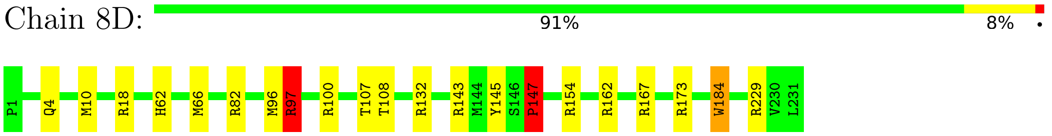
- Molecule 1: HIV-1 capsid protein

Chain 7D:



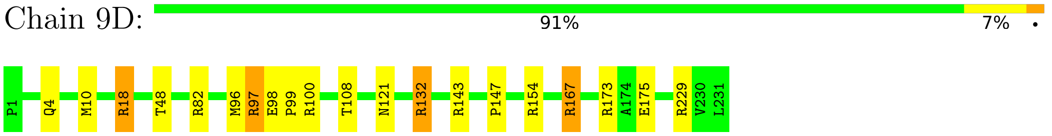
- Molecule 1: HIV-1 capsid protein

Chain 8D:



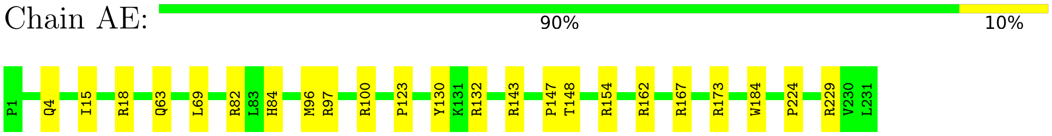
- Molecule 1: HIV-1 capsid protein

Chain 9D:



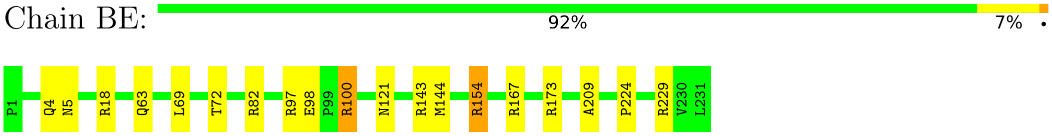
- Molecule 1: HIV-1 capsid protein

Chain AE:



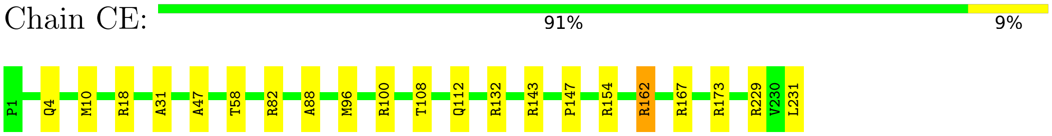
- Molecule 1: HIV-1 capsid protein

Chain BE:



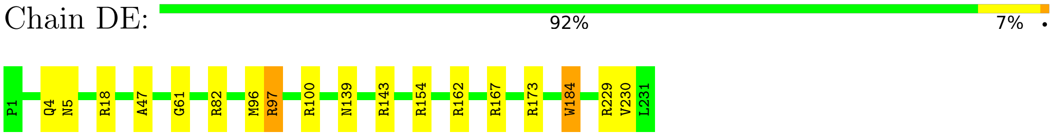
- Molecule 1: HIV-1 capsid protein

Chain CE:



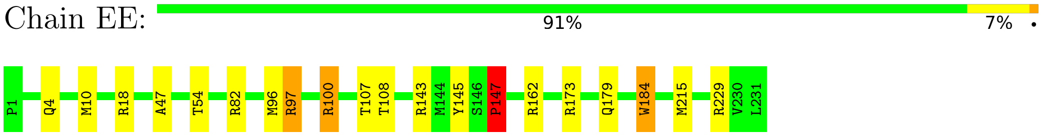
- Molecule 1: HIV-1 capsid protein

Chain DE:



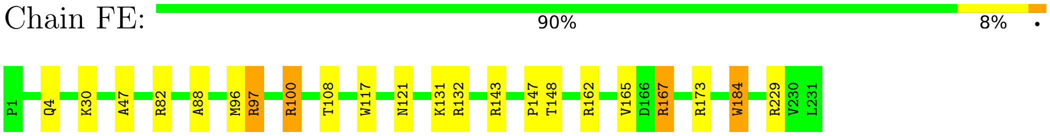
- Molecule 1: HIV-1 capsid protein

Chain EE:



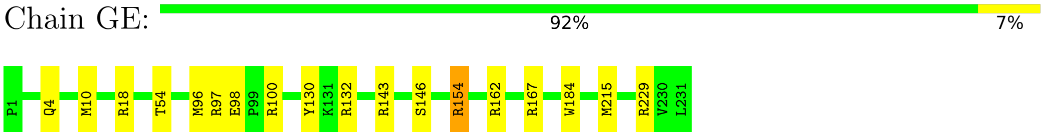
- Molecule 1: HIV-1 capsid protein

Chain FE:



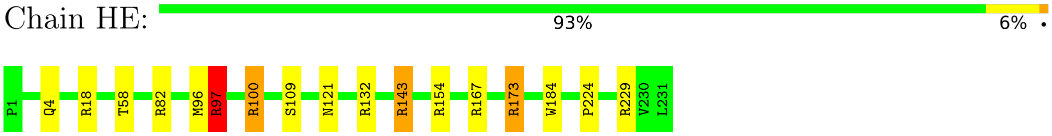
- Molecule 1: HIV-1 capsid protein

Chain GE:



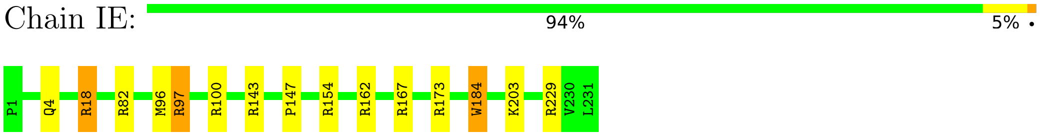
- Molecule 1: HIV-1 capsid protein

Chain HE:



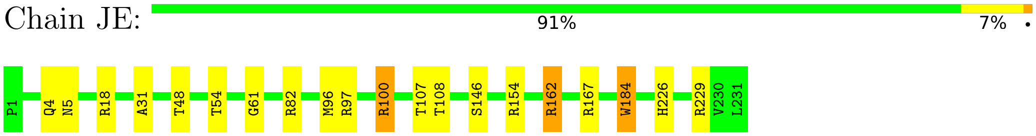
- Molecule 1: HIV-1 capsid protein

Chain IE:



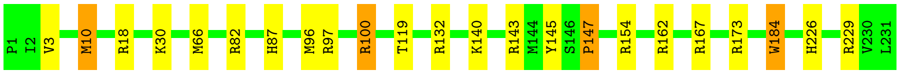
- Molecule 1: HIV-1 capsid protein

Chain JE:



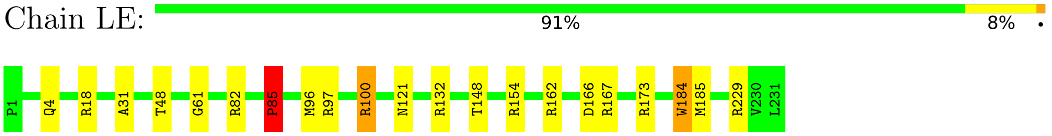
- Molecule 1: HIV-1 capsid protein

Chain KE:



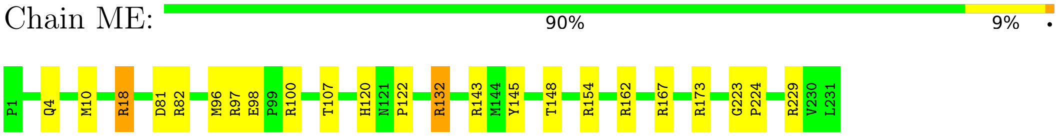
- Molecule 1: HIV-1 capsid protein

Chain LE:



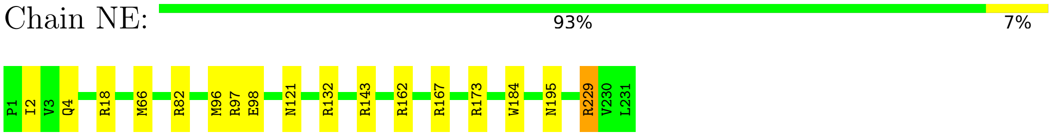
- Molecule 1: HIV-1 capsid protein

Chain ME:



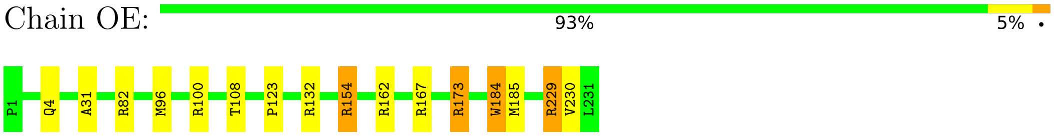
- Molecule 1: HIV-1 capsid protein

Chain NE:



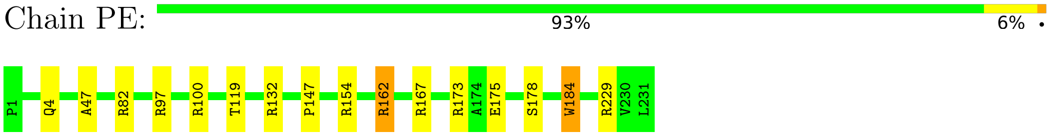
- Molecule 1: HIV-1 capsid protein

Chain OE:



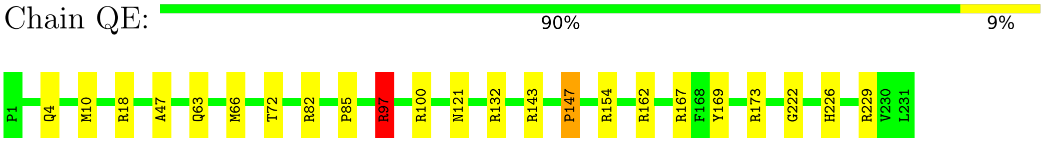
- Molecule 1: HIV-1 capsid protein

Chain PE:



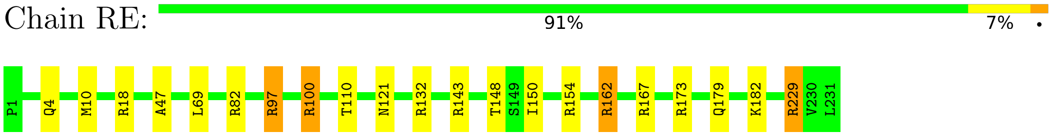
- Molecule 1: HIV-1 capsid protein

Chain QE:



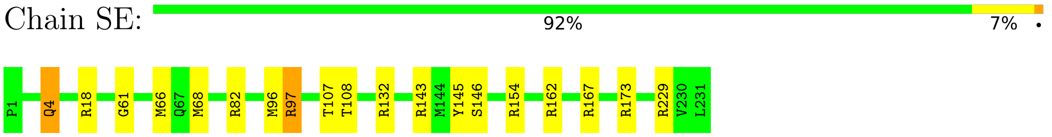
- Molecule 1: HIV-1 capsid protein

Chain RE:



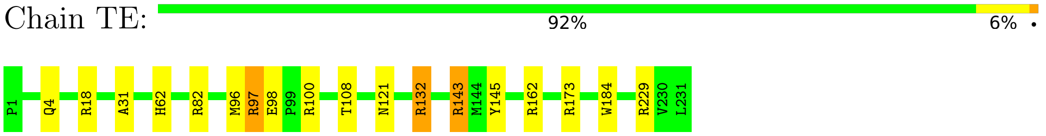
- Molecule 1: HIV-1 capsid protein

Chain SE:



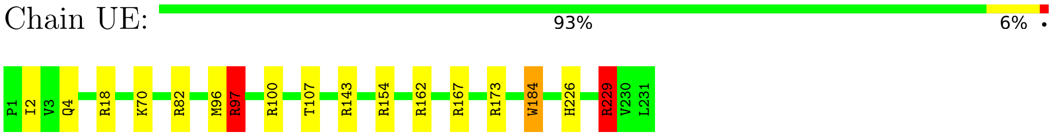
- Molecule 1: HIV-1 capsid protein

Chain TE:



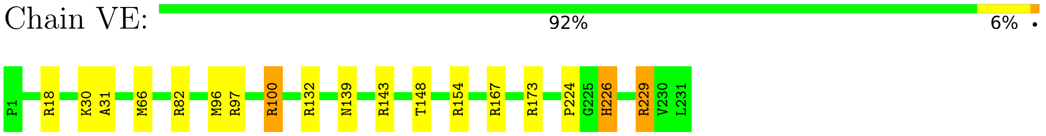
- Molecule 1: HIV-1 capsid protein

Chain UE:



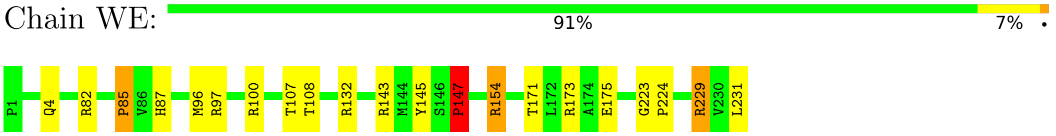
- Molecule 1: HIV-1 capsid protein

Chain VE:



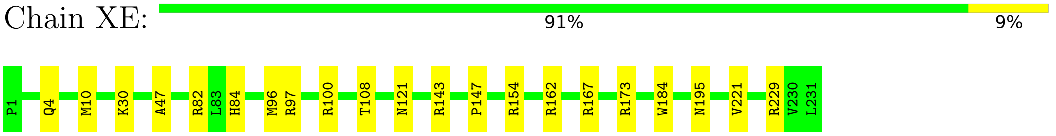
- Molecule 1: HIV-1 capsid protein

Chain WE:



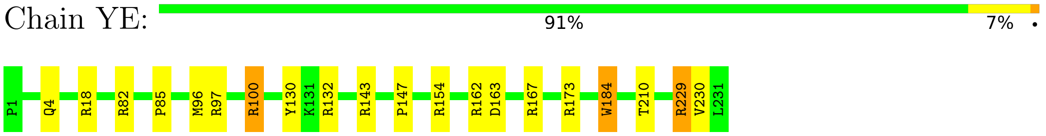
- Molecule 1: HIV-1 capsid protein

Chain XE:



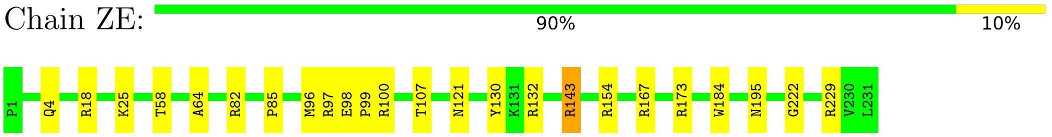
- Molecule 1: HIV-1 capsid protein

Chain YE:



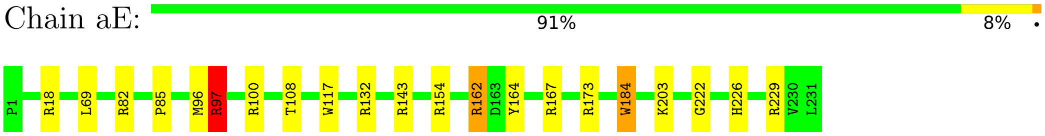
- Molecule 1: HIV-1 capsid protein

Chain ZE:



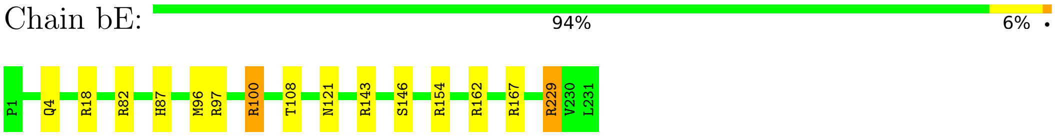
- Molecule 1: HIV-1 capsid protein

Chain aE:



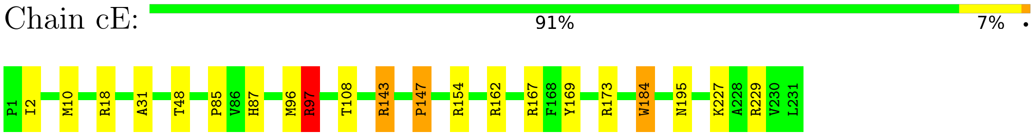
- Molecule 1: HIV-1 capsid protein

Chain bE:



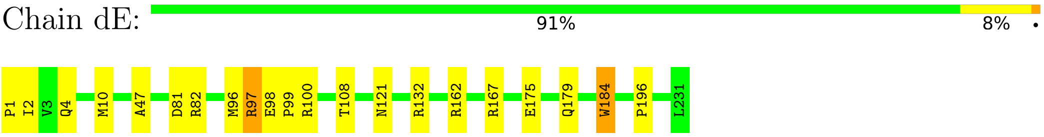
- Molecule 1: HIV-1 capsid protein

Chain cE:



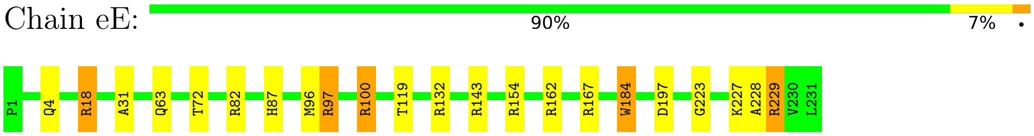
- Molecule 1: HIV-1 capsid protein

Chain dE:



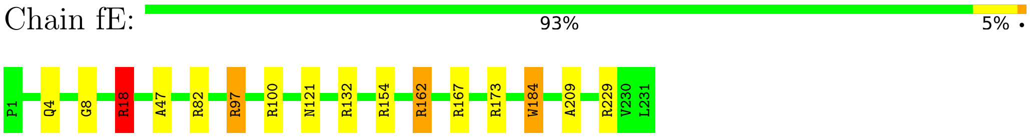
- Molecule 1: HIV-1 capsid protein

Chain eE:



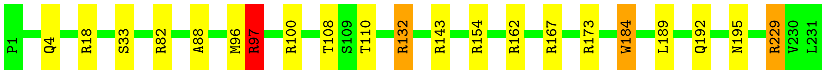
- Molecule 1: HIV-1 capsid protein

Chain fE:



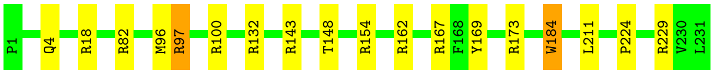
- Molecule 1: HIV-1 capsid protein

Chain gE:



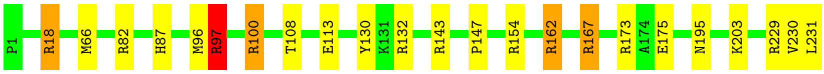
- Molecule 1: HIV-1 capsid protein

Chain hE:



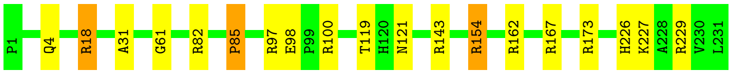
- Molecule 1: HIV-1 capsid protein

Chain iE:



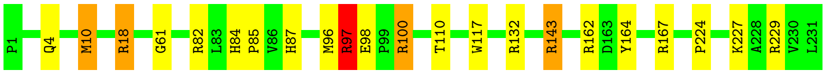
- Molecule 1: HIV-1 capsid protein

Chain jE:



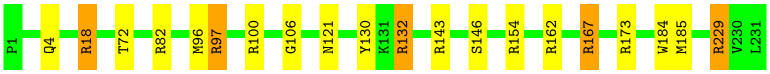
- Molecule 1: HIV-1 capsid protein

Chain kE:



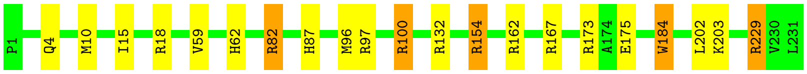
- Molecule 1: HIV-1 capsid protein

Chain lE:



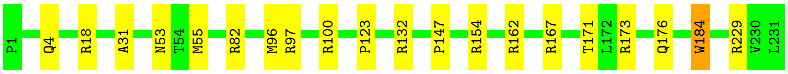
- Molecule 1: HIV-1 capsid protein

Chain mE:

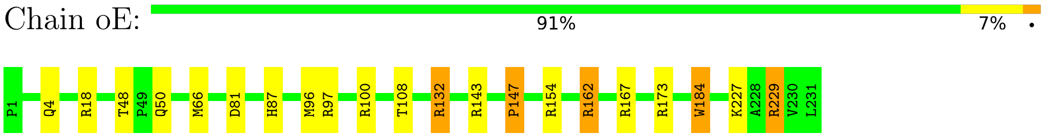


- Molecule 1: HIV-1 capsid protein

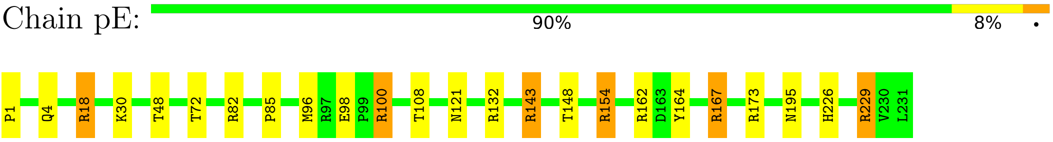
Chain nE:



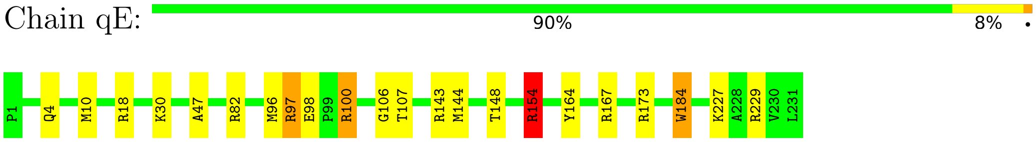
- Molecule 1: HIV-1 capsid protein



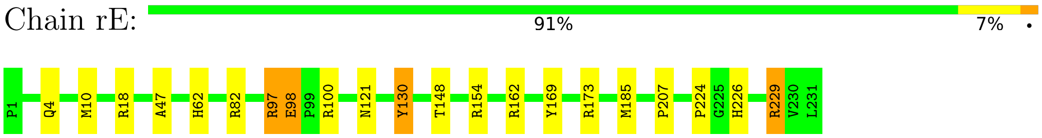
- Molecule 1: HIV-1 capsid protein



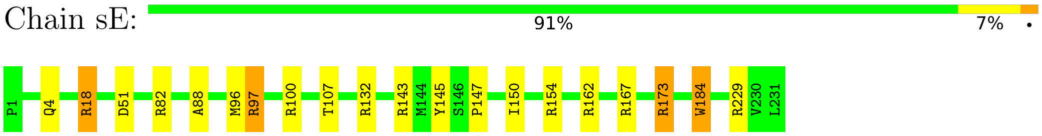
- Molecule 1: HIV-1 capsid protein



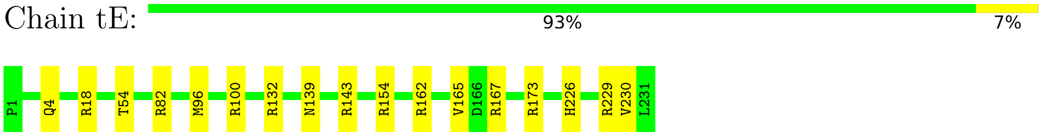
- Molecule 1: HIV-1 capsid protein



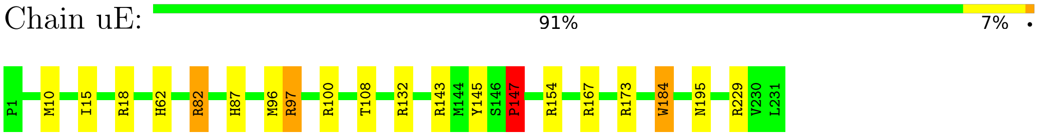
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

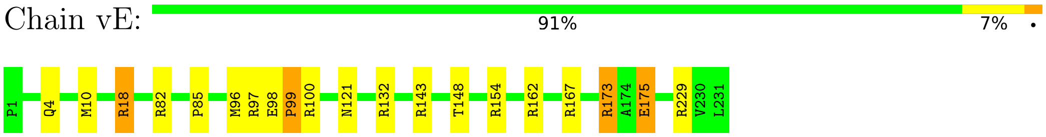


- Molecule 1: HIV-1 capsid protein



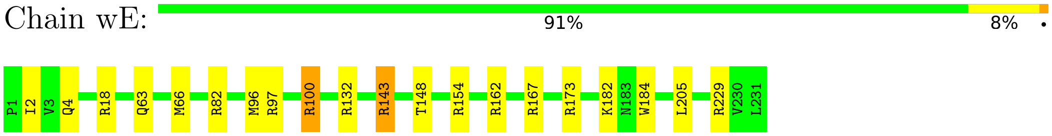
- Molecule 1: HIV-1 capsid protein

Chain vE:



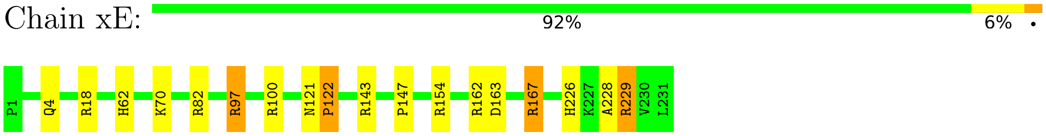
- Molecule 1: HIV-1 capsid protein

Chain wE:



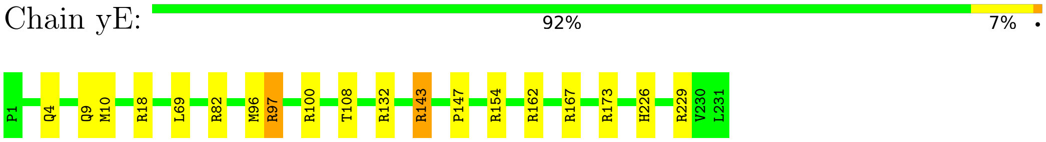
- Molecule 1: HIV-1 capsid protein

Chain xE:



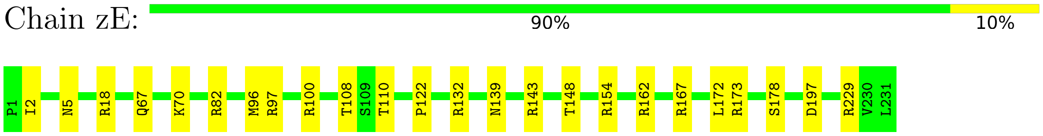
- Molecule 1: HIV-1 capsid protein

Chain yE:



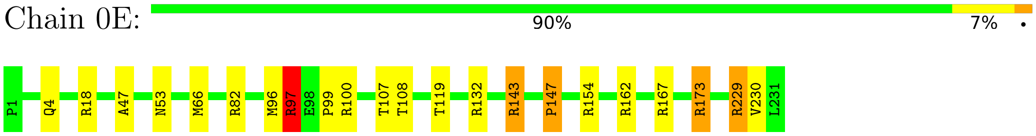
- Molecule 1: HIV-1 capsid protein

Chain zE:



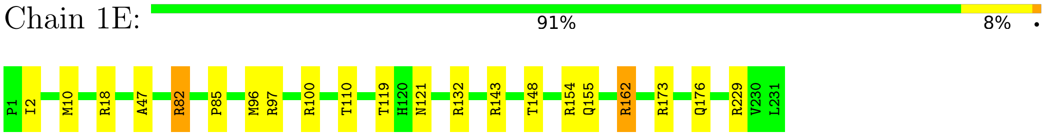
- Molecule 1: HIV-1 capsid protein

Chain 0E:



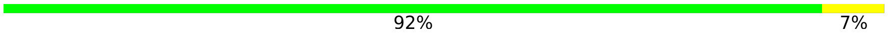
- Molecule 1: HIV-1 capsid protein

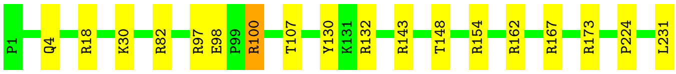
Chain 1E:



- Molecule 1: HIV-1 capsid protein

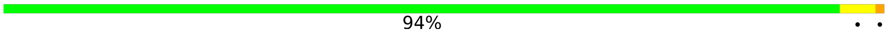
Chain 2E:

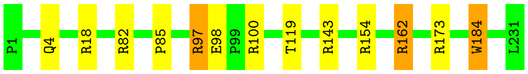




- Molecule 1: HIV-1 capsid protein

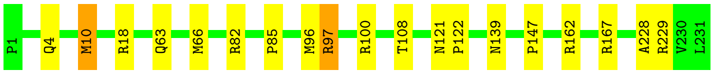
Chain 3E:





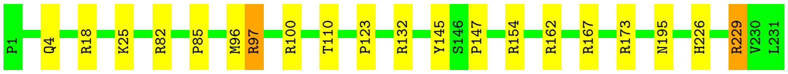
- Molecule 1: HIV-1 capsid protein

Chain 4E:



- Molecule 1: HIV-1 capsid protein

Chain 5E:



- Molecule 1: HIV-1 capsid protein

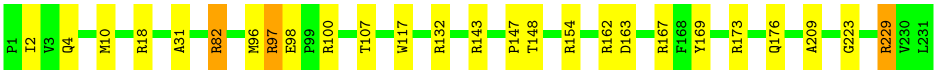
Chain 6E:

- Molecule 1: HIV-1 capsid protein

Chain 7E:

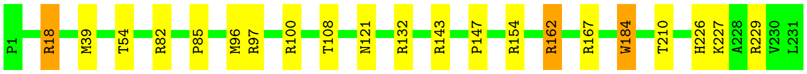
- Molecule 1: HIV-1 capsid protein

Chain 8E:



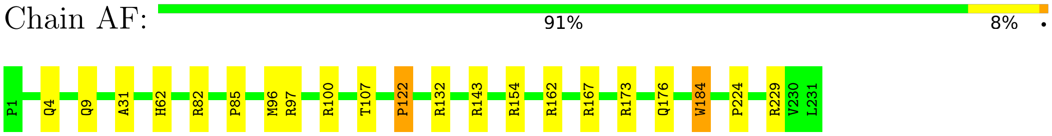
- Molecule 1: HIV-1 capsid protein

Chain 9E:



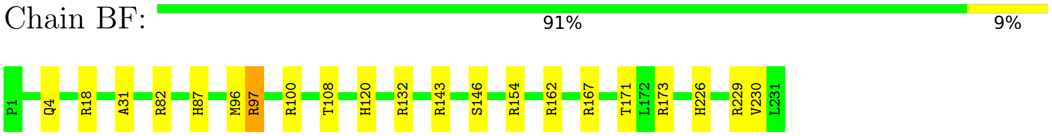
- Molecule 1: HIV-1 capsid protein

Chain AF:



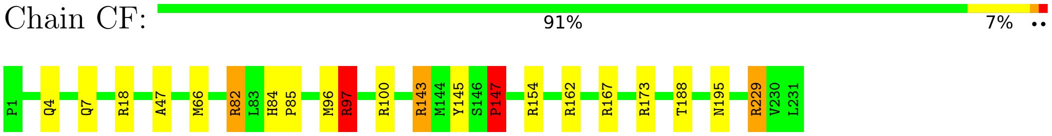
- Molecule 1: HIV-1 capsid protein

Chain BF:



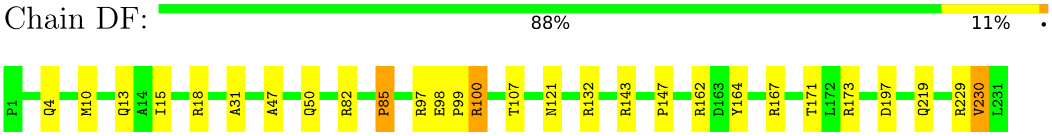
- Molecule 1: HIV-1 capsid protein

Chain CF:



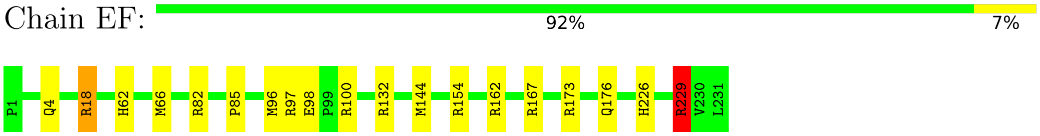
- Molecule 1: HIV-1 capsid protein

Chain DF:



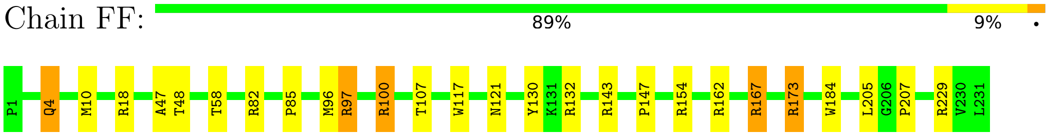
- Molecule 1: HIV-1 capsid protein

Chain EF:



- Molecule 1: HIV-1 capsid protein

Chain FF:



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	0.68	0/1836 (0.0%)	1.13	14/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.18	14/2493 (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	0.69	0/1836 (0.0%)	1.14	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	0.69	0/1836 (0.0%)	1.15	17/2493 (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	0.68	0/1836 (0.0%)	1.18	18/2493 (0.7%)
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	0.68	0/1836 (0.0%)	1.18	18/2493 (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	0.69	0/1836 (0.0%)	1.10	15/2493 (0.6%)
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	0.70	0/1836 (0.0%)	1.15	16/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.13	15/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.16	12/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.09	10/2493 (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	0.69	0/1836 (0.0%)	1.15	16/2493 (0.6%)
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	0.68	0/1836 (0.0%)	1.11	13/2493 (0.5%)
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	0.68	0/1836 (0.0%)	1.14	13/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.12	15/2493 (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	0.69	0/1836 (0.0%)	1.13	16/2493 (0.6%)
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	0.68	0/1836 (0.0%)	1.13	13/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.11	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	0.69	0/1836 (0.0%)	1.07	10/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.18	14/2493 (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	0.70	0/1836 (0.0%)	1.17	18/2493 (0.7%)
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	0.69	0/1836 (0.0%)	1.11	14/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.14	15/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.13	16/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
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	0.68	0/1836 (0.0%)	1.09	13/2493 (0.5%)

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	0.69	0/1836 (0.0%)	1.20	17/2493 (0.7%)
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	0.69	0/1836 (0.0%)	1.15	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	0.69	0/1836 (0.0%)	1.18	19/2493 (0.8%)
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	0.69	0/1836 (0.0%)	1.12	15/2493 (0.6%)
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	0.68	0/1836 (0.0%)	1.16	14/2493 (0.6%)
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	0.68	0/1836 (0.0%)	1.08	11/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.10	10/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.09	10/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.14	14/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.24	21/2493 (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	0.69	0/1836 (0.0%)	1.20	15/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.21	17/2493 (0.7%)
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	0.69	0/1836 (0.0%)	1.15	12/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.15	15/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.10	13/2493 (0.5%)
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	0.70	0/1836 (0.0%)	1.11	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	0.70	0/1836 (0.0%)	1.16	15/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.15	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	0.69	0/1836 (0.0%)	1.13	13/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.12	13/2493 (0.5%)
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	0.69	0/1836 (0.0%)	1.18	20/2493 (0.8%)
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	0.69	0/1836 (0.0%)	1.13	15/2493 (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	0.68	0/1836 (0.0%)	1.10	7/2493 (0.3%)
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	0.68	0/1836 (0.0%)	1.09	10/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.14	13/2493 (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	0.70	0/1836 (0.0%)	1.13	13/2493 (0.5%)
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	0.68	0/1836 (0.0%)	1.21	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	0.70	0/1836 (0.0%)	1.10	13/2493 (0.5%)
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	0.68	0/1836 (0.0%)	1.16	12/2493 (0.5%)
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	0.68	0/1836 (0.0%)	1.14	17/2493 (0.7%)
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	0.69	0/1836 (0.0%)	1.09	11/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.14	11/2493 (0.4%)
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	0.69	0/1836 (0.0%)	1.13	14/2493 (0.6%)
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	0.69	0/1836 (0.0%)	1.21	22/2493 (0.9%)
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	0.68	0/1836 (0.0%)	1.11	12/2493 (0.5%)
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	0.69	0/694008 (0.0%)	1.14	5397/942354 (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(^{o})	Ideal(^{o})
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	r	162	ARG	NE-CZ-NH1	13.64	127.12	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	T	82	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	b	184	TRP	CB-CG-CD1	-12.28	111.04	127.00
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	p	154	ARG	NE-CZ-NH1	12.08	126.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	TC	82	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	R	132	ARG	NE-CZ-NH1	12.03	126.31	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
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	A	97	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	M	167	ARG	NE-CZ-NH1	11.68	126.14	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	a	154	ARG	NE-CZ-NH1	11.51	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	P	154	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	BB	100	ARG	NE-CZ-NH1	11.34	125.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	NE-CZ-NH1	11.32	125.96	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	L	167	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	U	173	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	Q	162	ARG	NE-CZ-NH1	11.24	125.92	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
1	4	132	ARG	NE-CZ-NH2	-11.22	114.69	120.30
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	o	162	ARG	NE-CZ-NH1	11.11	125.85	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	d	162	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	IA	18	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	lD	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	n	154	ARG	NE-CZ-NH1	10.99	125.79	120.30
1	9C	162	ARG	NE-CZ-NH1	10.98	125.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	v	154	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	1	167	ARG	NE-CZ-NH1	10.94	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	k	97	ARG	NE-CZ-NH1	10.86	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
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	a	184	TRP	CB-CG-CD2	10.76	140.59	126.60
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	h	100	ARG	NE-CZ-NH1	10.71	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	K	18	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	0	97	ARG	NE-CZ-NH2	-10.68	114.96	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	7	184	TRP	CB-CG-CD1	-10.57	113.25	127.00
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	c	184	TRP	CB-CG-CD2	-10.52	112.92	126.60
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
1	lB	18	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	d	167	ARG	NE-CZ-NH1	10.49	125.54	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	c	132	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	k	154	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	rC	100	ARG	NE-CZ-NH1	10.38	125.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	1D	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	1A	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	N	143	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	3	143	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	T	97	ARG	NE-CZ-NH1	10.31	125.45	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
1	E	154	ARG	NE-CZ-NH1	10.28	125.44	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	r	184	TRP	CB-CG-CD1	-10.22	113.72	127.00
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	g	229	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	uD	132	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	a	18	ARG	NE-CZ-NH1	10.21	125.40	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	w	162	ARG	NE-CZ-NH1	10.18	125.39	120.30
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	u	173	ARG	NE-CZ-NH1	10.16	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	a	184	TRP	CB-CG-CD1	-10.14	113.81	127.00
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	i	173	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	XA	82	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	2	184	TRP	CB-CG-CD1	-10.11	113.86	127.00
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	8	167	ARG	NE-CZ-NH1	10.05	125.32	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	R	100	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	S	184	TRP	CB-CG-CD1	-9.99	114.02	127.00
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	e	97	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	l	167	ARG	NE-CZ-NH1	9.96	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	X	82	ARG	NE-CZ-NH1	9.93	125.26	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	H	162	ARG	NE-CZ-NH1	9.92	125.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	A	132	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
1	q	18	ARG	NE-CZ-NH1	9.91	125.25	120.30
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	U	229	ARG	NE-CZ-NH2	-9.91	115.35	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	E	97	ARG	NE-CZ-NH2	-9.88	115.36	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	m	100	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	cE	18	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	Y	154	ARG	NE-CZ-NH1	9.86	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	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	K	100	ARG	NE-CZ-NH1	9.79	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	0	97	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
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	m	143	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	R	100	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	j	154	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	EA	154	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	G	162	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	0	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	8	18	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	t	184	TRP	CB-CG-CD1	-9.70	114.40	127.00
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	D	229	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	8	100	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	JA	154	ARG	NE-CZ-NH1	9.69	125.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	f	167	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
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	P	18	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	E	18	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	5A	184	TRP	CB-CG-CD1	-9.57	114.55	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	82	ARG	NE-CZ-NH1	9.57	125.09	120.30
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	4	82	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	X	229	ARG	NE-CZ-NH1	9.52	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	167	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	x	167	ARG	NE-CZ-NH1	9.47	125.03	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	lD	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	X	97	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	h	184	TRP	CB-CG-CD1	-9.44	114.73	127.00
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	y	162	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
1	P	167	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	A	162	ARG	NE-CZ-NH1	9.41	125.00	120.30
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	c	143	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	x	132	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	fE	162	ARG	NE-CZ-NH1	9.39	125.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	167	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	w	97	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	1B	82	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	S	162	ARG	NE-CZ-NH1	9.38	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	w	229	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	EA	229	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	c	100	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	YC	167	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	K	162	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	3	82	ARG	NE-CZ-NH1	9.31	124.96	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	z	173	ARG	NE-CZ-NH1	9.31	124.95	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	b	97	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	i	18	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	2	18	ARG	NE-CZ-NH1	9.30	124.95	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	4	229	ARG	NE-CZ-NH1	9.29	124.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2B	82	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	O	97	ARG	NE-CZ-NH2	-9.29	115.66	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
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	y	229	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	bD	143	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	b	162	ARG	NE-CZ-NH2	-9.24	115.68	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	F	132	ARG	NE-CZ-NH1	9.23	124.92	120.30
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	p	18	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	IB	154	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	1E	100	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	sB	173	ARG	NE-CZ-NH1	9.21	124.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	A	154	ARG	NE-CZ-NH1	9.20	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	M	154	ARG	NE-CZ-NH1	9.19	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
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	t	229	ARG	NE-CZ-NH1	9.18	124.89	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	1	18	ARG	NE-CZ-NH1	9.17	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	y	132	ARG	NE-CZ-NH1	9.16	124.88	120.30
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	l	184	TRP	CB-CG-CD1	-9.16	115.09	127.00
1	vB	167	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	v	82	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	SA	162	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	u	184	TRP	CB-CG-CD1	-9.15	115.10	127.00
1	nE	184	TRP	CB-CG-CD1	-9.15	115.10	127.00
1	a	154	ARG	NE-CZ-NH2	-9.15	115.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	167	ARG	NE-CZ-NH1	9.15	124.87	120.30
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	r	162	ARG	NE-CZ-NH2	-9.14	115.73	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	c	18	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	9	143	ARG	NE-CZ-NH1	9.12	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
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	w	82	ARG	NE-CZ-NH1	9.11	124.86	120.30
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	x	82	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	NB	167	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	h	173	ARG	NE-CZ-NH1	9.09	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	i	132	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	E	97	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Y	229	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	SE	154	ARG	NE-CZ-NH1	9.08	124.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	y	154	ARG	NE-CZ-NH1	9.06	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	H	143	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	r	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	r	173	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	lD	82	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	q	229	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	4	18	ARG	NE-CZ-NH2	-9.03	115.78	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	lD	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
1	pB	100	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	r	173	ARG	NE-CZ-NH2	-9.02	115.79	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	132	ARG	NE-CZ-NH1	9.01	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	m	154	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	9	82	ARG	NE-CZ-NH1	9.01	124.80	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	e	162	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	z	162	ARG	NE-CZ-NH1	8.99	124.80	120.30
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	K	184	TRP	CB-CG-CD1	-8.97	115.34	127.00
1	u	162	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	F	82	ARG	NE-CZ-NH1	8.93	124.77	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	F	18	ARG	NE-CZ-NH1	8.93	124.76	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	N	229	ARG	NE-CZ-NH2	-8.92	115.84	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	b	132	ARG	NE-CZ-NH2	-8.92	115.84	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	P	100	ARG	NE-CZ-NH1	8.91	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	L	154	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
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	I	82	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	nC	162	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	J	97	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	c	229	ARG	NE-CZ-NH2	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	Z	82	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	u	167	ARG	NE-CZ-NH1	8.83	124.71	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	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	5	184	TRP	CB-CG-CD1	-8.82	115.54	127.00
1	3D	18	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	c	154	ARG	NE-CZ-NH1	8.81	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	4	132	ARG	NE-CZ-NH1	8.80	124.70	120.30
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
1	2D	167	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	y	100	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	t	154	ARG	NE-CZ-NH1	8.79	124.69	120.30
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	U	154	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	e	154	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	t	97	ARG	NE-CZ-NH2	-8.78	115.91	120.30
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	G	229	ARG	NE-CZ-NH1	8.77	124.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	n	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
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	S	167	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	B	97	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	5	100	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	g	18	ARG	NE-CZ-NH1	8.72	124.66	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	g	162	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	1	143	ARG	NE-CZ-NH1	8.71	124.66	120.30
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	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	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	oA	132	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	B	167	ARG	NE-CZ-NH2	-8.65	115.98	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	N	173	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	6	167	ARG	NE-CZ-NH1	8.63	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
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	t	143	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	5	162	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	0A	82	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	2	162	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	i	173	ARG	NE-CZ-NH1	8.60	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	KA	173	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	W	167	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	n	132	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	A	18	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	FB	143	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	p	100	ARG	NE-CZ-NH1	8.56	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	y	167	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	3	132	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	d	132	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	V	97	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
1	U	82	ARG	NE-CZ-NH1	8.54	124.57	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	167	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	1	97	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	Z	143	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	1	173	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	1B	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	V	18	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	o	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	y	184	TRP	CB-CG-CD1	-8.49	115.96	127.00
1	IA	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	W	82	ARG	NE-CZ-NH1	8.48	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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	n	154	ARG	NE-CZ-NH2	-8.47	116.07	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	e	97	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	UD	143	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	a	162	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	R	173	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	4	82	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	O	18	ARG	NE-CZ-NH1	8.45	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	K	162	ARG	NE-CZ-NH1	8.45	124.52	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	M	229	ARG	NE-CZ-NH1	8.44	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	x	143	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	hB	184	TRP	CB-CG-CD1	-8.43	116.04	127.00
1	a	18	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	b	100	ARG	NE-CZ-NH1	8.43	124.51	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	wB	132	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	q	167	ARG	NE-CZ-NH1	8.42	124.51	120.30
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	r	100	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	d	167	ARG	NE-CZ-NH2	-8.41	116.09	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	u	154	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	PB	162	ARG	NE-CZ-NH1	8.41	124.50	120.30
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	V	173	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	P	82	ARG	NE-CZ-NH1	8.40	124.50	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	I	143	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	K	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	F	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	fC	97	ARG	NE-CZ-NH1	8.39	124.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	1	18	ARG	NE-CZ-NH2	-8.37	116.11	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	d	97	ARG	NE-CZ-NH1	8.37	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	m	18	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	I	82	ARG	NE-CZ-NH1	8.36	124.48	120.30
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
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	N	18	ARG	NE-CZ-NH2	-8.35	116.13	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	1B	167	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	JE	82	ARG	NE-CZ-NH1	8.34	124.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	h	82	ARG	NE-CZ-NH1	8.33	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	7	97	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	fA	143	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	7	229	ARG	NE-CZ-NH1	8.32	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	t	18	ARG	NE-CZ-NH2	-8.32	116.14	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	H	132	ARG	NE-CZ-NH2	-8.31	116.14	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	1D	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	j	18	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	0A	130	TYR	CB-CG-CD2	-8.29	116.02	121.00
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	L	143	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	d	18	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	I	18	ARG	NE-CZ-NH1	8.29	124.44	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	143	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	E	173	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	Z	184	TRP	CB-CG-CD1	-8.28	116.24	127.00
1	z	97	ARG	NE-CZ-NH1	8.28	124.44	120.30
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	7	167	ARG	NE-CZ-NH1	8.25	124.42	120.30
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	M	132	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	gE	132	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	V	100	ARG	NE-CZ-NH1	8.23	124.42	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	4	18	ARG	NE-CZ-NH1	8.23	124.41	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	Q	167	ARG	NE-CZ-NH2	-8.22	116.19	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	l	143	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	9	18	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	YE	154	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	a	82	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	5	167	ARG	NE-CZ-NH1	8.21	124.40	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	3	18	ARG	NE-CZ-NH1	8.20	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	d	82	ARG	NE-CZ-NH1	8.19	124.39	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	7	162	ARG	NE-CZ-NH1	8.19	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	lD	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
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	E	229	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	b	143	ARG	NE-CZ-NH1	8.17	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	D	154	ARG	NE-CZ-NH2	-8.17	116.21	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	B	154	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	XB	100	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	i	132	ARG	NE-CZ-NH2	-8.16	116.22	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	b	162	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	l	162	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	rC	82	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	H	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	V	167	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	y	97	ARG	NE-CZ-NH1	8.13	124.37	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
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	7	154	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	i	100	ARG	NE-CZ-NH1	8.11	124.36	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	b	82	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	kB	173	ARG	NE-CZ-NH1	8.09	124.34	120.30
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	H	132	ARG	NE-CZ-NH1	8.09	124.34	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	d	229	ARG	NE-CZ-NH1	8.05	124.33	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	r	229	ARG	NE-CZ-NH1	8.05	124.32	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	j	97	ARG	NE-CZ-NH1	8.04	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HD	97	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	V	184	TRP	CB-CG-CD1	-8.02	116.57	127.00
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	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	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
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	v	167	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	T	184	TRP	CB-CG-CD1	-8.00	116.60	127.00
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	z	167	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6B	132	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	IE	82	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	1A	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	G	100	ARG	NE-CZ-NH1	7.97	124.28	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	E	82	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	i	97	ARG	NE-CZ-NH1	7.97	124.28	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	u	82	ARG	NE-CZ-NH2	-7.97	116.32	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
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	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	9	162	ARG	NE-CZ-NH1	7.95	124.27	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	R	162	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	hA	143	ARG	NE-CZ-NH1	7.95	124.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	97	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	wB	167	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	e	167	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	2	97	ARG	NE-CZ-NH2	-7.94	116.33	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	9	173	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	100	ARG	NE-CZ-NH1	7.91	124.26	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	a	173	ARG	NE-CZ-NH1	7.89	124.25	120.30
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	8	97	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	j	82	ARG	NE-CZ-NH2	-7.88	116.36	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	b	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	R	167	ARG	NE-CZ-NH2	-7.87	116.36	120.30
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	l	167	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	gD	143	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	w	100	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	3	82	ARG	NE-CZ-NH2	-7.86	116.37	120.30

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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	6	18	ARG	NE-CZ-NH2	-7.86	116.37	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	0	154	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	vE	167	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	c	100	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	xA	154	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	0	82	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	5	18	ARG	NE-CZ-NH1	7.85	124.22	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	N	100	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	l	173	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	18	ARG	NE-CZ-NH2	-7.83	116.38	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
1	G	100	ARG	NE-CZ-NH2	-7.82	116.39	120.30
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	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	A	143	ARG	NE-CZ-NH1	7.82	124.21	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	B	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	K	82	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	RE	229	ARG	NE-CZ-NH2	-7.79	116.40	120.30
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
1	jD	132	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	D	167	ARG	NE-CZ-NH1	7.78	124.19	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	x	229	ARG	NE-CZ-NH2	-7.78	116.41	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	T	18	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	a	184	TRP	CA-CB-CG	7.77	128.46	113.70
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	6	162	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	j	18	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	iD	162	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	T	100	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	c	173	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	z	154	ARG	NE-CZ-NH1	7.76	124.18	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	Z	154	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	154	ARG	NE-CZ-NH1	7.76	124.18	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	l	100	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	y	97	ARG	NE-CZ-NH2	-7.74	116.43	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
1	f	162	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	ND	229	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	N	132	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	9	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	6	18	ARG	NE-CZ-NH1	7.73	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	2	82	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	QA	173	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	1	82	ARG	NE-CZ-NH1	7.72	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	b	154	ARG	NE-CZ-NH1	7.72	124.16	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	i	167	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	B	167	ARG	NE-CZ-NH1	7.71	124.16	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	vA	162	ARG	NE-CZ-NH2	-7.70	116.45	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KD	229	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	L	18	ARG	NE-CZ-NH2	-7.69	116.45	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	e	162	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	2	18	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	g	162	ARG	NE-CZ-NH2	-7.68	116.46	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	B	18	ARG	NE-CZ-NH2	-7.68	116.46	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	x	100	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	O	82	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	0A	100	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	f	82	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	o	167	ARG	NE-CZ-NH1	7.67	124.13	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	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
1	3	167	ARG	NE-CZ-NH2	-7.66	116.47	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	G	97	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	t	100	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	j	82	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	2	162	ARG	NE-CZ-NH1	7.63	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	h	229	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	k	97	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	cD	97	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	F	100	ARG	NE-CZ-NH1	7.62	124.11	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	J	18	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	l	132	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	q	132	ARG	NE-CZ-NH2	-7.59	116.51	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	q	154	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	0	167	ARG	NE-CZ-NH1	7.59	124.09	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	zD	82	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	X	97	ARG	NE-CZ-NH2	-7.57	116.52	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
1	nB	154	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	Z	18	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	u	82	ARG	NE-CZ-NH1	7.55	124.08	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	S	173	ARG	NE-CZ-NH1	7.54	124.07	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	F	167	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	r	82	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	z	100	ARG	NE-CZ-NH2	-7.54	116.53	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	V	143	ARG	NE-CZ-NH1	7.53	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	N	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	r	154	ARG	NE-CZ-NH2	-7.52	116.54	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
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	1	162	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	Q	162	ARG	NE-CZ-NH2	-7.50	116.55	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	s	162	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	8	154	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	c	229	ARG	NE-CZ-NH1	-7.50	116.55	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C	100	ARG	NE-CZ-NH1	7.48	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
1	gE	167	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	H	154	ARG	NE-CZ-NH2	-7.47	116.56	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	m	97	ARG	NE-CZ-NH2	-7.47	116.56	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	v	97	ARG	NE-CZ-NH1	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7	229	ARG	NE-CZ-NH2	-7.45	116.57	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	2	229	ARG	NE-CZ-NH1	7.44	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	S	18	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
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	x	162	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	y	132	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1D	173	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	K	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	E	167	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	S	229	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	m	167	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	6D	18	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	T	173	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
1	sB	97	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	c	82	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4	154	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	VC	167	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	r	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	v	82	ARG	NE-CZ-NH2	-7.37	116.62	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	l	18	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	g	132	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	1B	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	A	229	ARG	NE-CZ-NH1	7.35	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
1	nA	97	ARG	NE-CZ-NH1	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	3	154	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	5	167	ARG	NE-CZ-NH2	-7.33	116.63	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	C	143	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	j	97	ARG	NE-CZ-NH2	-7.33	116.64	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	5	229	ARG	NE-CZ-NH1	7.33	123.96	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	L	97	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	M	229	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	N	18	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	K	229	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	a	184	TRP	N-CA-CB	-7.31	97.44	110.60
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FA	173	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	C	173	ARG	NE-CZ-NH1	7.30	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
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	R	167	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	f	154	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	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	W	154	ARG	NE-CZ-NH1	7.29	123.95	120.30
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	s	132	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	w	143	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	PD	132	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	L	18	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	PE	100	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	OC	100	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	x	162	ARG	NE-CZ-NH2	-7.25	116.67	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	r	97	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	W	97	ARG	NE-CZ-NH1	7.25	123.92	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	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	y	18	ARG	NE-CZ-NH1	7.24	123.92	120.30
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	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	O	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	82	ARG	NE-CZ-NH1	7.22	123.91	120.30
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
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	Y	132	ARG	NE-CZ-NH1	7.21	123.90	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	q	82	ARG	NE-CZ-NH1	7.20	123.90	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	6	97	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	cB	18	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	L	229	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	7	18	ARG	NE-CZ-NH1	7.18	123.89	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	F	97	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	p	154	ARG	NE-CZ-NH2	-7.17	116.71	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
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	V	154	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	y	82	ARG	NE-CZ-NH1	7.15	123.88	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	F	229	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	w	162	ARG	NE-CZ-NH2	-7.14	116.73	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	6	132	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	u	162	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	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	0D	100	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	6E	97	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	hE	82	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	9	167	ARG	NE-CZ-NH1	7.13	123.86	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	g	100	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	aC	18	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	l	143	ARG	NE-CZ-NH2	-7.11	116.74	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	S	154	ARG	NE-CZ-NH1	7.11	123.85	120.30
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	1	229	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	6	97	ARG	NE-CZ-NH1	7.11	123.85	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	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	lD	162	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	1A	143	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	R	143	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	i	162	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	x	154	ARG	NE-CZ-NH1	7.10	123.85	120.30
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	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
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	N	130	TYR	CB-CG-CD2	-7.09	116.74	121.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	l	18	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	kA	184	TRP	CB-CG-CD1	-7.07	117.81	127.00
1	X	154	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	KA	132	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	q	132	ARG	NE-CZ-NH1	7.06	123.83	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	Z	162	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	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	f	97	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	M	132	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
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	lB	167	ARG	NE-CZ-NH2	-7.01	116.79	120.30
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	e	82	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	jA	97	ARG	NE-CZ-NH2	-7.01	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	q	100	ARG	NE-CZ-NH1	7.01	123.80	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	G	82	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
1	L	173	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	t	18	ARG	NE-CZ-NH1	6.98	123.79	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	O	162	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	Y	143	ARG	NE-CZ-NH1	6.97	123.79	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	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	a	145	TYR	CB-CG-CD2	-6.97	116.82	121.00
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	D	100	ARG	NE-CZ-NH1	6.96	123.78	120.30
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	H	18	ARG	NE-CZ-NH1	6.96	123.78	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	A	173	ARG	NE-CZ-NH1	6.96	123.78	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	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	v	162	ARG	NE-CZ-NH1	6.95	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	82	ARG	NE-CZ-NH2	-6.95	116.83	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	c	154	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	XE	97	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	8	173	ARG	NE-CZ-NH1	6.94	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	w	229	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	y	229	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	4	173	ARG	NE-CZ-NH1	6.93	123.77	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	e	173	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	K	167	ARG	NE-CZ-NH1	6.93	123.76	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	1	100	ARG	NE-CZ-NH1	6.92	123.76	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	e	229	ARG	NE-CZ-NH1	6.91	123.75	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
1	m	82	ARG	NE-CZ-NH1	6.91	123.75	120.30
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	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	5	82	ARG	NE-CZ-NH1	6.89	123.75	120.30
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	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	M	162	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	U	162	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	l	132	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	9B	184	TRP	CA-CB-CG	6.87	126.75	113.70
1	z	100	ARG	NE-CZ-NH1	6.87	123.73	120.30
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	9	100	ARG	NE-CZ-NH1	6.86	123.73	120.30
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	R	143	ARG	NE-CZ-NH2	-6.86	116.87	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	R	154	ARG	NE-CZ-NH1	6.85	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	q	162	ARG	NE-CZ-NH1	6.85	123.72	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	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	3	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	3A	100	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	3	132	ARG	NE-CZ-NH2	-6.83	116.89	120.30
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	O	143	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	iA	82	ARG	NE-CZ-NH1	6.83	123.71	120.30
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	K	154	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	4	97	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	rA	100	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	U	229	ARG	NE-CZ-NH1	6.81	123.70	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	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	Z	167	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	r	154	ARG	NE-CZ-NH1	6.79	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	5B	132	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	184	TRP	CB-CG-CD1	-6.78	118.18	127.00
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	d	229	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	2	167	ARG	NE-CZ-NH1	6.78	123.69	120.30
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
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	m	145	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	o	143	ARG	NE-CZ-NH1	6.77	123.68	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	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	7	18	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	P	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	J	18	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	97	ARG	NE-CZ-NH1	6.75	123.67	120.30
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	gC	154	ARG	NE-CZ-NH1	6.74	123.67	120.30
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	S	97	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	t	229	ARG	NE-CZ-NH2	-6.73	116.93	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	W	100	ARG	NE-CZ-NH1	6.72	123.66	120.30
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	M	18	ARG	NE-CZ-NH1	6.72	123.66	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	k	162	ARG	NE-CZ-NH2	-6.71	116.94	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	z	132	ARG	NE-CZ-NH1	6.70	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	a	143	ARG	NE-CZ-NH2	-6.70	116.95	120.30
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	S	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	N	229	ARG	NE-CZ-NH1	6.69	123.64	120.30
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	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	z	82	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	DE	143	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7	154	ARG	NE-CZ-NH2	-6.67	116.96	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	yB	143	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	d	173	ARG	NE-CZ-NH1	6.67	123.63	120.30
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	L	132	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	SD	167	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	82	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	I	132	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	nB	143	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	f	97	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	0	100	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	TA	173	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	N	184	TRP	CB-CG-CD1	-6.65	118.36	127.00
1	l	229	ARG	NE-CZ-NH1	6.65	123.62	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	X	143	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	9E	100	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	q	97	ARG	NE-CZ-NH2	-6.64	116.98	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
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	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	T	167	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	M	97	ARG	NE-CZ-NH2	-6.62	116.99	120.30
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	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	o	229	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	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
1	5	143	ARG	NE-CZ-NH2	-6.61	117.00	120.30
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	z	18	ARG	NE-CZ-NH1	6.61	123.60	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	D	162	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	mB	132	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	U	167	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	C	154	ARG	NE-CZ-NH1	6.58	123.59	120.30
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	D	162	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	k	143	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	E	100	ARG	NE-CZ-NH1	6.56	123.58	120.30
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	S	154	ARG	NE-CZ-NH2	-6.56	117.02	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	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	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	9	162	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	0	132	ARG	NE-CZ-NH2	-6.55	117.03	120.30
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	I	229	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	Z	97	ARG	NE-CZ-NH1	6.55	123.57	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
1	mE	100	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	x	97	ARG	NE-CZ-NH1	6.54	123.57	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	p	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	d	100	ARG	NE-CZ-NH1	6.53	123.56	120.30
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	Q	18	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	oA	100	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	k	82	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
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	N	130	TYR	CB-CG-CD1	6.51	124.91	121.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	hE	154	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	k	229	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	m	145	TYR	CB-CG-CD1	6.50	124.90	121.00
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	6	184	TRP	CB-CG-CD1	-6.50	118.55	127.00
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	T	82	ARG	NE-CZ-NH2	-6.50	117.05	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	i	154	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	X	100	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	5	143	ARG	NE-CZ-NH1	6.49	123.54	120.30
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
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	B	143	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	t	167	ARG	NE-CZ-NH1	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bE	154	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	a	132	ARG	NE-CZ-NH1	6.48	123.54	120.30
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	T	132	ARG	NE-CZ-NH1	6.47	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	h	162	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	1B	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	Q	82	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	T	162	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	l	97	ARG	NE-CZ-NH1	6.46	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	154	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	SC	229	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	s	173	ARG	NE-CZ-NH1	6.45	123.53	120.30
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	H	97	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	WC	132	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	y	100	ARG	NE-CZ-NH2	-6.45	117.08	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	J	154	ARG	NE-CZ-NH1	6.44	123.52	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	W	167	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	C	82	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	G	143	ARG	NE-CZ-NH1	6.44	123.52	120.30
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	2	173	ARG	NE-CZ-NH2	-6.43	117.09	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	Q	154	ARG	NE-CZ-NH1	6.42	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	D	154	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	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	J	162	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	oD	162	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	y	145	TYR	CB-CG-CD2	-6.41	117.16	121.00
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	p	184	TRP	CB-CG-CD1	-6.40	118.67	127.00
1	5	229	ARG	NE-CZ-NH2	-6.40	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	0	173	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	5	97	ARG	NE-CZ-NH1	6.39	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	G	18	ARG	NE-CZ-NH1	6.39	123.50	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	E	162	ARG	NE-CZ-NH1	6.38	123.49	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	5	184	TRP	CB-CG-CD2	6.38	134.89	126.60
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	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	n	100	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	7A	162	ARG	NE-CZ-NH1	6.37	123.48	120.30
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	7	82	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	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	6	229	ARG	NE-CZ-NH1	6.36	123.48	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	w	132	ARG	NE-CZ-NH1	6.36	123.48	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	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	y	143	ARG	NE-CZ-NH1	6.35	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	100	ARG	NE-CZ-NH1	6.34	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	O	145	TYR	CB-CG-CD1	6.34	124.81	121.00
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	k	18	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	KA	82	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	S	167	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	E	132	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	W	229	ARG	NE-CZ-NH1	6.33	123.47	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	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	0	132	ARG	NE-CZ-NH1	6.33	123.46	120.30
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
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	QD	100	ARG	NE-CZ-NH1	6.33	123.46	120.30
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	l	184	TRP	CB-CG-CD2	6.32	134.82	126.60
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	D	143	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	7B	143	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	4	145	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	X	162	ARG	NE-CZ-NH1	6.31	123.45	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	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	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	P	97	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	a	167	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	g	97	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	h	132	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	j	167	ARG	NE-CZ-NH1	6.30	123.45	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
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	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	r	132	ARG	NE-CZ-NH1	6.29	123.44	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	hD	97	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	1D	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	J	173	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	1B	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	u	97	ARG	NE-CZ-NH1	6.28	123.44	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	1E	82	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	1	154	ARG	NE-CZ-NH1	6.28	123.44	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	E	154	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	GB	132	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	T	100	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	yD	97	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	143	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	6	82	ARG	NE-CZ-NH1	6.27	123.43	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	g	82	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	IB	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	O	145	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	GA	82	ARG	NE-CZ-NH2	-6.26	117.17	120.30
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
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	DA	173	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	L	82	ARG	NE-CZ-NH1	6.25	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	x	97	ARG	NE-CZ-NH2	-6.25	117.18	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	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	Z	154	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	q	154	ARG	NE-CZ-NH2	-6.24	117.18	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	I	100	ARG	NE-CZ-NH2	-6.24	117.18	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	eD	173	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	G	184	TRP	CB-CG-CD1	-6.23	118.91	127.00
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
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	9	97	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	cB	132	ARG	NE-CZ-NH2	-6.22	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	O	100	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	e	132	ARG	NE-CZ-NH1	6.22	123.41	120.30
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	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	z	162	ARG	NE-CZ-NH2	-6.20	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	9	132	ARG	NE-CZ-NH1	6.20	123.40	120.30
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	j	154	ARG	NE-CZ-NH2	-6.20	117.20	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	h	18	ARG	NE-CZ-NH1	6.19	123.40	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	WD	143	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	4E	162	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	x	154	ARG	NE-CZ-NH2	-6.18	117.21	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	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	G	173	ARG	NE-CZ-NH1	6.17	123.39	120.30
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	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	L	154	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	l	82	ARG	NE-CZ-NH1	6.16	123.38	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
1	nB	82	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	H	82	ARG	NE-CZ-NH2	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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	eE	162	ARG	NE-CZ-NH1	6.14	123.37	120.30
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	a	145	TYR	CB-CG-CD1	6.14	124.69	121.00
1	XA	229	ARG	NE-CZ-NH1	6.14	123.37	120.30
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	A	173	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	zD	97	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	F	100	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	Y	97	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	c	132	ARG	NE-CZ-NH2	-6.13	117.23	120.30
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	H	100	ARG	NE-CZ-NH1	6.13	123.37	120.30
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	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	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	f	18	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	s	229	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	5	154	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	v	18	ARG	NE-CZ-NH1	6.12	123.36	120.30
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	EC	162	ARG	NE-CZ-NH1	6.12	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	gE	162	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	a	229	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	FA	143	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	I	100	ARG	NE-CZ-NH1	6.11	123.35	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	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	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	S	162	ARG	NE-CZ-NH2	-6.09	117.25	120.30
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	i	229	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	mE	184	TRP	CA-CB-CG	6.09	125.27	113.70
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	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	WD	162	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	R	82	ARG	NE-CZ-NH2	-6.08	117.26	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	I	162	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	J	82	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	u	97	ARG	NE-CZ-NH2	-6.07	117.26	120.30
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	y	145	TYR	CB-CG-CD1	6.07	124.64	121.00
1	6B	184	TRP	CB-CG-CD2	6.07	134.49	126.60
1	I	154	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	n	229	ARG	NE-CZ-NH1	6.07	123.33	120.30
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
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	rE	18	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	L	162	ARG	NE-CZ-NH1	6.06	123.33	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	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	9	100	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	6A	184	TRP	CB-CG-CD1	-6.05	119.14	127.00
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	v	229	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	uE	132	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	k	167	ARG	NE-CZ-NH1	6.04	123.32	120.30
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	97	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	4	154	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	2A	18	ARG	NE-CZ-NH2	-6.04	117.28	120.30
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	l	184	TRP	CA-CB-CG	6.03	125.16	113.70
1	6	167	ARG	NE-CZ-NH2	-6.03	117.28	120.30
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	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	b	167	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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	kD	145	TYR	CB-CG-CD1	6.02	124.61	121.00
1	3	169	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	4	100	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	ZE	130	TYR	CB-CG-CD1	6.02	124.61	121.00
1	o	162	ARG	NE-CZ-NH2	-6.02	117.29	120.30
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	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
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	G	82	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	H	154	ARG	NE-CZ-NH1	6.01	123.30	120.30
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	S	100	ARG	NE-CZ-NH1	6.00	123.30	120.30
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	W	162	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	v	100	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	0	143	ARG	NE-CZ-NH1	6.00	123.30	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	oC	184	TRP	CB-CG-CD1	-6.00	119.21	127.00
1	e	18	ARG	NE-CZ-NH1	5.99	123.30	120.30
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	F	162	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	8	167	ARG	NE-CZ-NH2	-5.99	117.30	120.30
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	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
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	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	v	184	TRP	CB-CG-CD1	-5.98	119.22	127.00
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	Z	173	ARG	NE-CZ-NH1	5.97	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	h	184	TRP	N-CA-CB	-5.97	99.85	110.60
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	Z	100	ARG	NE-CZ-NH1	5.97	123.28	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	nB	82	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	18	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	8C	167	ARG	NE-CZ-NH1	5.96	123.28	120.30
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	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	eA	184	TRP	CB-CG-CD1	-5.95	119.26	127.00
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	u	229	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	lA	184	TRP	CB-CG-CD2	-5.95	118.86	126.60
1	O	97	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	s	154	ARG	NE-CZ-NH1	5.95	123.28	120.30
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	4	162	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	bC	162	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	82	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	Q	229	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	w	173	ARG	NE-CZ-NH1	5.95	123.27	120.30
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	c	184	TRP	CA-CB-CG	5.94	124.99	113.70
1	C	132	ARG	NE-CZ-NH1	5.94	123.27	120.30
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	F	173	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	4	167	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	vB	132	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	FC	173	ARG	NE-CZ-NH1	5.94	123.27	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	184	TRP	N-CA-CB	-5.93	99.92	110.60
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	p	82	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	wB	173	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	2	100	ARG	NE-CZ-NH2	-5.92	117.34	120.30
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	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
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	FE	167	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	b	132	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	tD	162	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	AB	100	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	T	162	ARG	NE-CZ-NH2	-5.91	117.35	120.30
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	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	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	ZC	154	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	vD	167	ARG	NE-CZ-NH1	5.90	123.25	120.30
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	c	143	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	9	229	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	P	132	ARG	NE-CZ-NH1	5.89	123.25	120.30
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
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	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	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	Q	167	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	u	18	ARG	NE-CZ-NH1	5.87	123.23	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	M	82	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	YB	143	ARG	NE-CZ-NH2	-5.87	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	yC	145	TYR	CB-CG-CD1	5.87	124.52	121.00
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	HB	132	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	J	167	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
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	m	173	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	s	100	ARG	NE-CZ-NH1	5.85	123.22	120.30
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	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	v	173	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	BE	18	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	G	173	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	t	162	ARG	NE-CZ-NH2	-5.84	117.38	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	W	173	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	g	145	TYR	CB-CG-CD2	-5.84	117.50	121.00
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	D	167	ARG	NE-CZ-NH2	-5.84	117.38	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	173	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	k	132	ARG	NE-CZ-NH1	5.83	123.22	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
1	L	100	ARG	NE-CZ-NH1	5.83	123.22	120.30
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	k	100	ARG	NE-CZ-NH1	5.82	123.21	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	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	T	130	TYR	CB-CG-CD1	5.82	124.49	121.00
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	CE	173	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	T	130	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	aE	132	ARG	NE-CZ-NH1	5.81	123.21	120.30
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	8	184	TRP	CB-CG-CD1	-5.81	119.45	127.00
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	0	18	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	f	229	ARG	NE-CZ-NH2	5.80	123.20	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	RB	82	ARG	NE-CZ-NH1	5.79	123.20	120.30
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	s	97	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	P	154	ARG	NE-CZ-NH2	-5.79	117.41	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	f	132	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	m	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	f	100	ARG	NE-CZ-NH1	5.78	123.19	120.30
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	h	97	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	hC	229	ARG	NE-CZ-NH2	-5.77	117.41	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	143	ARG	NE-CZ-NH1	5.77	123.18	120.30
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	130	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	GB	132	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	N	100	ARG	NE-CZ-NH2	-5.76	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
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	T	154	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	l	154	ARG	NE-CZ-NH1	5.76	123.18	120.30
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	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	1D	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	U	100	ARG	NE-CZ-NH1	5.75	123.18	120.30
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	1	167	ARG	NE-CZ-NH2	-5.75	117.42	120.30
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	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	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	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	O	154	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	wB	100	ARG	NE-CZ-NH2	-5.74	117.43	120.30
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	s	18	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	18	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	0D	100	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	HE	184	TRP	CB-CG-CD2	-5.74	119.14	126.60
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	m	162	ARG	NE-CZ-NH1	5.73	123.17	120.30
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	cC	143	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	C	167	ARG	NE-CZ-NH1	5.73	123.17	120.30
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	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	k	162	ARG	NE-CZ-NH1	5.72	123.16	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	2	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	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	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	P	143	ARG	NE-CZ-NH1	5.71	123.16	120.30
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	Q	184	TRP	CB-CG-CD1	-5.71	119.58	127.00
1	q	229	ARG	NE-CZ-NH2	-5.71	117.44	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	y	147	PRO	CA-N-CD	-5.70	103.52	111.50
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	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	P	173	ARG	NE-CZ-NH1	5.70	123.15	120.30
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	7	100	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	5B	144	MET	CG-SD-CE	-5.69	91.09	100.20
1	iB	143	ARG	NE-CZ-NH2	-5.69	117.45	120.30
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	lD	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
1	Q	100	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	a	100	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	u	130	TYR	CB-CG-CD1	5.69	124.41	121.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	S	173	ARG	NE-CZ-NH2	-5.68	117.46	120.30
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	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	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	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	d	162	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	j	81	ASP	CB-CG-OD2	5.67	123.40	118.30
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	8	100	ARG	NE-CZ-NH2	-5.67	117.47	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	s	154	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	uC	229	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	f	143	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	WE	147	PRO	CA-N-CD	-5.66	103.57	111.50
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	o	143	ARG	NE-CZ-NH2	-5.66	117.47	120.30
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	C	173	ARG	NE-CZ-NH2	-5.65	117.47	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	F	143	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	R	18	ARG	NE-CZ-NH1	5.65	123.12	120.30
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	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	QB	162	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	M	173	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	8D	100	ARG	NE-CZ-NH1	5.64	123.12	120.30
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	X	18	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	8A	229	ARG	NE-CZ-NH1	5.64	123.12	120.30
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	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	G	167	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	U	162	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	b	18	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	WE	145	TYR	CB-CG-CD2	-5.62	117.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	229	ARG	NE-CZ-NH1	5.62	123.11	120.30
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	l	184	TRP	N-CA-CB	-5.62	100.49	110.60
1	oB	184	TRP	N-CA-CB	-5.62	100.49	110.60
1	FD	143	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	k	100	ARG	NE-CZ-NH2	-5.61	117.49	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	O	167	ARG	NE-CZ-NH1	5.61	123.11	120.30
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
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	GA	100	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	TB	173	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	R	184	TRP	CB-CG-CD1	-5.59	119.73	127.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	r	184	TRP	CA-CB-CG	5.59	124.31	113.70
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	3	100	ARG	NE-CZ-NH2	-5.58	117.51	120.30
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	H	162	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	p	152	ASP	CB-CG-OD2	5.58	123.33	118.30
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	9D	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	R	132	ARG	NE-CZ-NH2	-5.58	117.51	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	Y	100	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	sB	162	ARG	NE-CZ-NH1	5.58	123.09	120.30
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	M	18	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	G	154	ARG	NE-CZ-NH1	5.57	123.08	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	82	ARG	NE-CZ-NH2	-5.57	117.52	120.30
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	X	167	ARG	NE-CZ-NH1	5.57	123.08	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	5A	100	ARG	NE-CZ-NH2	-5.56	117.52	120.30
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	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	kD	143	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	z	173	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	QA	167	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	7	143	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	aD	162	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	6	143	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	S	97	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	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	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	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	B	82	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	p	82	ARG	NE-CZ-NH1	5.53	123.07	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	t	132	ARG	NE-CZ-NH1	5.53	123.06	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	167	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	YC	167	ARG	NE-CZ-NH2	-5.53	117.54	120.30
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	r	100	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	JE	167	ARG	NE-CZ-NH2	-5.52	117.54	120.30
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	2	143	ARG	NE-CZ-NH2	-5.52	117.54	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	g	229	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	cC	167	ARG	NE-CZ-NH2	-5.52	117.54	120.30
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	4B	18	ARG	NE-CZ-NH1	5.51	123.06	120.30
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	W	132	ARG	NE-CZ-NH1	5.51	123.05	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	8	229	ARG	NE-CZ-NH1	5.50	123.05	120.30
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	U	167	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	1	130	TYR	CB-CG-CD2	-5.50	117.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0B	147	PRO	CA-N-CD	-5.50	103.80	111.50
1	8	173	ARG	NE-CZ-NH2	-5.50	117.55	120.30
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	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	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	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	h	154	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	3	162	ARG	NE-CZ-NH1	5.49	123.05	120.30
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	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	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
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	ZA	85	PRO	CA-N-CD	-5.48	103.83	111.50
1	2	97	ARG	NE-CZ-NH1	5.47	123.04	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	I	173	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	j	10	MET	CG-SD-CE	-5.47	91.45	100.20
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	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	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
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	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	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	3	154	ARG	NE-CZ-NH2	-5.45	117.57	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	Q	184	TRP	CA-CB-CG	5.45	124.05	113.70
1	g	82	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	q	143	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	7	173	ARG	NE-CZ-NH1	5.45	123.03	120.30
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	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	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	S	82	ARG	NE-CZ-NH2	-5.44	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	V	184	TRP	CA-CB-CG	5.44	124.04	113.70
1	Y	167	ARG	NE-CZ-NH1	5.44	123.02	120.30
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	3	18	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	Z	184	TRP	N-CA-CB	-5.44	100.81	110.60
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	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	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	Q	173	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	5E	132	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	SA	167	ARG	NE-CZ-NH1	5.43	123.01	120.30
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	V	162	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	0	229	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	o	130	TYR	CB-CG-CD2	-5.42	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	oC	132	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	ZD	97	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	T	143	ARG	NE-CZ-NH2	-5.42	117.59	120.30
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	2	132	ARG	NE-CZ-NH2	-5.42	117.59	120.30
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	a	167	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	zD	97	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	82	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	YA	147	PRO	CA-N-CD	-5.41	103.92	111.50
1	P	143	ARG	NE-CZ-NH2	-5.41	117.59	120.30
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	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	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	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
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	O	173	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	7	143	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	FB	162	ARG	NE-CZ-NH2	-5.40	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	R	229	ARG	NE-CZ-NH1	5.39	123.00	120.30
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	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	f	167	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	m	100	ARG	NE-CZ-NH2	-5.38	117.61	120.30
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	YB	184	TRP	CB-CG-CD2	-5.38	119.60	126.60
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
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	n	97	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	kC	162	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	8	132	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	6C	229	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	h	154	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	vA	169	TYR	CB-CG-CD2	-5.37	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	Y	173	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	2	154	ARG	NE-CZ-NH1	5.37	122.99	120.30
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	b	173	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	W	132	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	e	173	ARG	NE-CZ-NH2	-5.37	117.62	120.30
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	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	Z	229	ARG	NE-CZ-NH1	5.37	122.98	120.30
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	E	82	ARG	NE-CZ-NH2	-5.36	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	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	D	100	ARG	NE-CZ-NH2	-5.36	117.62	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	oE	18	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	j	100	ARG	NE-CZ-NH1	5.35	122.98	120.30
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	GE	184	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	g	100	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	4	100	ARG	NE-CZ-NH1	5.35	122.97	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	ARG	NE-CZ-NH2	-5.35	117.63	120.30
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	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
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	6	100	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	aA	173	ARG	NE-CZ-NH1	5.34	122.97	120.30
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	C	145	TYR	CB-CG-CD2	-5.33	117.80	121.00
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	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	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	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BF	143	ARG	NE-CZ-NH2	-5.32	117.64	120.30
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	I	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	N	167	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	DC	143	ARG	NE-CZ-NH1	5.32	122.96	120.30
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	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	h	184	TRP	CB-CA-C	5.31	121.02	110.40
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	I	145	TYR	CB-CG-CD2	-5.31	117.82	121.00
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	7C	154	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	a	184	TRP	CB-CA-C	5.30	121.00	110.40
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	nB	143	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	7	100	ARG	NE-CZ-NH1	5.29	122.95	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	O	82	ARG	NE-CZ-NH1	5.29	122.95	120.30
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	2	132	ARG	NE-CZ-NH1	5.29	122.94	120.30
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	y	184	TRP	N-CA-CB	-5.29	101.09	110.60
1	gB	229	ARG	NE-CZ-NH1	5.29	122.94	120.30
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	YE	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
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	L	97	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	V	229	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	4C	184	TRP	CB-CG-CD2	5.28	133.46	126.60
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	R	169	TYR	CB-CG-CD2	5.27	124.16	121.00
1	Z	132	ARG	NE-CZ-NH1	5.27	122.94	120.30
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	y	154	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	3E	184	TRP	CB-CG-CD1	-5.27	120.15	127.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	L	184	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	4	145	TYR	CB-CG-CD1	5.26	124.16	121.00
1	5	173	ARG	NE-CZ-NH1	5.26	122.93	120.30
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	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
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	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	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	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	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	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	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	18	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	o	130	TYR	CB-CG-CD1	5.24	124.14	121.00
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	e	39	MET	CG-SD-CE	-5.23	91.83	100.20
1	oD	173	ARG	NE-CZ-NH1	5.23	122.92	120.30
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	5E	229	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	2	184	TRP	CA-CB-CG	5.23	123.63	113.70
1	DF	132	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	V	229	ARG	NE-CZ-NH2	-5.23	117.69	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	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
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	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	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	s	145	TYR	CB-CG-CD2	-5.21	117.87	121.00
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	sB	184	TRP	N-CA-CB	-5.21	101.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	G	144	MET	CG-SD-CE	-5.21	91.87	100.20
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	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
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	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	x	143	ARG	NE-CZ-NH2	-5.20	117.70	120.30
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	L	82	ARG	NE-CZ-NH2	-5.20	117.70	120.30
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	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	N	167	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	m	147	PRO	CA-N-CD	-5.19	104.23	111.50
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	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	YE	18	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	I	147	PRO	CA-N-CD	-5.18	104.24	111.50
1	sC	184	TRP	N-CA-CB	-5.18	101.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	97	ARG	NE-CZ-NH1	5.18	122.89	120.30
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	132	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	mC	147	PRO	CA-N-CD	-5.18	104.25	111.50
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	i	143	ARG	NE-CZ-NH1	5.18	122.89	120.30
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	0	143	ARG	NE-CZ-NH2	-5.17	117.71	120.30
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	oB	173	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	4	147	PRO	CA-N-CD	-5.17	104.26	111.50
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	5	82	ARG	NE-CZ-NH2	-5.17	117.72	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	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	4C	184	TRP	CA-CB-CG	5.17	123.51	113.70
1	F	118	MET	CG-SD-CE	-5.16	91.94	100.20
1	K	143	ARG	NE-CZ-NH1	5.16	122.88	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	IB	97	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	3	97	ARG	NE-CZ-NH1	5.16	122.88	120.30
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	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	f	173	ARG	NE-CZ-NH1	5.15	122.88	120.30
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
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	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	97	ARG	NE-CZ-NH1	5.14	122.87	120.30
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	S	184	TRP	N-CA-CB	-5.14	101.35	110.60
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	O	147	PRO	CA-N-CD	-5.14	104.31	111.50
1	x	100	ARG	NE-CZ-NH2	-5.14	117.73	120.30
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	BD	96	MET	CG-SD-CE	-5.13	91.98	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3D	167	ARG	NE-CZ-NH2	-5.13	117.73	120.30
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	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	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	s	132	ARG	NE-CZ-NH2	-5.13	117.74	120.30
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	U	132	ARG	NE-CZ-NH1	5.13	122.86	120.30
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	bB	173	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	229	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	J	162	ARG	NE-CZ-NH1	5.12	122.86	120.30
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	K	132	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	y	82	ARG	NE-CZ-NH2	-5.12	117.74	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	3	167	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
1	oE	184	TRP	CA-CB-CG	5.12	123.42	113.70
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	8	97	ARG	NE-CZ-NH2	-5.12	117.74	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	J	100	ARG	NE-CZ-NH2	-5.11	117.75	120.30
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	M	143	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	O	132	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	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	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	K	144	MET	CG-SD-CE	-5.10	92.04	100.20
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	L	229	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	y	173	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	yA	154	ARG	NE-CZ-NH2	-5.09	117.75	120.30
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	C	145	TYR	CB-CG-CD1	5.09	124.05	121.00
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	l	144	MET	CG-SD-CE	-5.09	92.06	100.20
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	147	PRO	CA-N-CD	-5.08	104.38	111.50
1	r	143	ARG	NE-CZ-NH1	5.08	122.84	120.30
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	T	184	TRP	N-CA-CB	-5.08	101.45	110.60
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	u	100	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	5C	154	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	KA	229	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	h	184	TRP	CA-CB-CG	5.08	123.34	113.70
1	6	173	ARG	NE-CZ-NH1	5.08	122.84	120.30
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	P	167	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	1	229	ARG	NE-CZ-NH2	-5.07	117.76	120.30
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	4E	229	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	T	167	ARG	NE-CZ-NH2	-5.07	117.77	120.30
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	A	132	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	M	97	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	g	147	PRO	CA-N-CD	-5.07	104.41	111.50
1	3	143	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	yD	132	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	F	154	ARG	NE-CZ-NH2	-5.06	117.77	120.30
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	U	173	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	Y	82	ARG	NE-CZ-NH1	5.06	122.83	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	97	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	iD	100	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	s	82	ARG	NE-CZ-NH1	5.06	122.83	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	I	145	TYR	CB-CG-CD1	5.06	124.03	121.00
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	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	e	143	ARG	NE-CZ-NH1	5.05	122.83	120.30
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	C	162	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	bC	100	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	o	154	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	jA	169	TYR	CB-CG-CD2	5.04	124.03	121.00
1	B	132	ARG	NE-CZ-NH1	5.04	122.82	120.30
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	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	s	162	ARG	NE-CZ-NH2	-5.04	117.78	120.30
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	FA	167	ARG	NE-CZ-NH1	5.04	122.82	120.30
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	mB	144	MET	CG-SD-CE	-5.03	92.15	100.20
1	1C	100	ARG	NE-CZ-NH2	-5.03	117.78	120.30
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	u	100	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	V	132	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	MA	145	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	3B	143	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	tE	173	ARG	NE-CZ-NH1	5.03	122.81	120.30
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	SA	145	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	L	132	ARG	NE-CZ-NH2	-5.02	117.79	120.30
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	j	229	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	dA	132	ARG	NE-CZ-NH2	-5.02	117.79	120.30
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	2	143	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	9	144	MET	CG-SD-CE	-5.02	92.17	100.20
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	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
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	8C	162	ARG	NE-CZ-NH2	-5.01	117.80	120.30
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	147	PRO	CA-N-CD	-5.01	104.49	111.50
1	p	162	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	BF	229	ARG	NE-CZ-NH1	5.00	122.80	120.30
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	p	97	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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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
All	All	678510	680778	680778	-

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 -.

There are no clashes.

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%)	38	78
1	0A	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	10	49
1	0B	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	0C	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	0D	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	0E	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	13	56
1	1	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	1A	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	5	32
1	1B	229/231 (99%)	207 (90%)	12 (5%)	10 (4%)	4	29
1	1C	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	1D	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	10	49
1	1E	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	2	229/231 (99%)	215 (94%)	9 (4%)	5 (2%)	10	49
1	2A	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	2B	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	6	35
1	2C	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	2D	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	8	44
1	2E	229/231 (99%)	199 (87%)	27 (12%)	3 (1%)	16	63
1	3	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	6	35
1	3A	229/231 (99%)	213 (93%)	10 (4%)	6 (3%)	8	44
1	3B	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	13	56
1	3C	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	3D	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	3E	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	4	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	8	44
1	4A	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	4B	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	4C	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	4D	229/231 (99%)	203 (89%)	18 (8%)	8 (3%)	6	35
1	4E	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	7	39
1	5	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	16	63
1	5A	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5B	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	5C	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	5D	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	5E	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	6	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39
1	6A	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	13	56
1	6B	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	13	56
1	6C	229/231 (99%)	200 (87%)	23 (10%)	6 (3%)	8	44
1	6D	229/231 (99%)	215 (94%)	10 (4%)	4 (2%)	13	56
1	6E	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	8	44
1	7	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	6	35
1	7A	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	16	63
1	7B	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	7C	229/231 (99%)	205 (90%)	15 (7%)	9 (4%)	5	32
1	7D	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	7E	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	7	39
1	8	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	8A	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	16	63
1	8B	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	8C	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	16	63
1	8D	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	8E	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	7	39
1	9	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	10	49
1	9A	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	9B	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	10	49
1	9C	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	9D	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	16	63
1	9E	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	16	63
1	A	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	8	44
1	AA	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	21	69
1	AB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	229/231 (99%)	215 (94%)	12 (5%)	2 (1%)	21	69
1	AD	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	AE	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	8	44
1	AF	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	B	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	21	69
1	BA	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	BB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	BC	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	7	39
1	BD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	10	49
1	BE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	BF	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	7	39
1	C	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	CA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	CB	229/231 (99%)	214 (93%)	12 (5%)	3 (1%)	16	63
1	CC	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	10	49
1	CD	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	16	63
1	CE	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	CF	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	D	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	DA	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	DB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	DC	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	DD	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	5	32
1	DE	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	DF	229/231 (99%)	200 (87%)	21 (9%)	8 (3%)	6	35
1	E	229/231 (99%)	206 (90%)	14 (6%)	9 (4%)	5	32
1	EA	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	EB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	EC	229/231 (99%)	200 (87%)	24 (10%)	5 (2%)	10	49
1	ED	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	10	49
1	EE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EF	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	7	39
1	F	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	FA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	FB	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	FC	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	FD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	FE	229/231 (99%)	213 (93%)	12 (5%)	4 (2%)	13	56
1	FF	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	G	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	7	39
1	GA	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	13	56
1	GB	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	GC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	GD	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39
1	GE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	H	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	HA	229/231 (99%)	199 (87%)	22 (10%)	8 (3%)	6	35
1	HB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	HC	229/231 (99%)	201 (88%)	21 (9%)	7 (3%)	7	39
1	HD	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	HE	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	I	229/231 (99%)	201 (88%)	25 (11%)	3 (1%)	16	63
1	IA	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	IB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	IC	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	21	69
1	ID	229/231 (99%)	202 (88%)	21 (9%)	6 (3%)	8	44
1	IE	229/231 (99%)	207 (90%)	20 (9%)	2 (1%)	21	69
1	J	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	JA	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	JB	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	7	39
1	JC	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	JD	229/231 (99%)	210 (92%)	17 (7%)	2 (1%)	21	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JE	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	K	229/231 (99%)	205 (90%)	16 (7%)	8 (3%)	6	35
1	KA	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	10	49
1	KB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	KC	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39
1	KD	229/231 (99%)	211 (92%)	17 (7%)	1 (0%)	38	78
1	KE	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	L	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	16	63
1	LA	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	LB	229/231 (99%)	206 (90%)	14 (6%)	9 (4%)	5	32
1	LC	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	6	35
1	LD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	LE	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	M	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	MA	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	13	56
1	MB	229/231 (99%)	210 (92%)	17 (7%)	2 (1%)	21	69
1	MC	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	13	56
1	MD	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	16	63
1	ME	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	N	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	13	56
1	NA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	NB	229/231 (99%)	205 (90%)	15 (7%)	9 (4%)	5	32
1	NC	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	6	35
1	ND	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	16	63
1	NE	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	16	63
1	O	229/231 (99%)	212 (93%)	12 (5%)	5 (2%)	10	49
1	OA	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	10	49
1	OB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	OC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	OD	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	OE	229/231 (99%)	217 (95%)	8 (3%)	4 (2%)	13	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	PA	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	16	63
1	PB	229/231 (99%)	204 (89%)	16 (7%)	9 (4%)	5	32
1	PC	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	PD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	PE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	Q	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39
1	QA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	QB	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	16	63
1	QC	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	QD	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	QE	229/231 (99%)	209 (91%)	11 (5%)	9 (4%)	5	32
1	R	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	13	56
1	RA	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	13	56
1	RB	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	13	56
1	RC	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	RD	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	RE	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	S	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	SA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	16	63
1	SB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	SC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	SD	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	SE	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	13	56
1	T	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	TA	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	TB	229/231 (99%)	210 (92%)	12 (5%)	7 (3%)	7	39
1	TC	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	TD	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	TE	229/231 (99%)	213 (93%)	12 (5%)	4 (2%)	13	56
1	U	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	8	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	16	63
1	UB	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	13	56
1	UC	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	10	49
1	UD	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	UE	229/231 (99%)	205 (90%)	22 (10%)	2 (1%)	21	69
1	V	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	VA	229/231 (99%)	209 (91%)	10 (4%)	10 (4%)	4	29
1	VB	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	VC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	VD	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	VE	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	16	63
1	W	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	13	56
1	WA	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	13	56
1	WB	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	WC	229/231 (99%)	203 (89%)	25 (11%)	1 (0%)	38	78
1	WD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	10	49
1	WE	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	X	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	8	44
1	XA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	XB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	XC	229/231 (99%)	211 (92%)	9 (4%)	9 (4%)	5	32
1	XD	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	16	63
1	XE	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	Y	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	YA	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	16	63
1	YB	229/231 (99%)	202 (88%)	21 (9%)	6 (3%)	8	44
1	YC	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	YD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	YE	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	Z	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	ZA	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZB	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	13	56
1	ZC	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	ZD	229/231 (99%)	209 (91%)	18 (8%)	2 (1%)	21	69
1	ZE	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	a	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	aA	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	aB	229/231 (99%)	206 (90%)	21 (9%)	2 (1%)	21	69
1	aC	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	aD	229/231 (99%)	206 (90%)	15 (7%)	8 (3%)	6	35
1	aE	229/231 (99%)	204 (89%)	23 (10%)	2 (1%)	21	69
1	b	229/231 (99%)	208 (91%)	12 (5%)	9 (4%)	5	32
1	bA	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	bB	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	13	56
1	bC	229/231 (99%)	203 (89%)	16 (7%)	10 (4%)	4	29
1	bD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	bE	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	c	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	cA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	16	63
1	cB	229/231 (99%)	205 (90%)	16 (7%)	8 (3%)	6	35
1	cC	229/231 (99%)	202 (88%)	20 (9%)	7 (3%)	7	39
1	cD	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	13	56
1	cE	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	d	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	10	49
1	dA	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	dB	229/231 (99%)	210 (92%)	13 (6%)	6 (3%)	8	44
1	dC	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	dD	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	8	44
1	dE	229/231 (99%)	202 (88%)	23 (10%)	4 (2%)	13	56
1	e	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	16	63
1	eA	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	eB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	eC	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	21	69
1	eD	229/231 (99%)	215 (94%)	10 (4%)	4 (2%)	13	56
1	eE	229/231 (99%)	206 (90%)	15 (7%)	8 (3%)	6	35
1	f	229/231 (99%)	205 (90%)	17 (7%)	7 (3%)	7	39
1	fA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	fB	229/231 (99%)	209 (91%)	18 (8%)	2 (1%)	21	69
1	fC	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	fD	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	fE	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	g	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	10	49
1	gA	229/231 (99%)	207 (90%)	14 (6%)	8 (3%)	6	35
1	gB	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	16	63
1	gC	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	21	69
1	gD	229/231 (99%)	203 (89%)	18 (8%)	8 (3%)	6	35
1	gE	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	13	56
1	h	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	hA	229/231 (99%)	209 (91%)	15 (7%)	5 (2%)	10	49
1	hB	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	21	69
1	hC	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	21	69
1	hD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	hE	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	21	69
1	i	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	iA	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	16	63
1	iB	229/231 (99%)	206 (90%)	16 (7%)	7 (3%)	7	39
1	iC	229/231 (99%)	209 (91%)	11 (5%)	9 (4%)	5	32
1	iD	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	10	49
1	iE	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	21	69
1	j	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	jA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	jB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	jC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	jD	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	jE	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	k	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	16	63
1	kA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	kB	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	kC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	kD	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	kE	229/231 (99%)	207 (90%)	13 (6%)	9 (4%)	5	32
1	l	229/231 (99%)	211 (92%)	12 (5%)	6 (3%)	8	44
1	lA	229/231 (99%)	209 (91%)	19 (8%)	1 (0%)	38	78
1	lB	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	lC	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	lD	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	lE	229/231 (99%)	210 (92%)	16 (7%)	3 (1%)	16	63
1	m	229/231 (99%)	204 (89%)	17 (7%)	8 (3%)	6	35
1	mA	229/231 (99%)	204 (89%)	20 (9%)	5 (2%)	10	49
1	mB	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	mC	229/231 (99%)	205 (90%)	18 (8%)	6 (3%)	8	44
1	mD	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63
1	mE	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	13	56
1	n	229/231 (99%)	205 (90%)	19 (8%)	5 (2%)	10	49
1	nA	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	nB	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	10	49
1	nC	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	nD	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	nE	229/231 (99%)	203 (89%)	21 (9%)	5 (2%)	10	49
1	o	229/231 (99%)	208 (91%)	13 (6%)	8 (3%)	6	35
1	oA	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	oB	229/231 (99%)	204 (89%)	21 (9%)	4 (2%)	13	56
1	oC	229/231 (99%)	203 (89%)	19 (8%)	7 (3%)	7	39
1	oD	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	16	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	oE	229/231 (99%)	213 (93%)	13 (6%)	3 (1%)	16	63
1	p	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	pA	229/231 (99%)	201 (88%)	25 (11%)	3 (1%)	16	63
1	pB	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	pC	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	pD	229/231 (99%)	209 (91%)	12 (5%)	8 (3%)	6	35
1	pE	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	13	56
1	q	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	7	39
1	qA	229/231 (99%)	209 (91%)	13 (6%)	7 (3%)	7	39
1	qB	229/231 (99%)	203 (89%)	20 (9%)	6 (3%)	8	44
1	qC	229/231 (99%)	213 (93%)	9 (4%)	7 (3%)	7	39
1	qD	229/231 (99%)	212 (93%)	11 (5%)	6 (3%)	8	44
1	qE	229/231 (99%)	201 (88%)	23 (10%)	5 (2%)	10	49
1	r	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	13	56
1	rA	229/231 (99%)	208 (91%)	14 (6%)	7 (3%)	7	39
1	rB	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	rC	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	rD	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	rE	229/231 (99%)	207 (90%)	13 (6%)	9 (4%)	5	32
1	s	229/231 (99%)	212 (93%)	14 (6%)	3 (1%)	16	63
1	sA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	sB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	21	69
1	sC	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	sD	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	sE	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	t	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	13	56
1	tA	229/231 (99%)	206 (90%)	19 (8%)	4 (2%)	13	56
1	tB	229/231 (99%)	210 (92%)	11 (5%)	8 (3%)	6	35
1	tC	229/231 (99%)	200 (87%)	21 (9%)	8 (3%)	6	35
1	tD	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	tE	229/231 (99%)	206 (90%)	20 (9%)	3 (1%)	16	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	229/231 (99%)	207 (90%)	18 (8%)	4 (2%)	13	56
1	uA	229/231 (99%)	208 (91%)	15 (7%)	6 (3%)	8	44
1	uB	229/231 (99%)	211 (92%)	14 (6%)	4 (2%)	13	56
1	uC	229/231 (99%)	207 (90%)	19 (8%)	3 (1%)	16	63
1	uD	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49
1	uE	229/231 (99%)	208 (91%)	17 (7%)	4 (2%)	13	56
1	v	229/231 (99%)	211 (92%)	11 (5%)	7 (3%)	7	39
1	vA	229/231 (99%)	207 (90%)	20 (9%)	2 (1%)	21	69
1	vB	229/231 (99%)	209 (91%)	16 (7%)	4 (2%)	13	56
1	vC	229/231 (99%)	210 (92%)	12 (5%)	7 (3%)	7	39
1	vD	229/231 (99%)	201 (88%)	21 (9%)	7 (3%)	7	39
1	vE	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	w	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	wA	229/231 (99%)	205 (90%)	20 (9%)	4 (2%)	13	56
1	wB	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	wC	229/231 (99%)	214 (93%)	10 (4%)	5 (2%)	10	49
1	wD	229/231 (99%)	213 (93%)	11 (5%)	5 (2%)	10	49
1	wE	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	21	69
1	x	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	16	63
1	xA	229/231 (99%)	206 (90%)	18 (8%)	5 (2%)	10	49
1	xB	229/231 (99%)	204 (89%)	19 (8%)	6 (3%)	8	44
1	xC	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	16	63
1	xD	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	xE	229/231 (99%)	206 (90%)	17 (7%)	6 (3%)	8	44
1	y	229/231 (99%)	207 (90%)	17 (7%)	5 (2%)	10	49
1	yA	229/231 (99%)	209 (91%)	17 (7%)	3 (1%)	16	63
1	yB	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	21	69
1	yC	229/231 (99%)	209 (91%)	14 (6%)	6 (3%)	8	44
1	yD	229/231 (99%)	210 (92%)	15 (7%)	4 (2%)	13	56
1	yE	229/231 (99%)	214 (93%)	11 (5%)	4 (2%)	13	56
1	z	229/231 (99%)	210 (92%)	14 (6%)	5 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	zA	229/231 (99%)	207 (90%)	16 (7%)	6 (3%)	8	44
1	zB	229/231 (99%)	208 (91%)	18 (8%)	3 (1%)	16	63
1	zC	229/231 (99%)	207 (90%)	15 (7%)	7 (3%)	7	39
1	zD	229/231 (99%)	212 (93%)	11 (5%)	6 (3%)	8	44
1	zE	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	16	63
All	All	86562/87318 (99%)	78634 (91%)	6023 (7%)	1905 (2%)	10	49

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	66	95
1	0A	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	0B	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	0C	194/194 (100%)	187 (96%)	7 (4%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0D	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	0E	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	1	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	1A	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	1B	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	1C	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	1D	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	1E	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	2	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	2A	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	2B	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	2C	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	2D	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	2E	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	3	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	3A	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	3B	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	3C	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	3D	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	3E	194/194 (100%)	193 (99%)	1 (1%)	89	97
1	4	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	4A	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	4B	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	4C	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	4D	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	4E	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	5	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	5A	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	5B	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	5C	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	5D	194/194 (100%)	189 (97%)	5 (3%)	49	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5E	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	6	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	6A	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	6B	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	6C	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	6D	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	6E	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	7	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	7A	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	7B	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	7C	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	7D	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	7E	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	8	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	8A	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	8B	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	8C	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	8D	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	8E	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	9	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	9A	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	9B	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	9C	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	9D	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	9E	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	A	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	AA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	AB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	AC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	AD	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	AE	194/194 (100%)	190 (98%)	4 (2%)	56	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AF	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	B	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	BA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	BB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	BC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	BD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	BE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	BF	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	C	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	CA	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	CB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	CC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	CD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	CE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	CF	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	D	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	DA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	DB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	DC	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	DD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	DE	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	DF	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	E	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	EA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	EB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	EC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	ED	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	EE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	EF	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	F	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	FA	194/194 (100%)	187 (96%)	7 (4%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	FC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	FD	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	FE	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	FF	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	G	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	GA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	GB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	GC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	GD	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	GE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	H	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	HA	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	HB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	HC	194/194 (100%)	193 (99%)	1 (1%)	89	97
1	HD	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	HE	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	I	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	IA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	IB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	IC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	ID	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	IE	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	J	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	JA	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	JB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	JC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	JD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	JE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	K	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	KA	194/194 (100%)	187 (96%)	7 (4%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KB	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	KC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	KD	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	KE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	L	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	LA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	LB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	LC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	LD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	LE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	M	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	MA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	MB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	MC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	MD	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	ME	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	N	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	NA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	NB	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	NC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	ND	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	NE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	O	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	OA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	OB	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	OC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	OD	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	OE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	P	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	PA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	PB	194/194 (100%)	187 (96%)	7 (4%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PC	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	PD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	PE	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	Q	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	QA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	QB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	QC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	QD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	QE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	R	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	RA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	RB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	RC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	RD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	RE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	S	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	SA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	SB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	SC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	SD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	SE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	T	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	TA	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	TB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	TC	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	TD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	TE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	U	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	UA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	UB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	UC	194/194 (100%)	189 (97%)	5 (3%)	49	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UD	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	UE	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	V	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	VA	194/194 (100%)	181 (93%)	13 (7%)	20	68
1	VB	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	VC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	VD	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	VE	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	W	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	WA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	WB	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	WC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	WD	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	WE	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	X	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	XA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	XB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	XC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	XD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	XE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	Y	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	YA	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	YB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	YC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	YD	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	YE	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	Z	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	ZA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	ZB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	ZC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	ZD	194/194 (100%)	185 (95%)	9 (5%)	31	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ZE	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	a	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	aA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	aB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	aC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	aD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	aE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	b	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	bA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	bB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	bC	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	bD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	bE	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	c	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	cA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	cB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	cC	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	cD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	cE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	d	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	dA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	dB	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	dC	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	dD	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	dE	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	e	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	eA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	eB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	eC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	eD	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	eE	194/194 (100%)	186 (96%)	8 (4%)	34	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	fA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	fB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	fC	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	fD	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	fE	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	g	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	gA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	gB	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	gC	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	gD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	gE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	h	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	hA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	hB	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	hC	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	hD	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	hE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	i	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	iA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	iB	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	iC	194/194 (100%)	193 (99%)	1 (1%)	89	97
1	iD	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	iE	194/194 (100%)	182 (94%)	12 (6%)	22	71
1	j	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	jA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	jB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	jC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	jD	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	jE	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	k	194/194 (100%)	184 (95%)	10 (5%)	27	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	kA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	kB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	kC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	kD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	kE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	l	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	lA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	lB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	lC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	lD	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	lE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	m	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	mA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	mB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	mC	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	mD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	mE	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	n	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	nA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	nB	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	nC	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	nD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	nE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	o	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	oA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	oB	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	oC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	oD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	oE	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	p	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	pA	194/194 (100%)	186 (96%)	8 (4%)	34	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	pB	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	pC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	pD	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	pE	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	q	194/194 (100%)	183 (94%)	11 (6%)	24	73
1	qA	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	qB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	qC	194/194 (100%)	191 (98%)	3 (2%)	66	95
1	qD	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	qE	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	r	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	rA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	rB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	rC	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	rD	194/194 (100%)	184 (95%)	10 (5%)	27	76
1	rE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	s	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	sA	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	sB	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	sC	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	sD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	sE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	t	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	tA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	tB	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	tC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	tD	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	tE	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	u	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	uA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	uB	194/194 (100%)	187 (96%)	7 (4%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	uC	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	uD	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	uE	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	v	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	vA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	vB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	vC	194/194 (100%)	185 (95%)	9 (5%)	31	79
1	vD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	vE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	w	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	wA	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	wB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	wC	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	wD	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	wE	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	x	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	xA	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	xB	194/194 (100%)	187 (96%)	7 (4%)	38	86
1	xC	194/194 (100%)	192 (99%)	2 (1%)	77	96
1	xD	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	xE	194/194 (100%)	188 (97%)	6 (3%)	43	88
1	y	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	yA	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	yB	194/194 (100%)	186 (96%)	8 (4%)	34	82
1	yC	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	yD	194/194 (100%)	193 (99%)	1 (1%)	89	97
1	yE	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	z	194/194 (100%)	190 (98%)	4 (2%)	56	93
1	zA	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	zB	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	zC	194/194 (100%)	186 (96%)	8 (4%)	34	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	zD	194/194 (100%)	189 (97%)	5 (3%)	49	91
1	zE	194/194 (100%)	184 (95%)	10 (5%)	27	76
All	All	73332/73332 (100%)	70942 (97%)	2390 (3%)	41	87

All 2390 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	10	MET
1	A	96	MET
1	A	97	ARG
1	A	108	THR
1	A	154	ARG
1	A	184	TRP
1	A	200	THR
1	B	10	MET
1	B	63	GLN
1	B	96	MET
1	B	108	THR
1	C	15	ILE
1	C	96	MET
1	C	97	ARG
1	C	112	GLN
1	C	119	THR
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	85	PRO
1	E	117	TRP
1	E	144	MET
1	E	148	THR
1	F	48	THR
1	F	54	THR
1	F	96	MET

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Mol	Chain	Res	Type
1	F	97	ARG
1	F	108	THR
1	F	148	THR
1	F	182	LYS
1	F	184	TRP
1	G	85	PRO
1	G	96	MET
1	G	97	ARG
1	G	184	TRP
1	H	3	VAL
1	H	4	GLN
1	H	10	MET
1	H	25	LYS
1	H	96	MET
1	H	141	ILE
1	H	175	GLU
1	I	51	ASP
1	I	70	LYS
1	I	96	MET
1	I	97	ARG
1	I	108	THR
1	I	121	ASN
1	I	147	PRO
1	I	195	ASN
1	J	10	MET
1	J	66	MET
1	J	108	THR
1	J	121	ASN
1	J	195	ASN
1	J	231	LEU
1	K	96	MET
1	K	97	ARG
1	K	108	THR
1	K	131	LYS
1	K	184	TRP
1	K	214	MET
1	L	2	ILE
1	L	5	ASN
1	L	18	ARG
1	L	72	THR
1	L	96	MET
1	L	97	ARG

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Mol	Chain	Res	Type
1	L	107	THR
1	L	143	ARG
1	L	148	THR
1	L	154	ARG
1	L	184	TRP
1	M	54	THR
1	M	96	MET
1	M	97	ARG
1	M	107	THR
1	M	108	THR
1	N	13	GLN
1	N	53	ASN
1	N	74	ASN
1	N	81	ASP
1	N	96	MET
1	N	139	ASN
1	N	184	TRP
1	N	215	MET
1	O	63	GLN
1	O	96	MET
1	O	97	ARG
1	O	108	THR
1	O	147	PRO
1	O	192	GLN
1	O	226	HIS
1	P	96	MET
1	P	108	THR
1	P	148	THR
1	P	195	ASN
1	Q	10	MET
1	Q	67	GLN
1	Q	96	MET
1	Q	184	TRP
1	Q	200	THR
1	R	4	GLN
1	R	30	LYS
1	R	51	ASP
1	R	96	MET
1	R	117	TRP
1	R	173	ARG
1	R	184	TRP
1	R	200	THR

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Mol	Chain	Res	Type
1	R	226	HIS
1	S	10	MET
1	S	54	THR
1	S	96	MET
1	S	97	ARG
1	S	108	THR
1	S	122	PRO
1	S	184	TRP
1	S	195	ASN
1	T	96	MET
1	T	108	THR
1	T	130	TYR
1	T	148	THR
1	T	154	ARG
1	T	184	TRP
1	U	75	GLU
1	U	96	MET
1	U	97	ARG
1	U	108	THR
1	V	1	PRO
1	V	9	GLN
1	V	15	ILE
1	V	53	ASN
1	V	85	PRO
1	V	96	MET
1	V	121	ASN
1	V	182	LYS
1	V	184	TRP
1	W	18	ARG
1	W	96	MET
1	W	97	ARG
1	W	205	LEU
1	X	10	MET
1	X	72	THR
1	X	96	MET
1	X	117	TRP
1	X	121	ASN
1	Y	54	THR
1	Y	96	MET
1	Y	97	ARG
1	Y	107	THR
1	Y	108	THR

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Mol	Chain	Res	Type
1	Y	144	MET
1	Z	58	THR
1	Z	66	MET
1	Z	96	MET
1	Z	108	THR
1	Z	175	GLU
1	Z	184	TRP
1	Z	185	MET
1	Z	203	LYS
1	a	9	GLN
1	a	10	MET
1	a	96	MET
1	a	97	ARG
1	a	108	THR
1	a	147	PRO
1	a	184	TRP
1	b	48	THR
1	b	108	THR
1	b	121	ASN
1	b	175	GLU
1	b	184	TRP
1	b	188	THR
1	b	221	VAL
1	b	229	ARG
1	b	230	VAL
1	c	2	ILE
1	c	66	MET
1	c	96	MET
1	c	112	GLN
1	c	117	TRP
1	d	30	LYS
1	d	63	GLN
1	d	66	MET
1	d	96	MET
1	d	110	THR
1	d	145	TYR
1	d	154	ARG
1	e	96	MET
1	e	108	THR
1	e	121	ASN
1	e	164	TYR
1	e	184	TRP

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Mol	Chain	Res	Type
1	f	54	THR
1	f	96	MET
1	f	139	ASN
1	f	182	LYS
1	g	15	ILE
1	g	48	THR
1	g	67	GLN
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	66	MET
1	h	96	MET
1	h	121	ASN
1	h	148	THR
1	h	184	TRP
1	i	10	MET
1	i	97	ARG
1	i	188	THR
1	j	2	ILE
1	j	4	GLN
1	j	63	GLN
1	j	96	MET
1	j	108	THR
1	j	230	VAL
1	k	54	THR
1	k	96	MET
1	k	97	ARG
1	k	99	PRO
1	k	108	THR
1	k	143	ARG
1	k	162	ARG
1	k	175	GLU
1	k	184	TRP
1	k	203	LYS
1	l	48	THR
1	l	66	MET
1	l	69	LEU

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Mol	Chain	Res	Type
1	l	95	GLN
1	l	96	MET
1	l	108	THR
1	l	184	TRP
1	m	10	MET
1	m	48	THR
1	m	59	VAL
1	m	66	MET
1	m	96	MET
1	m	97	ARG
1	m	147	PRO
1	m	175	GLU
1	m	229	ARG
1	n	10	MET
1	n	48	THR
1	n	96	MET
1	n	97	ARG
1	n	103	ASP
1	n	108	THR
1	n	119	THR
1	n	121	ASN
1	n	162	ARG
1	o	62	HIS
1	o	96	MET
1	o	107	THR
1	o	117	TRP
1	p	18	ARG
1	p	69	LEU
1	p	97	ARG
1	p	100	ARG
1	p	107	THR
1	p	184	TRP
1	p	187	GLU
1	p	229	ARG
1	q	4	GLN
1	q	10	MET
1	q	25	LYS
1	q	54	THR
1	q	66	MET
1	q	85	PRO
1	q	96	MET
1	q	97	ARG

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Mol	Chain	Res	Type
1	q	108	THR
1	q	114	GLN
1	q	182	LYS
1	r	10	MET
1	r	96	MET
1	r	99	PRO
1	r	184	TRP
1	s	48	THR
1	s	50	GLN
1	s	66	MET
1	s	72	THR
1	s	96	MET
1	s	147	PRO
1	s	154	ARG
1	s	188	THR
1	t	97	ARG
1	t	121	ASN
1	t	148	THR
1	t	150	ILE
1	t	184	TRP
1	t	216	THR
1	t	230	VAL
1	u	10	MET
1	u	96	MET
1	u	117	TRP
1	u	184	TRP
1	u	211	LEU
1	v	18	ARG
1	v	96	MET
1	v	97	ARG
1	v	108	THR
1	v	184	TRP
1	v	195	ASN
1	v	205	LEU
1	w	85	PRO
1	w	96	MET
1	w	97	ARG
1	w	108	THR
1	x	30	LYS
1	x	96	MET
1	x	108	THR
1	x	145	TYR

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Mol	Chain	Res	Type
1	x	162	ARG
1	x	226	HIS
1	y	53	ASN
1	y	66	MET
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	121	ASN
1	z	171	THR
1	0	18	ARG
1	0	69	LEU
1	0	97	ARG
1	1	15	ILE
1	1	63	GLN
1	1	72	THR
1	1	81	ASP
1	1	87	HIS
1	1	96	MET
1	1	107	THR
1	1	158	LYS
1	1	173	ARG
1	2	15	ILE
1	2	96	MET
1	2	97	ARG
1	2	154	ARG
1	2	158	LYS
1	2	182	LYS
1	2	184	TRP
1	3	25	LYS
1	3	96	MET
1	3	97	ARG
1	3	107	THR
1	4	30	LYS
1	4	66	MET
1	4	96	MET
1	4	108	THR
1	4	147	PRO

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Mol	Chain	Res	Type
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	80	TRP
1	6	84	HIS
1	6	96	MET
1	6	97	ARG
1	6	182	LYS
1	6	184	TRP
1	6	205	LEU
1	7	4	GLN
1	7	96	MET
1	7	97	ARG
1	7	107	THR
1	7	182	LYS
1	7	184	TRP
1	7	195	ASN
1	8	13	GLN
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	97	ARG
1	9	108	THR
1	9	175	GLU
1	9	179	GLN
1	9	219	GLN
1	AA	21	ASN
1	AA	96	MET
1	AA	97	ARG
1	AA	131	LYS
1	AA	147	PRO
1	AA	184	TRP
1	BA	10	MET

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Mol	Chain	Res	Type
1	BA	30	LYS
1	BA	108	THR
1	BA	148	THR
1	BA	196	PRO
1	CA	69	LEU
1	CA	96	MET
1	CA	158	LYS
1	DA	96	MET
1	DA	97	ARG
1	DA	184	TRP
1	DA	185	MET
1	DA	201	ILE
1	DA	227	LYS
1	EA	63	GLN
1	EA	96	MET
1	EA	108	THR
1	EA	185	MET
1	FA	53	ASN
1	FA	62	HIS
1	FA	66	MET
1	FA	69	LEU
1	FA	96	MET
1	FA	108	THR
1	FA	227	LYS
1	GA	2	ILE
1	GA	96	MET
1	GA	143	ARG
1	GA	184	TRP
1	GA	229	ARG
1	HA	15	ILE
1	HA	85	PRO
1	HA	121	ASN
1	IA	66	MET
1	IA	96	MET
1	IA	117	TRP
1	IA	148	THR
1	JA	96	MET
1	JA	97	ARG
1	KA	53	ASN
1	KA	96	MET
1	KA	107	THR
1	KA	139	ASN

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Mol	Chain	Res	Type
1	KA	175	GLU
1	KA	184	TRP
1	KA	221	VAL
1	LA	10	MET
1	LA	48	THR
1	LA	96	MET
1	LA	108	THR
1	LA	175	GLU
1	LA	184	TRP
1	LA	195	ASN
1	MA	48	THR
1	MA	84	HIS
1	MA	97	ARG
1	MA	108	THR
1	MA	147	PRO
1	MA	184	TRP
1	MA	207	PRO
1	MA	229	ARG
1	NA	48	THR
1	NA	70	LYS
1	NA	113	GLU
1	NA	148	THR
1	NA	173	ARG
1	NA	188	THR
1	OA	2	ILE
1	OA	18	ARG
1	OA	25	LYS
1	OA	66	MET
1	OA	96	MET
1	OA	97	ARG
1	OA	121	ASN
1	OA	203	LYS
1	PA	96	MET
1	PA	97	ARG
1	PA	130	TYR
1	PA	182	LYS
1	PA	200	THR
1	QA	10	MET
1	QA	48	THR
1	QA	96	MET
1	QA	107	THR
1	QA	145	TYR

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Mol	Chain	Res	Type
1	QA	164	TYR
1	QA	195	ASN
1	RA	4	GLN
1	RA	48	THR
1	RA	96	MET
1	RA	108	THR
1	RA	148	THR
1	RA	175	GLU
1	RA	229	ARG
1	SA	53	ASN
1	SA	54	THR
1	SA	72	THR
1	SA	96	MET
1	SA	97	ARG
1	SA	143	ARG
1	SA	147	PRO
1	SA	184	TRP
1	TA	69	LEU
1	TA	72	THR
1	TA	85	PRO
1	UA	2	ILE
1	UA	51	ASP
1	UA	97	ARG
1	UA	107	THR
1	VA	4	GLN
1	VA	18	ARG
1	VA	28	GLU
1	VA	51	ASP
1	VA	54	THR
1	VA	66	MET
1	VA	96	MET
1	VA	107	THR
1	VA	131	LYS
1	VA	184	TRP
1	VA	192	GLN
1	VA	195	ASN
1	VA	229	ARG
1	WA	10	MET
1	WA	66	MET
1	WA	96	MET
1	WA	97	ARG
1	WA	184	TRP

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Mol	Chain	Res	Type
1	WA	192	GLN
1	XA	67	GLN
1	XA	96	MET
1	XA	108	THR
1	XA	110	THR
1	XA	185	MET
1	XA	229	ARG
1	YA	10	MET
1	YA	48	THR
1	YA	96	MET
1	YA	97	ARG
1	YA	108	THR
1	YA	147	PRO
1	YA	154	ARG
1	YA	171	THR
1	YA	229	ARG
1	ZA	15	ILE
1	ZA	85	PRO
1	ZA	154	ARG
1	ZA	184	TRP
1	aA	4	GLN
1	aA	74	ASN
1	aA	96	MET
1	aA	117	TRP
1	bA	2	ILE
1	bA	18	ARG
1	bA	96	MET
1	bA	97	ARG
1	bA	108	THR
1	bA	195	ASN
1	bA	229	ARG
1	cA	54	THR
1	cA	96	MET
1	cA	97	ARG
1	cA	107	THR
1	cA	184	TRP
1	dA	10	MET
1	dA	32	PHE
1	dA	80	TRP
1	dA	96	MET
1	dA	108	THR
1	dA	145	TYR

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Mol	Chain	Res	Type
1	dA	175	GLU
1	dA	196	PRO
1	eA	2	ILE
1	eA	96	MET
1	eA	108	THR
1	eA	112	GLN
1	eA	117	TRP
1	eA	147	PRO
1	eA	175	GLU
1	eA	184	TRP
1	fA	15	ILE
1	fA	30	LYS
1	fA	66	MET
1	fA	68	MET
1	fA	85	PRO
1	fA	121	ASN
1	fA	182	LYS
1	gA	18	ARG
1	gA	48	THR
1	gA	70	LYS
1	gA	96	MET
1	gA	184	TRP
1	gA	205	LEU
1	hA	45	GLU
1	hA	54	THR
1	hA	66	MET
1	hA	95	GLN
1	hA	96	MET
1	hA	148	THR
1	hA	184	TRP
1	hA	185	MET
1	iA	10	MET
1	iA	96	MET
1	iA	107	THR
1	iA	154	ARG
1	iA	195	ASN
1	iA	226	HIS
1	iA	229	ARG
1	jA	2	ILE
1	jA	96	MET
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	21	ASN
1	kA	63	GLN
1	kA	96	MET
1	kA	108	THR
1	lA	1	PRO
1	lA	10	MET
1	lA	48	THR
1	lA	96	MET
1	lA	152	ASP
1	mA	10	MET
1	mA	66	MET
1	mA	84	HIS
1	mA	96	MET
1	mA	107	THR
1	mA	154	ARG
1	nA	10	MET
1	nA	18	ARG
1	nA	50	GLN
1	nA	51	ASP
1	nA	96	MET
1	nA	97	ARG
1	nA	180	GLU
1	oA	96	MET
1	oA	97	ARG
1	oA	103	ASP
1	oA	108	THR
1	pA	54	THR
1	pA	96	MET
1	pA	97	ARG
1	pA	132	ARG
1	pA	139	ASN
1	pA	148	THR
1	pA	195	ASN
1	pA	205	LEU
1	qA	96	MET
1	qA	108	THR
1	qA	147	PRO

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Mol	Chain	Res	Type
1	qA	226	HIS
1	rA	54	THR
1	rA	72	THR
1	rA	95	GLN
1	rA	97	ARG
1	rA	108	THR
1	rA	171	THR
1	rA	184	TRP
1	sA	4	GLN
1	sA	21	ASN
1	sA	66	MET
1	sA	96	MET
1	sA	107	THR
1	sA	123	PRO
1	sA	148	THR
1	sA	179	GLN
1	sA	227	LYS
1	tA	5	ASN
1	tA	10	MET
1	tA	72	THR
1	tA	96	MET
1	tA	97	ARG
1	tA	107	THR
1	tA	121	ASN
1	uA	25	LYS
1	uA	66	MET
1	uA	96	MET
1	uA	107	THR
1	uA	108	THR
1	uA	184	TRP
1	vA	96	MET
1	vA	97	ARG
1	vA	108	THR
1	vA	113	GLU
1	vA	148	THR
1	vA	229	ARG
1	wA	66	MET
1	wA	85	PRO
1	wA	96	MET
1	wA	108	THR
1	wA	141	ILE
1	wA	147	PRO

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Mol	Chain	Res	Type
1	wA	184	TRP
1	xA	2	ILE
1	xA	7	GLN
1	xA	48	THR
1	xA	96	MET
1	xA	121	ASN
1	xA	231	LEU
1	yA	10	MET
1	yA	63	GLN
1	yA	66	MET
1	yA	84	HIS
1	yA	96	MET
1	yA	107	THR
1	yA	148	THR
1	yA	184	TRP
1	zA	67	GLN
1	zA	97	ARG
1	zA	108	THR
1	zA	121	ASN
1	zA	173	ARG
1	0A	10	MET
1	0A	70	LYS
1	0A	96	MET
1	0A	108	THR
1	0A	110	THR
1	0A	184	TRP
1	0A	229	ARG
1	1A	53	ASN
1	1A	54	THR
1	1A	69	LEU
1	1A	96	MET
1	1A	108	THR
1	1A	226	HIS
1	2A	96	MET
1	2A	97	ARG
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

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Mol	Chain	Res	Type
1	3A	108	THR
1	3A	117	TRP
1	3A	121	ASN
1	3A	130	TYR
1	3A	184	TRP
1	4A	96	MET
1	4A	117	TRP
1	4A	148	THR
1	4A	149	SER
1	4A	184	TRP
1	5A	10	MET
1	5A	81	ASP
1	5A	96	MET
1	5A	97	ARG
1	5A	118	MET
1	5A	130	TYR
1	5A	184	TRP
1	6A	30	LYS
1	6A	96	MET
1	6A	108	THR
1	6A	184	TRP
1	6A	203	LYS
1	7A	48	THR
1	7A	96	MET
1	7A	139	ASN
1	7A	175	GLU
1	7A	184	TRP
1	8A	15	ILE
1	8A	48	THR
1	8A	96	MET
1	8A	97	ARG
1	8A	108	THR
1	8A	147	PRO
1	9A	10	MET
1	9A	96	MET
1	9A	121	ASN
1	9A	171	THR
1	9A	173	ARG
1	9A	200	THR
1	AB	10	MET
1	AB	15	ILE
1	AB	63	GLN

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Mol	Chain	Res	Type
1	AB	66	MET
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	97	ARG
1	BB	108	THR
1	BB	154	ARG
1	CB	5	ASN
1	CB	96	MET
1	CB	119	THR
1	CB	184	TRP
1	DB	54	THR
1	DB	96	MET
1	DB	107	THR
1	DB	162	ARG
1	EB	63	GLN
1	EB	96	MET
1	EB	97	ARG
1	EB	188	THR
1	FB	10	MET
1	FB	51	ASP
1	FB	72	THR
1	FB	82	ARG
1	FB	96	MET
1	FB	121	ASN
1	FB	175	GLU
1	FB	182	LYS
1	FB	184	TRP
1	GB	148	THR
1	GB	184	TRP
1	GB	188	THR
1	GB	226	HIS
1	HB	4	GLN
1	HB	96	MET
1	HB	97	ARG
1	HB	108	THR
1	HB	184	TRP
1	IB	10	MET

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Mol	Chain	Res	Type
1	IB	96	MET
1	IB	113	GLU
1	IB	165	VAL
1	JB	96	MET
1	JB	108	THR
1	JB	148	THR
1	JB	151	LEU
1	JB	227	LYS
1	KB	48	THR
1	KB	75	GLU
1	KB	81	ASP
1	KB	96	MET
1	KB	144	MET
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	175	GLU
1	LB	226	HIS
1	MB	10	MET
1	MB	84	HIS
1	MB	97	ARG
1	MB	107	THR
1	MB	130	TYR
1	MB	185	MET
1	NB	72	THR
1	NB	87	HIS
1	NB	96	MET
1	NB	97	ARG
1	NB	117	TRP
1	NB	184	TRP
1	NB	185	MET
1	NB	205	LEU
1	OB	5	ASN
1	OB	21	ASN
1	OB	96	MET
1	OB	97	ARG

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Mol	Chain	Res	Type
1	OB	108	THR
1	OB	112	GLN
1	OB	148	THR
1	OB	179	GLN
1	PB	10	MET
1	PB	30	LYS
1	PB	96	MET
1	PB	108	THR
1	PB	148	THR
1	PB	154	ARG
1	PB	180	GLU
1	QB	96	MET
1	QB	97	ARG
1	QB	108	THR
1	QB	147	PRO
1	QB	184	TRP
1	QB	195	ASN
1	RB	10	MET
1	RB	15	ILE
1	RB	48	THR
1	RB	121	ASN
1	SB	7	GLN
1	SB	15	ILE
1	SB	63	GLN
1	SB	66	MET
1	SB	96	MET
1	SB	107	THR
1	SB	117	TRP
1	SB	119	THR
1	SB	148	THR
1	TB	96	MET
1	TB	107	THR
1	TB	184	TRP
1	TB	219	GLN
1	UB	96	MET
1	UB	97	ARG
1	UB	107	THR
1	UB	184	TRP
1	UB	229	ARG
1	VB	10	MET
1	VB	96	MET
1	VB	219	GLN

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Mol	Chain	Res	Type
1	WB	58	THR
1	WB	72	THR
1	WB	96	MET
1	WB	97	ARG
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	121	ASN
1	YB	10	MET
1	YB	69	LEU
1	YB	110	THR
1	YB	171	THR
1	YB	184	TRP
1	ZB	4	GLN
1	ZB	10	MET
1	ZB	69	LEU
1	ZB	72	THR
1	ZB	96	MET
1	ZB	130	TYR
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	162	ARG
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	dB	10	MET
1	dB	66	MET
1	dB	85	PRO
1	dB	95	GLN

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Mol	Chain	Res	Type
1	dB	96	MET
1	dB	108	THR
1	dB	110	THR
1	eB	18	ARG
1	eB	53	ASN
1	eB	96	MET
1	eB	107	THR
1	eB	148	THR
1	fB	10	MET
1	fB	54	THR
1	fB	58	THR
1	fB	121	ASN
1	fB	184	TRP
1	fB	227	LYS
1	gB	70	LYS
1	gB	95	GLN
1	gB	96	MET
1	gB	97	ARG
1	gB	132	ARG
1	gB	175	GLU
1	gB	184	TRP
1	gB	226	HIS
1	hB	10	MET
1	hB	30	LYS
1	hB	67	GLN
1	hB	95	GLN
1	hB	96	MET
1	hB	108	THR
1	hB	162	ARG
1	hB	184	TRP
1	iB	70	LYS
1	iB	96	MET
1	iB	97	ARG
1	iB	108	THR
1	iB	147	PRO
1	iB	184	TRP
1	iB	230	VAL
1	jB	66	MET
1	jB	67	GLN
1	jB	96	MET
1	jB	97	ARG
1	jB	108	THR

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Mol	Chain	Res	Type
1	jB	121	ASN
1	jB	154	ARG
1	jB	171	THR
1	jB	230	VAL
1	kB	69	LEU
1	kB	96	MET
1	kB	107	THR
1	kB	143	ARG
1	kB	201	ILE
1	lB	2	ILE
1	lB	72	THR
1	lB	97	ARG
1	lB	130	TYR
1	lB	184	TRP
1	mB	48	THR
1	mB	66	MET
1	mB	96	MET
1	mB	108	THR
1	mB	175	GLU
1	mB	184	TRP
1	nB	10	MET
1	nB	139	ASN
1	oB	51	ASP
1	oB	53	ASN
1	oB	66	MET
1	oB	69	LEU
1	oB	91	ILE
1	oB	97	ARG
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	96	MET
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	66	MET

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Mol	Chain	Res	Type
1	qB	85	PRO
1	qB	96	MET
1	qB	97	ARG
1	qB	148	THR
1	qB	176	GLN
1	rB	72	THR
1	rB	96	MET
1	rB	97	ARG
1	rB	117	TRP
1	rB	184	TRP
1	sB	66	MET
1	sB	85	PRO
1	sB	96	MET
1	sB	108	THR
1	sB	139	ASN
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	97	ARG
1	tB	108	THR
1	uB	1	PRO
1	uB	75	GLU
1	uB	96	MET
1	uB	97	ARG
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	226	HIS
1	wB	18	ARG
1	wB	69	LEU
1	wB	96	MET
1	wB	183	ASN
1	wB	229	ARG
1	xB	54	THR
1	xB	96	MET

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Mol	Chain	Res	Type
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	96	MET
1	yB	121	ASN
1	yB	152	ASP
1	yB	168	PHE
1	yB	183	ASN
1	yB	184	TRP
1	yB	192	GLN
1	zB	30	LYS
1	zB	96	MET
1	zB	154	ARG
1	zB	162	ARG
1	zB	184	TRP
1	0B	10	MET
1	0B	58	THR
1	0B	63	GLN
1	0B	72	THR
1	0B	96	MET
1	0B	97	ARG
1	0B	139	ASN
1	0B	184	TRP
1	0B	227	LYS
1	1B	10	MET
1	1B	85	PRO
1	1B	108	THR
1	1B	175	GLU
1	2B	2	ILE
1	2B	10	MET
1	2B	70	LYS
1	2B	96	MET
1	3B	72	THR
1	3B	96	MET
1	3B	182	LYS
1	3B	226	HIS
1	3B	229	ARG
1	4B	10	MET
1	4B	66	MET

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Mol	Chain	Res	Type
1	4B	70	LYS
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	96	MET
1	5B	107	THR
1	5B	108	THR
1	5B	122	PRO
1	5B	139	ASN
1	5B	148	THR
1	5B	215	MET
1	5B	229	ARG
1	6B	25	LYS
1	6B	48	THR
1	6B	96	MET
1	6B	97	ARG
1	6B	107	THR
1	6B	108	THR
1	6B	147	PRO
1	6B	184	TRP
1	6B	230	VAL
1	7B	10	MET
1	7B	15	ILE
1	7B	48	THR
1	7B	66	MET
1	7B	99	PRO
1	7B	186	THR
1	8B	3	VAL
1	8B	84	HIS
1	8B	96	MET
1	8B	107	THR
1	8B	117	TRP
1	8B	148	THR
1	9B	5	ASN
1	9B	10	MET
1	9B	96	MET
1	9B	148	THR
1	9B	184	TRP
1	AC	69	LEU

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Mol	Chain	Res	Type
1	AC	91	ILE
1	AC	96	MET
1	AC	97	ARG
1	AC	184	TRP
1	AC	185	MET
1	BC	54	THR
1	BC	96	MET
1	BC	108	THR
1	BC	171	THR
1	BC	175	GLU
1	BC	182	LYS
1	CC	10	MET
1	CC	96	MET
1	CC	97	ARG
1	CC	107	THR
1	CC	147	PRO
1	CC	175	GLU
1	CC	196	PRO
1	CC	231	LEU
1	DC	1	PRO
1	DC	7	GLN
1	DC	10	MET
1	DC	107	THR
1	DC	108	THR
1	DC	121	ASN
1	DC	144	MET
1	DC	148	THR
1	DC	175	GLU
1	EC	62	HIS
1	EC	63	GLN
1	EC	96	MET
1	EC	107	THR
1	EC	148	THR
1	EC	210	THR
1	EC	226	HIS
1	FC	10	MET
1	FC	18	ARG
1	FC	96	MET
1	FC	97	ARG
1	FC	108	THR
1	FC	121	ASN
1	FC	184	TRP

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Mol	Chain	Res	Type
1	GC	69	LEU
1	GC	96	MET
1	GC	97	ARG
1	GC	107	THR
1	GC	108	THR
1	GC	148	THR
1	GC	182	LYS
1	HC	108	THR
1	IC	108	THR
1	IC	147	PRO
1	IC	171	THR
1	IC	180	GLU
1	IC	184	TRP
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	KC	18	ARG
1	KC	107	THR
1	KC	179	GLN
1	KC	184	TRP
1	KC	185	MET
1	LC	15	ILE
1	LC	18	ARG
1	LC	63	GLN
1	LC	97	ARG
1	LC	165	VAL
1	LC	185	MET
1	MC	96	MET
1	MC	97	ARG
1	MC	107	THR
1	MC	108	THR
1	MC	154	ARG
1	MC	171	THR
1	MC	182	LYS
1	MC	229	ARG
1	NC	1	PRO
1	NC	30	LYS

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Mol	Chain	Res	Type
1	NC	96	MET
1	NC	108	THR
1	NC	221	VAL
1	NC	227	LYS
1	OC	66	MET
1	OC	96	MET
1	OC	97	ARG
1	OC	147	PRO
1	OC	166	ASP
1	OC	171	THR
1	OC	205	LEU
1	OC	227	LYS
1	PC	85	PRO
1	PC	96	MET
1	PC	108	THR
1	PC	110	THR
1	PC	121	ASN
1	PC	185	MET
1	PC	195	ASN
1	PC	201	ILE
1	PC	229	ARG
1	QC	84	HIS
1	QC	91	ILE
1	QC	96	MET
1	QC	131	LYS
1	QC	184	TRP
1	RC	18	ARG
1	RC	96	MET
1	RC	97	ARG
1	RC	108	THR
1	RC	121	ASN
1	RC	148	THR
1	RC	182	LYS
1	RC	184	TRP
1	SC	72	THR
1	SC	96	MET
1	SC	108	THR
1	SC	175	GLU
1	SC	184	TRP
1	SC	226	HIS
1	TC	96	MET
1	TC	107	THR

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Mol	Chain	Res	Type
1	TC	108	THR
1	TC	175	GLU
1	UC	10	MET
1	UC	15	ILE
1	UC	96	MET
1	UC	108	THR
1	UC	184	TRP
1	VC	1	PRO
1	VC	48	THR
1	VC	96	MET
1	VC	108	THR
1	VC	121	ASN
1	VC	161	PHE
1	VC	195	ASN
1	VC	227	LYS
1	WC	4	GLN
1	WC	58	THR
1	WC	192	GLN
1	WC	226	HIS
1	WC	227	LYS
1	XC	10	MET
1	XC	18	ARG
1	XC	96	MET
1	XC	140	LYS
1	XC	148	THR
1	XC	184	TRP
1	XC	230	VAL
1	YC	53	ASN
1	YC	96	MET
1	YC	171	THR
1	YC	175	GLU
1	YC	203	LYS
1	ZC	25	LYS
1	ZC	53	ASN
1	ZC	108	THR
1	ZC	148	THR
1	ZC	154	ARG
1	ZC	175	GLU
1	ZC	211	LEU
1	aC	5	ASN
1	aC	10	MET
1	aC	70	LYS

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Mol	Chain	Res	Type
1	aC	96	MET
1	aC	107	THR
1	aC	147	PRO
1	bC	10	MET
1	bC	108	THR
1	bC	175	GLU
1	cC	69	LEU
1	cC	81	ASP
1	cC	96	MET
1	cC	199	LYS
1	dC	66	MET
1	dC	96	MET
1	dC	97	ARG
1	dC	121	ASN
1	eC	30	LYS
1	eC	96	MET
1	eC	184	TRP
1	eC	188	THR
1	eC	226	HIS
1	fC	25	LYS
1	fC	96	MET
1	fC	139	ASN
1	fC	175	GLU
1	gC	7	GLN
1	gC	48	THR
1	gC	63	GLN
1	gC	66	MET
1	gC	96	MET
1	gC	97	ARG
1	gC	108	THR
1	gC	147	PRO
1	gC	184	TRP
1	hC	13	GLN
1	hC	108	THR
1	hC	188	THR
1	iC	10	MET
1	jC	4	GLN
1	jC	18	ARG
1	jC	108	THR
1	jC	184	TRP
1	jC	192	GLN
1	jC	226	HIS

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Mol	Chain	Res	Type
1	kC	66	MET
1	kC	96	MET
1	kC	97	ARG
1	kC	107	THR
1	kC	131	LYS
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	226	HIS
1	lC	230	VAL
1	mC	10	MET
1	mC	48	THR
1	mC	96	MET
1	mC	107	THR
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	143	ARG
1	nC	145	TYR
1	nC	175	GLU
1	nC	185	MET
1	nC	196	PRO
1	oC	96	MET
1	oC	107	THR
1	oC	148	THR
1	oC	184	TRP
1	oC	205	LEU
1	oC	215	MET
1	oC	219	GLN
1	pC	4	GLN
1	pC	66	MET
1	pC	96	MET

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Mol	Chain	Res	Type
1	pC	100	ARG
1	pC	108	THR
1	pC	121	ASN
1	pC	182	LYS
1	qC	96	MET
1	qC	108	THR
1	qC	149	SER
1	rC	96	MET
1	rC	195	ASN
1	sC	10	MET
1	sC	66	MET
1	sC	72	THR
1	sC	96	MET
1	sC	108	THR
1	sC	147	PRO
1	sC	184	TRP
1	tC	10	MET
1	tC	62	HIS
1	tC	107	THR
1	tC	122	PRO
1	tC	179	GLN
1	uC	96	MET
1	uC	97	ARG
1	uC	162	ARG
1	uC	184	TRP
1	vC	69	LEU
1	vC	96	MET
1	vC	97	ARG
1	vC	107	THR
1	vC	110	THR
1	vC	121	ASN
1	vC	173	ARG
1	vC	192	GLN
1	vC	229	ARG
1	wC	33	SER
1	wC	54	THR
1	wC	66	MET
1	wC	96	MET
1	wC	107	THR
1	wC	231	LEU
1	xC	96	MET
1	xC	184	TRP

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Mol	Chain	Res	Type
1	yC	66	MET
1	yC	96	MET
1	yC	97	ARG
1	yC	147	PRO
1	yC	183	ASN
1	zC	1	PRO
1	zC	10	MET
1	zC	33	SER
1	zC	107	THR
1	zC	121	ASN
1	zC	182	LYS
1	zC	184	TRP
1	zC	229	ARG
1	0C	53	ASN
1	0C	66	MET
1	0C	69	LEU
1	0C	96	MET
1	0C	108	THR
1	0C	145	TYR
1	0C	154	ARG
1	1C	4	GLN
1	1C	10	MET
1	1C	96	MET
1	1C	107	THR
1	1C	117	TRP
1	1C	148	THR
1	1C	184	TRP
1	1C	205	LEU
1	2C	21	ASN
1	2C	53	ASN
1	2C	66	MET
1	2C	96	MET
1	2C	108	THR
1	2C	182	LYS
1	2C	184	TRP
1	2C	229	ARG
1	3C	96	MET
1	3C	108	THR
1	3C	148	THR
1	4C	70	LYS
1	4C	96	MET
1	4C	97	ARG

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Mol	Chain	Res	Type
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	85	PRO
1	5C	108	THR
1	5C	121	ASN
1	5C	123	PRO
1	5C	173	ARG
1	5C	184	TRP
1	6C	10	MET
1	6C	85	PRO
1	6C	97	ARG
1	7C	15	ILE
1	7C	18	ARG
1	7C	30	LYS
1	7C	63	GLN
1	7C	96	MET
1	7C	97	ARG
1	7C	148	THR
1	8C	48	THR
1	8C	96	MET
1	8C	97	ARG
1	8C	100	ARG
1	8C	107	THR
1	8C	184	TRP
1	8C	195	ASN
1	8C	226	HIS
1	8C	229	ARG
1	9C	13	GLN
1	9C	96	MET
1	9C	108	THR
1	9C	139	ASN
1	AD	1	PRO
1	AD	15	ILE
1	AD	66	MET
1	AD	96	MET
1	AD	143	ARG

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Mol	Chain	Res	Type
1	AD	147	PRO
1	AD	227	LYS
1	AD	229	ARG
1	BD	66	MET
1	BD	69	LEU
1	BD	85	PRO
1	BD	148	THR
1	BD	184	TRP
1	BD	229	ARG
1	CD	51	ASP
1	CD	66	MET
1	CD	84	HIS
1	CD	96	MET
1	CD	107	THR
1	DD	82	ARG
1	DD	85	PRO
1	DD	107	THR
1	DD	148	THR
1	DD	159	GLU
1	ED	54	THR
1	ED	96	MET
1	ED	100	ARG
1	ED	107	THR
1	ED	184	TRP
1	FD	10	MET
1	FD	96	MET
1	FD	182	LYS
1	GD	10	MET
1	GD	48	THR
1	GD	66	MET
1	GD	85	PRO
1	GD	96	MET
1	GD	97	ARG
1	GD	108	THR
1	GD	147	PRO
1	GD	184	TRP
1	GD	230	VAL
1	HD	1	PRO
1	HD	3	VAL
1	HD	10	MET
1	HD	21	ASN
1	HD	48	THR

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Mol	Chain	Res	Type
1	HD	66	MET
1	HD	96	MET
1	HD	99	PRO
1	HD	108	THR
1	HD	121	ASN
1	HD	195	ASN
1	ID	10	MET
1	ID	84	HIS
1	ID	96	MET
1	ID	97	ARG
1	ID	184	TRP
1	JD	4	GLN
1	JD	18	ARG
1	JD	54	THR
1	JD	82	ARG
1	JD	96	MET
1	JD	148	THR
1	JD	162	ARG
1	KD	50	GLN
1	KD	53	ASN
1	KD	66	MET
1	KD	96	MET
1	LD	25	LYS
1	LD	66	MET
1	LD	96	MET
1	LD	162	ARG
1	LD	200	THR
1	LD	226	HIS
1	MD	53	ASN
1	MD	58	THR
1	MD	91	ILE
1	MD	97	ARG
1	MD	108	THR
1	MD	147	PRO
1	MD	184	TRP
1	MD	226	HIS
1	ND	10	MET
1	ND	30	LYS
1	ND	85	PRO
1	ND	96	MET
1	ND	148	THR
1	ND	182	LYS

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Mol	Chain	Res	Type
1	ND	184	TRP
1	ND	188	THR
1	OD	10	MET
1	OD	63	GLN
1	OD	148	THR
1	OD	184	TRP
1	PD	48	THR
1	PD	96	MET
1	PD	97	ARG
1	PD	107	THR
1	PD	108	THR
1	QD	54	THR
1	QD	63	GLN
1	QD	74	ASN
1	QD	96	MET
1	QD	97	ARG
1	QD	108	THR
1	QD	184	TRP
1	RD	96	MET
1	RD	107	THR
1	RD	112	GLN
1	RD	139	ASN
1	RD	205	LEU
1	SD	48	THR
1	SD	96	MET
1	SD	97	ARG
1	SD	147	PRO
1	SD	179	GLN
1	SD	184	TRP
1	SD	226	HIS
1	TD	10	MET
1	TD	48	THR
1	TD	62	HIS
1	TD	66	MET
1	TD	121	ASN
1	UD	2	ILE
1	UD	66	MET
1	UD	69	LEU
1	UD	81	ASP
1	UD	96	MET
1	UD	97	ARG
1	UD	126	VAL

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Mol	Chain	Res	Type
1	UD	130	TYR
1	UD	184	TRP
1	UD	227	LYS
1	VD	51	ASP
1	VD	54	THR
1	VD	96	MET
1	VD	97	ARG
1	VD	108	THR
1	VD	121	ASN
1	VD	162	ARG
1	VD	184	TRP
1	VD	185	MET
1	VD	195	ASN
1	VD	227	LYS
1	WD	66	MET
1	WD	97	ARG
1	WD	108	THR
1	WD	184	TRP
1	XD	10	MET
1	XD	70	LYS
1	XD	96	MET
1	XD	108	THR
1	XD	175	GLU
1	XD	184	TRP
1	XD	195	ASN
1	YD	10	MET
1	YD	63	GLN
1	YD	66	MET
1	YD	70	LYS
1	YD	96	MET
1	YD	108	THR
1	YD	143	ARG
1	YD	147	PRO
1	YD	184	TRP
1	YD	216	THR
1	ZD	48	THR
1	ZD	96	MET
1	ZD	99	PRO
1	ZD	108	THR
1	ZD	121	ASN
1	ZD	154	ARG
1	ZD	171	THR

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Mol	Chain	Res	Type
1	ZD	184	TRP
1	ZD	196	PRO
1	aD	2	ILE
1	aD	69	LEU
1	aD	85	PRO
1	aD	96	MET
1	aD	107	THR
1	aD	148	THR
1	aD	185	MET
1	bD	4	GLN
1	bD	10	MET
1	bD	97	ARG
1	bD	173	ARG
1	bD	182	LYS
1	cD	54	THR
1	cD	96	MET
1	cD	97	ARG
1	cD	108	THR
1	cD	184	TRP
1	cD	226	HIS
1	dD	33	SER
1	dD	53	ASN
1	dD	69	LEU
1	dD	95	GLN
1	dD	96	MET
1	dD	97	ARG
1	dD	108	THR
1	dD	171	THR
1	dD	175	GLU
1	dD	184	TRP
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	97	ARG
1	fD	108	THR
1	fD	121	ASN
1	fD	148	THR
1	fD	150	ILE
1	fD	184	TRP

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Mol	Chain	Res	Type
1	fD	185	MET
1	gD	66	MET
1	gD	69	LEU
1	gD	96	MET
1	gD	107	THR
1	gD	131	LYS
1	gD	143	ARG
1	gD	184	TRP
1	hD	4	GLN
1	hD	96	MET
1	hD	97	ARG
1	iD	85	PRO
1	iD	96	MET
1	iD	97	ARG
1	iD	108	THR
1	iD	117	TRP
1	iD	154	ARG
1	iD	184	TRP
1	iD	188	THR
1	iD	230	VAL
1	jD	30	LYS
1	jD	96	MET
1	jD	108	THR
1	jD	139	ASN
1	kD	63	GLN
1	kD	96	MET
1	kD	97	ARG
1	kD	110	THR
1	kD	147	PRO
1	kD	205	LEU
1	lD	1	PRO
1	lD	54	THR
1	lD	66	MET
1	lD	96	MET
1	lD	121	ASN
1	lD	148	THR
1	lD	196	PRO
1	lD	219	GLN
1	mD	15	ILE
1	mD	48	THR
1	mD	69	LEU
1	mD	96	MET

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Mol	Chain	Res	Type
1	mD	97	ARG
1	mD	107	THR
1	mD	164	TYR
1	nD	4	GLN
1	nD	63	GLN
1	nD	96	MET
1	nD	97	ARG
1	nD	139	ASN
1	oD	62	HIS
1	oD	66	MET
1	oD	96	MET
1	oD	97	ARG
1	oD	154	ARG
1	oD	184	TRP
1	pD	96	MET
1	pD	97	ARG
1	qD	1	PRO
1	qD	48	THR
1	qD	96	MET
1	qD	107	THR
1	qD	141	ILE
1	qD	144	MET
1	qD	147	PRO
1	qD	175	GLU
1	qD	201	ILE
1	rD	9	GLN
1	rD	10	MET
1	rD	62	HIS
1	rD	66	MET
1	rD	85	PRO
1	rD	108	THR
1	rD	121	ASN
1	rD	139	ASN
1	rD	148	THR
1	rD	182	LYS
1	sD	10	MET
1	sD	66	MET
1	sD	84	HIS
1	sD	96	MET
1	sD	107	THR
1	tD	2	ILE
1	tD	66	MET

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Mol	Chain	Res	Type
1	tD	96	MET
1	tD	108	THR
1	tD	143	ARG
1	tD	154	ARG
1	tD	188	THR
1	tD	229	ARG
1	uD	21	ASN
1	uD	66	MET
1	uD	96	MET
1	uD	97	ARG
1	uD	108	THR
1	uD	184	TRP
1	uD	197	ASP
1	uD	219	GLN
1	uD	230	VAL
1	vD	54	THR
1	vD	96	MET
1	vD	108	THR
1	vD	122	PRO
1	vD	184	TRP
1	vD	200	THR
1	vD	229	ARG
1	wD	10	MET
1	wD	25	LYS
1	wD	48	THR
1	wD	96	MET
1	wD	108	THR
1	wD	147	PRO
1	wD	175	GLU
1	xD	10	MET
1	xD	30	LYS
1	xD	96	MET
1	xD	148	THR
1	xD	189	LEU
1	xD	231	LEU
1	yD	97	ARG
1	zD	97	ARG
1	zD	107	THR
1	zD	108	THR
1	zD	121	ASN
1	zD	227	LYS
1	0D	96	MET

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Mol	Chain	Res	Type
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
1	1D	182	LYS
1	2D	10	MET
1	2D	15	ILE
1	2D	87	HIS
1	2D	96	MET
1	2D	97	ARG
1	2D	113	GLU
1	2D	147	PRO
1	2D	184	TRP
1	2D	203	LYS
1	3D	10	MET
1	3D	48	THR
1	3D	69	LEU
1	3D	87	HIS
1	3D	121	ASN
1	3D	148	THR
1	3D	175	GLU
1	3D	185	MET
1	4D	10	MET
1	4D	63	GLN
1	4D	96	MET
1	4D	97	ARG
1	4D	143	ARG
1	4D	148	THR
1	4D	184	TRP
1	5D	4	GLN
1	5D	66	MET
1	5D	96	MET
1	5D	97	ARG
1	5D	185	MET
1	6D	96	MET
1	6D	97	ARG
1	6D	103	ASP
1	6D	108	THR

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Mol	Chain	Res	Type
1	6D	154	ARG
1	6D	184	TRP
1	7D	30	LYS
1	7D	69	LEU
1	7D	96	MET
1	7D	108	THR
1	7D	145	TYR
1	7D	175	GLU
1	8D	10	MET
1	8D	62	HIS
1	8D	66	MET
1	8D	96	MET
1	8D	97	ARG
1	8D	107	THR
1	8D	108	THR
1	8D	147	PRO
1	8D	184	TRP
1	8D	229	ARG
1	9D	10	MET
1	9D	48	THR
1	9D	96	MET
1	9D	97	ARG
1	9D	99	PRO
1	9D	108	THR
1	9D	121	ASN
1	9D	175	GLU
1	AE	15	ILE
1	AE	69	LEU
1	AE	96	MET
1	AE	148	THR
1	BE	4	GLN
1	BE	5	ASN
1	BE	63	GLN
1	BE	69	LEU
1	BE	72	THR
1	BE	121	ASN
1	CE	10	MET
1	CE	58	THR
1	CE	96	MET
1	CE	108	THR
1	CE	112	GLN
1	CE	231	LEU

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Mol	Chain	Res	Type
1	DE	96	MET
1	DE	97	ARG
1	DE	139	ASN
1	DE	184	TRP
1	EE	54	THR
1	EE	96	MET
1	EE	97	ARG
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	96	MET
1	FE	97	ARG
1	FE	108	THR
1	FE	117	TRP
1	FE	121	ASN
1	FE	131	LYS
1	FE	148	THR
1	FE	165	VAL
1	FE	184	TRP
1	GE	10	MET
1	GE	54	THR
1	GE	96	MET
1	GE	154	ARG
1	GE	215	MET
1	HE	58	THR
1	HE	96	MET
1	HE	97	ARG
1	HE	109	SER
1	IE	96	MET
1	IE	184	TRP
1	IE	203	LYS
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	10	MET

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Mol	Chain	Res	Type
1	KE	30	LYS
1	KE	66	MET
1	KE	96	MET
1	KE	140	LYS
1	KE	147	PRO
1	KE	184	TRP
1	KE	226	HIS
1	LE	48	THR
1	LE	85	PRO
1	LE	96	MET
1	LE	121	ASN
1	LE	148	THR
1	LE	166	ASP
1	LE	184	TRP
1	LE	185	MET
1	ME	10	MET
1	ME	18	ARG
1	ME	81	ASP
1	ME	96	MET
1	ME	107	THR
1	ME	145	TYR
1	ME	148	THR
1	NE	2	ILE
1	NE	66	MET
1	NE	96	MET
1	NE	121	ASN
1	NE	195	ASN
1	OE	96	MET
1	OE	108	THR
1	OE	154	ARG
1	OE	184	TRP
1	OE	185	MET
1	PE	119	THR
1	PE	175	GLU
1	PE	184	TRP
1	QE	63	GLN
1	QE	66	MET
1	QE	72	THR
1	QE	97	ARG
1	QE	147	PRO
1	RE	10	MET
1	RE	69	LEU

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Mol	Chain	Res	Type
1	RE	110	THR
1	RE	121	ASN
1	RE	148	THR
1	RE	162	ARG
1	RE	179	GLN
1	RE	182	LYS
1	SE	4	GLN
1	SE	66	MET
1	SE	96	MET
1	SE	107	THR
1	SE	108	THR
1	SE	145	TYR
1	TE	62	HIS
1	TE	96	MET
1	TE	97	ARG
1	TE	108	THR
1	TE	143	ARG
1	TE	184	TRP
1	UE	2	ILE
1	UE	70	LYS
1	UE	96	MET
1	UE	97	ARG
1	UE	107	THR
1	UE	184	TRP
1	UE	229	ARG
1	VE	30	LYS
1	VE	66	MET
1	VE	96	MET
1	VE	139	ASN
1	VE	148	THR
1	VE	226	HIS
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	147	PRO
1	WE	171	THR
1	WE	175	GLU
1	WE	231	LEU
1	XE	10	MET

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Mol	Chain	Res	Type
1	XE	30	LYS
1	XE	96	MET
1	XE	108	THR
1	XE	121	ASN
1	XE	195	ASN
1	YE	96	MET
1	YE	163	ASP
1	YE	184	TRP
1	ZE	4	GLN
1	ZE	25	LYS
1	ZE	58	THR
1	ZE	96	MET
1	ZE	107	THR
1	ZE	143	ARG
1	ZE	195	ASN
1	aE	69	LEU
1	aE	96	MET
1	aE	97	ARG
1	aE	108	THR
1	aE	117	TRP
1	aE	184	TRP
1	aE	203	LYS
1	aE	226	HIS
1	bE	96	MET
1	bE	108	THR
1	bE	229	ARG
1	cE	10	MET
1	cE	48	THR
1	cE	96	MET
1	cE	97	ARG
1	cE	108	THR
1	cE	184	TRP
1	cE	195	ASN
1	cE	227	LYS
1	dE	1	PRO
1	dE	10	MET
1	dE	81	ASP
1	dE	96	MET
1	dE	99	PRO
1	dE	108	THR
1	dE	121	ASN
1	dE	175	GLU

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Mol	Chain	Res	Type
1	dE	179	GLN
1	dE	184	TRP
1	dE	196	PRO
1	eE	18	ARG
1	eE	72	THR
1	eE	96	MET
1	eE	97	ARG
1	eE	184	TRP
1	eE	197	ASP
1	eE	227	LYS
1	eE	229	ARG
1	fE	18	ARG
1	fE	121	ASN
1	fE	184	TRP
1	gE	33	SER
1	gE	96	MET
1	gE	97	ARG
1	gE	108	THR
1	gE	110	THR
1	gE	184	TRP
1	gE	189	LEU
1	gE	195	ASN
1	hE	96	MET
1	hE	97	ARG
1	hE	148	THR
1	hE	184	TRP
1	hE	211	LEU
1	iE	18	ARG
1	iE	66	MET
1	iE	96	MET
1	iE	97	ARG
1	iE	100	ARG
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

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Mol	Chain	Res	Type
1	kE	10	MET
1	kE	18	ARG
1	kE	84	HIS
1	kE	96	MET
1	kE	97	ARG
1	kE	110	THR
1	kE	117	TRP
1	kE	164	TYR
1	lE	18	ARG
1	lE	72	THR
1	lE	96	MET
1	lE	97	ARG
1	lE	121	ASN
1	lE	185	MET
1	mE	10	MET
1	mE	15	ILE
1	mE	87	HIS
1	mE	96	MET
1	mE	154	ARG
1	mE	175	GLU
1	mE	184	TRP
1	mE	202	LEU
1	mE	203	LYS
1	nE	53	ASN
1	nE	55	MET
1	nE	96	MET
1	nE	171	THR
1	nE	184	TRP
1	oE	48	THR
1	oE	50	GLN
1	oE	66	MET
1	oE	81	ASP
1	oE	96	MET
1	oE	97	ARG
1	oE	108	THR
1	oE	147	PRO
1	oE	184	TRP
1	oE	227	LYS
1	oE	229	ARG
1	pE	1	PRO
1	pE	48	THR
1	pE	72	THR

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Mol	Chain	Res	Type
1	pE	96	MET
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	10	MET
1	qE	30	LYS
1	qE	96	MET
1	qE	97	ARG
1	qE	107	THR
1	qE	148	THR
1	qE	154	ARG
1	qE	184	TRP
1	rE	97	ARG
1	rE	98	GLU
1	rE	121	ASN
1	rE	130	TYR
1	rE	148	THR
1	rE	185	MET
1	sE	51	ASP
1	sE	96	MET
1	sE	97	ARG
1	sE	107	THR
1	sE	154	ARG
1	sE	184	TRP
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	97	ARG
1	uE	108	THR
1	uE	147	PRO
1	uE	184	TRP
1	uE	195	ASN
1	vE	10	MET
1	vE	96	MET
1	vE	99	PRO
1	vE	148	THR

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Mol	Chain	Res	Type
1	vE	175	GLU
1	wE	2	ILE
1	wE	18	ARG
1	wE	66	MET
1	wE	96	MET
1	wE	148	THR
1	wE	182	LYS
1	wE	205	LEU
1	xE	70	LYS
1	xE	97	ARG
1	xE	121	ASN
1	xE	122	PRO
1	xE	163	ASP
1	xE	226	HIS
1	yE	9	GLN
1	yE	10	MET
1	yE	69	LEU
1	yE	96	MET
1	yE	108	THR
1	zE	2	ILE
1	zE	67	GLN
1	zE	70	LYS
1	zE	96	MET
1	zE	108	THR
1	zE	110	THR
1	zE	139	ASN
1	zE	148	THR
1	zE	172	LEU
1	zE	197	ASP
1	0E	53	ASN
1	0E	66	MET
1	0E	96	MET
1	0E	97	ARG
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	96	MET
1	1E	110	THR
1	1E	121	ASN

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Mol	Chain	Res	Type
1	1E	148	THR
1	1E	155	GLN
1	2E	30	LYS
1	2E	107	THR
1	2E	148	THR
1	2E	231	LEU
1	3E	184	TRP
1	4E	10	MET
1	4E	63	GLN
1	4E	66	MET
1	4E	96	MET
1	4E	108	THR
1	4E	121	ASN
1	4E	139	ASN
1	5E	25	LYS
1	5E	96	MET
1	5E	110	THR
1	5E	195	ASN
1	6E	10	MET
1	6E	15	ILE
1	6E	21	ASN
1	6E	75	GLU
1	6E	96	MET
1	6E	97	ARG
1	6E	108	THR
1	6E	139	ASN
1	6E	147	PRO
1	6E	227	LYS
1	7E	10	MET
1	7E	15	ILE
1	7E	30	LYS
1	7E	85	PRO
1	7E	107	THR
1	7E	121	ASN
1	7E	182	LYS
1	7E	183	ASN
1	8E	2	ILE
1	8E	10	MET
1	8E	96	MET
1	8E	97	ARG
1	8E	107	THR
1	8E	117	TRP

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Mol	Chain	Res	Type
1	8E	148	THR
1	9E	18	ARG
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	9E	226	HIS
1	AF	9	GLN
1	AF	96	MET
1	AF	97	ARG
1	AF	107	THR
1	AF	122	PRO
1	AF	184	TRP
1	BF	96	MET
1	BF	108	THR
1	BF	171	THR
1	CF	7	GLN
1	CF	66	MET
1	CF	96	MET
1	CF	97	ARG
1	CF	147	PRO
1	CF	188	THR
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	121	ASN
1	DF	171	THR
1	DF	219	GLN
1	DF	230	VAL
1	EF	66	MET
1	EF	96	MET
1	FF	4	GLN
1	FF	48	THR
1	FF	58	THR
1	FF	96	MET
1	FF	97	ARG

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Mol	Chain	Res	Type
1	FF	107	THR
1	FF	117	TRP
1	FF	121	ASN
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 monosaccharides 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 ⓘ

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 ⓘ

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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	223	-0.48 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	205	0.47 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	190	-0.48 ± 0.14	None needed (< 0.5 ppm)
^{15}N	209	0.38 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

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	^{1}H	^{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	^{1}H	^{13}C	^{15}N
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	^{1}H	^{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%)
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.

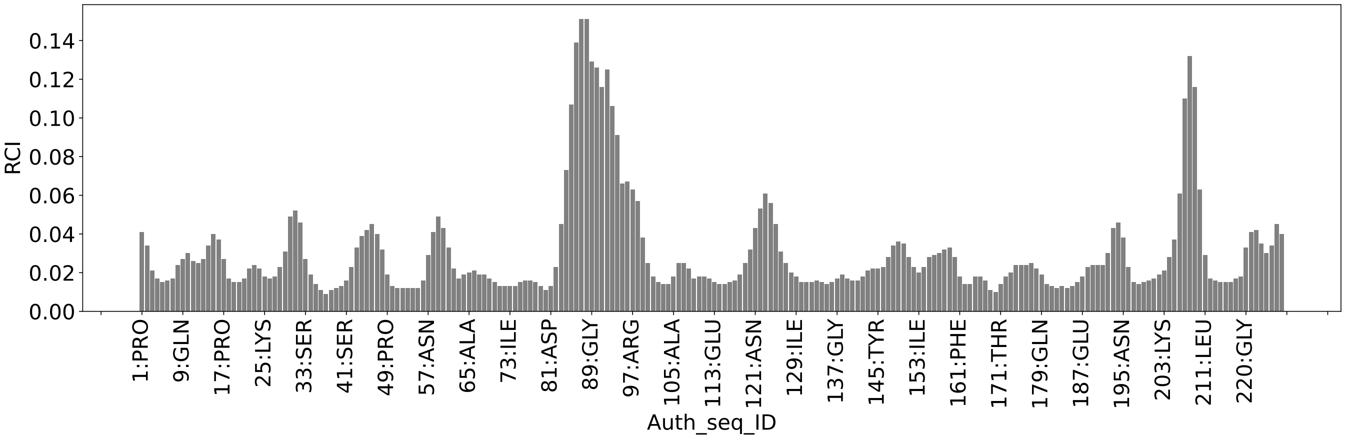
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:


RCI
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:PRO
9:GLN
17:PRO
25:LYS
33:SER
41:SER
49:PRO
57:ASN
65:ALA
73:ILE
81:ASP
89:GLY
97:ARG
105:ALA
113:GLU
121:ASN
129:ILE
137:GLY
145:TYR
153:ILE
161:PHE
171:THR
179:GLN
187:GLU
195:ASN
203:LYS
211:LEU
220:GLY
Auth_seq_ID

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 ($\|i-j\|\geq5$)	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

[1] Long 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)	16.0	0.45
>0.5 (Large)	35.0	3.5

8.2.2 Average number of dihedral-angle violations per model ⓘ

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	19.4
>20.0 (Large)	24.0	147.8

9 Distance violation analysis ⓘ

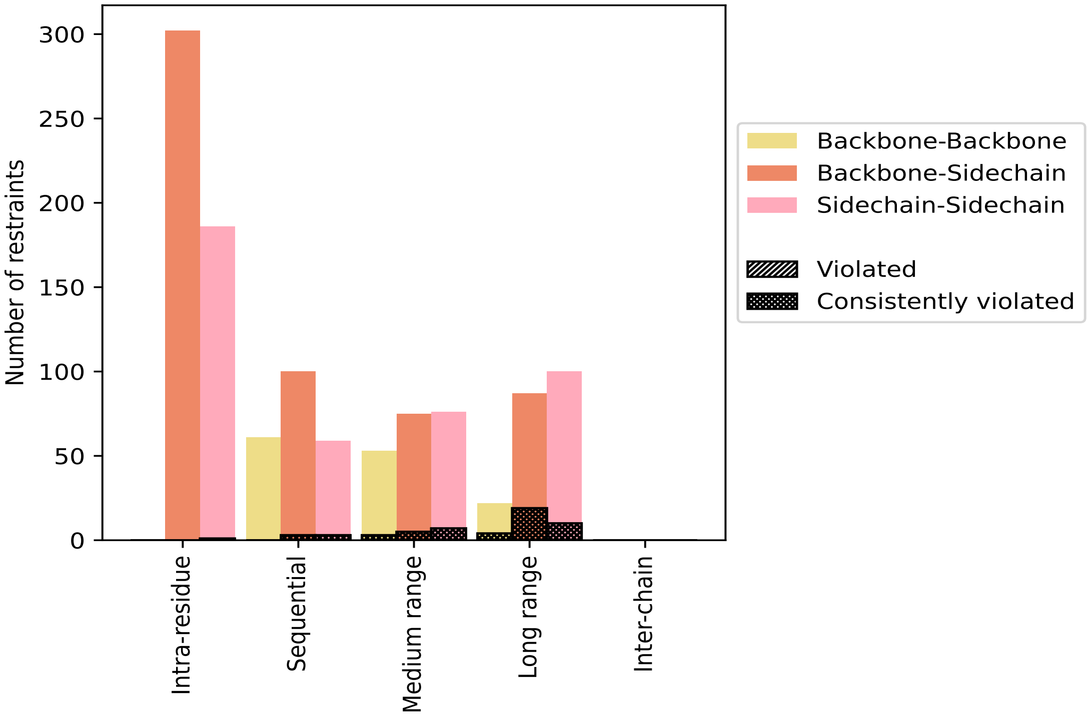
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	488	43.5	1	0.2	0.1	1	0.2	0.1
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	1	0.5	0.1	1	0.5	0.1
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|≥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	55	4.9	4.9	55	4.9	4.9
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	21	5.0	1.9	21	5.0	1.9

[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 ⓘ



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

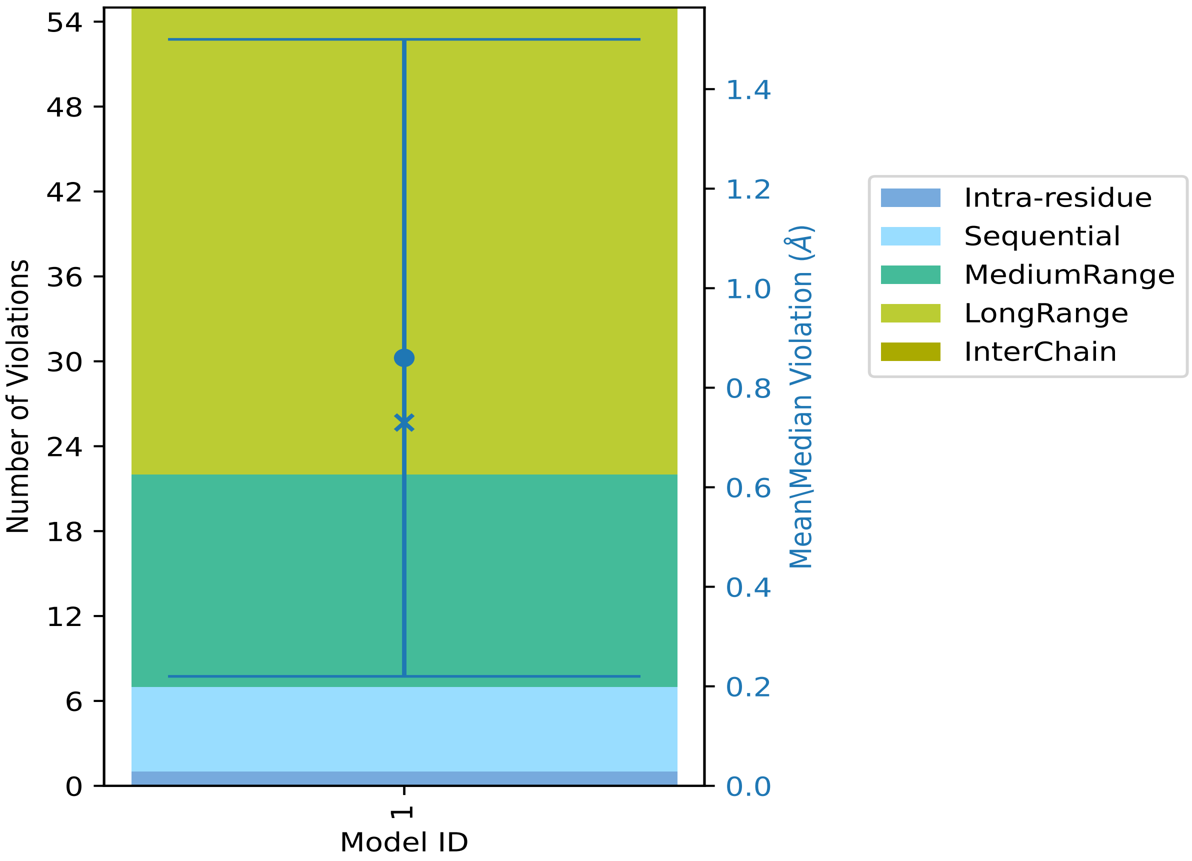
9.2 Distance violation statistics for each model ⓘ

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	1	6	15	33	0	55	0.86	3.5	0.64	0.73

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

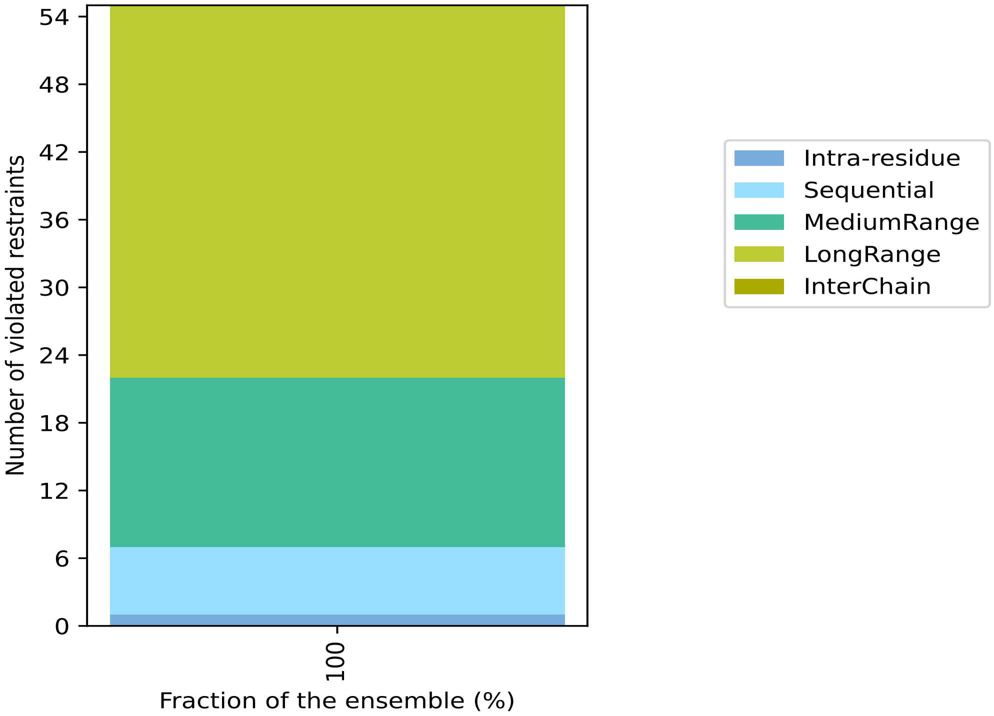
9.3 Distance violation statistics for the ensemble ⓘ

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, 1066(IR:487, 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]	%
1	6	15	33	0	55	1	100.0

[1] Intra-residue restraints, [2] Sequential restraints, [3] Medium range restraints, [4] Long range restraints, [5] Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



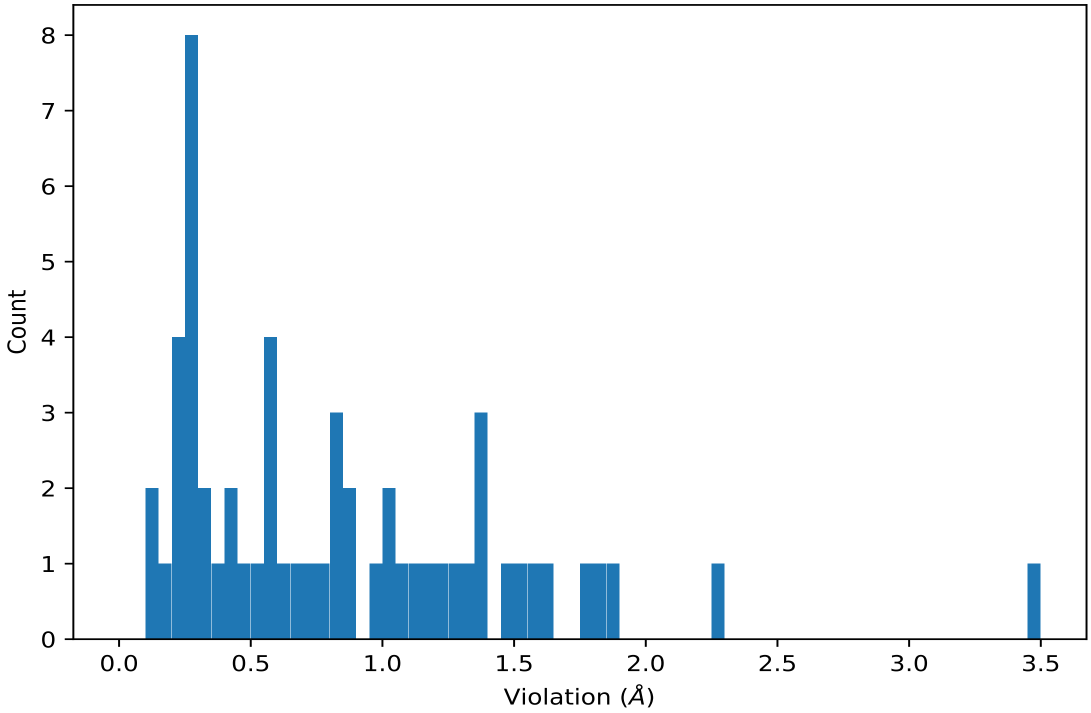
9.4 Most violated distance restraints in the ensemble ⓘ

No violations found

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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 ⓘ

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:A:23:TRP:CZ2	1:A:36:VAL:CA	1	1.11
(1,885)	1:A:159:GLU:CG	1:A:158:LYS:CG	1	1.06
(1,1121)	1:A:153:ILE:CB	1:A:151:LEU:CG	1	1.04
(1,985)	1:A:131:LYS:CE	1:A:127:GLY:CA	1	1.01
(1,766)	1:A:103:ASP:CA	1:A:107:THR:CA	1	0.98
(1,131)	1:A:102:SER:CB	1:A:107:THR:CB	1	0.87
(1,130)	1:A:102:SER:CB	1:A:107:THR:CA	1	0.87
(1,163)	1:A:118:MET:CA	1:A:125:PRO:CD	1	0.83
(1,1004)	1:A:80:TRP:CG	1:A:83:LEU:CB	1	0.83
(1,1078)	1:A:153:ILE:CB	1:A:154:ARG:CD	1	0.81
(1,82)	1:A:49:PRO:CA	1:A:126:VAL:CG1	1	0.77
(1,206)	1:A:202:LEU:CD2	1:A:214:MET:CA	1	0.73
(1,1017)	1:A:47:ALA:CA	1:A:51:ASP:CA	1	0.7
(1,1118)	1:A:80:TRP:CE3	1:A:76:GLU:CA	1	0.62
(1,192)	1:A:161:PHE:CD1	1:A:202:LEU:CA	1	0.6
(1,106)	1:A:80:TRP:CZ2	1:A:101:GLY:CA	1	0.6
(1,179)	1:A:154:ARG:CA	1:A:194:ALA:CB	1	0.59
(1,880)	1:A:117:TRP:CE3	1:A:118:MET:CB	1	0.58
(1,715)	1:A:84:HIS:C	1:A:81:ASP:CB	1	0.52
(1,164)	1:A:118:MET:CA	1:A:126:VAL:CA	1	0.45
(1,45)	1:A:24:VAL:CG1	1:A:58:THR:CA	1	0.44
(1,175)	1:A:153:ILE:CA	1:A:171:THR:CB	1	0.44
(1,14)	1:A:15:ILE:CA	1:A:51:ASP:CA	1	0.36
(1,2)	1:A:1:PRO:CB	1:A:47:ALA:CB	1	0.31
(1,190)	1:A:161:PHE:CB	1:A:194:ALA:CB	1	0.31
(1,702)	1:A:121:ASN:CA	1:A:123:PRO:CG	1	0.3
(1,41)	1:A:23:TRP:CD1	1:A:59:VAL:CG1	1	0.3
(1,207)	1:A:202:LEU:CD2	1:A:214:MET:CB	1	0.29
(1,138)	1:A:103:ASP:CB	1:A:108:THR:CG2	1	0.29
(1,1072)	1:A:139:ASN:CA	1:A:140:LYS:CE	1	0.28
(1,884)	1:A:117:TRP:CE3	1:A:118:MET:CA	1	0.26
(1,343)	1:A:23:TRP:CG	1:A:23:TRP:CD1	1	0.25
(1,343)	1:A:23:TRP:CG	1:A:23:TRP:CD2	1	0.25
(1,29)	1:A:23:TRP:CA	1:A:40:PHE:CA	1	0.24
(1,24)	1:A:20:LEU:CG	1:A:55:MET:CA	1	0.22
(1,128)	1:A:99:PRO:CA	1:A:126:VAL:CB	1	0.22
(1,974)	1:A:184:TRP:CG	1:A:182:LYS:CA	1	0.2
(1,64)	1:A:40:PHE:CD1	1:A:131:LYS:CG	1	0.16
(1,740)	1:A:80:TRP:CD1	1:A:79:GLU:CA	1	0.11
(1,172)	1:A:153:ILE:CB	1:A:164:TYR:CA	1	0.11

10 Dihedral-angle violation analysis ⓘ

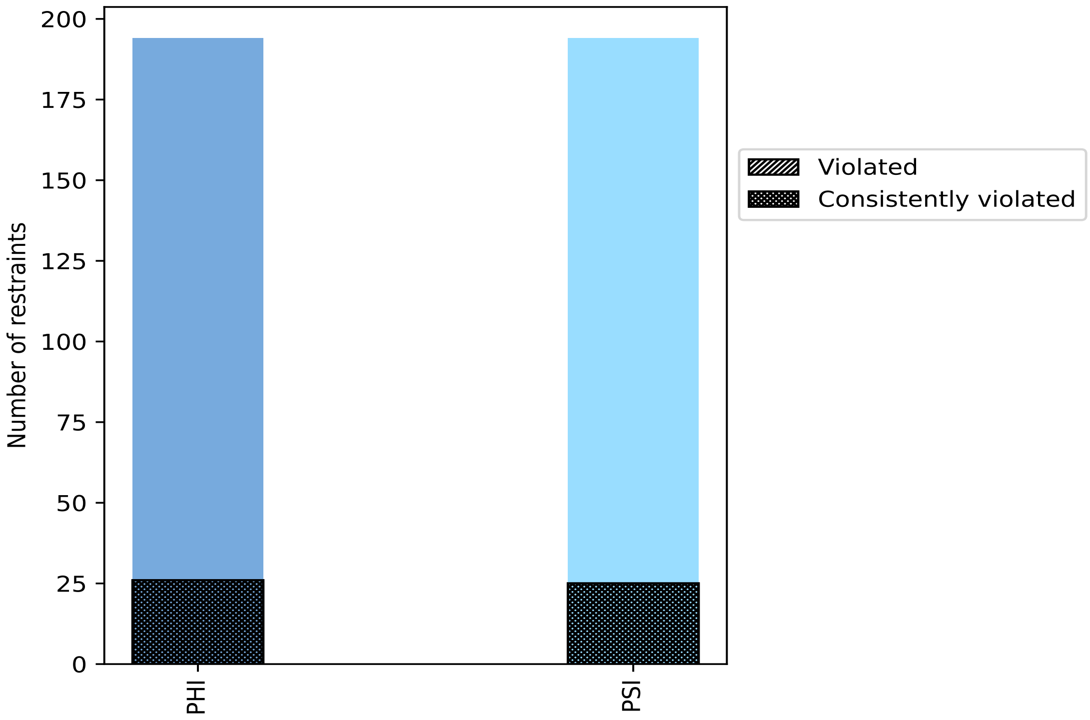
10.1 Summary of dihedral-angle violations ⓘ

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]
PHI	194	50.0	26	13.4	6.7	26	13.4	6.7
PSI	194	50.0	25	12.9	6.4	25	12.9	6.4
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 ⓘ



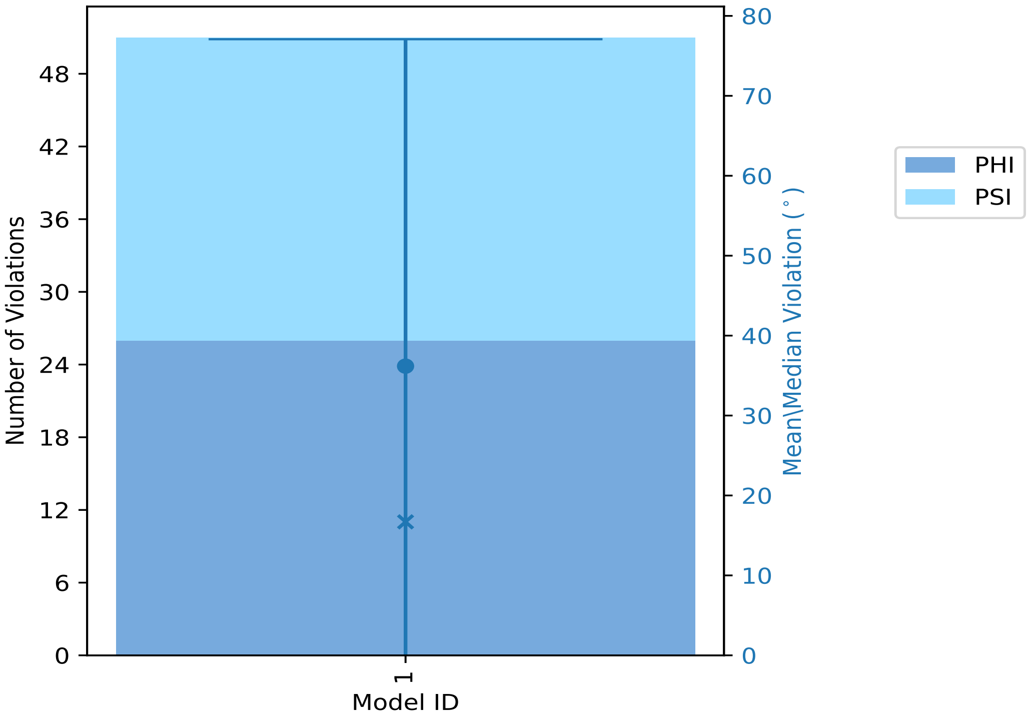
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	26	25	51	36.18	147.8	40.9	16.7

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

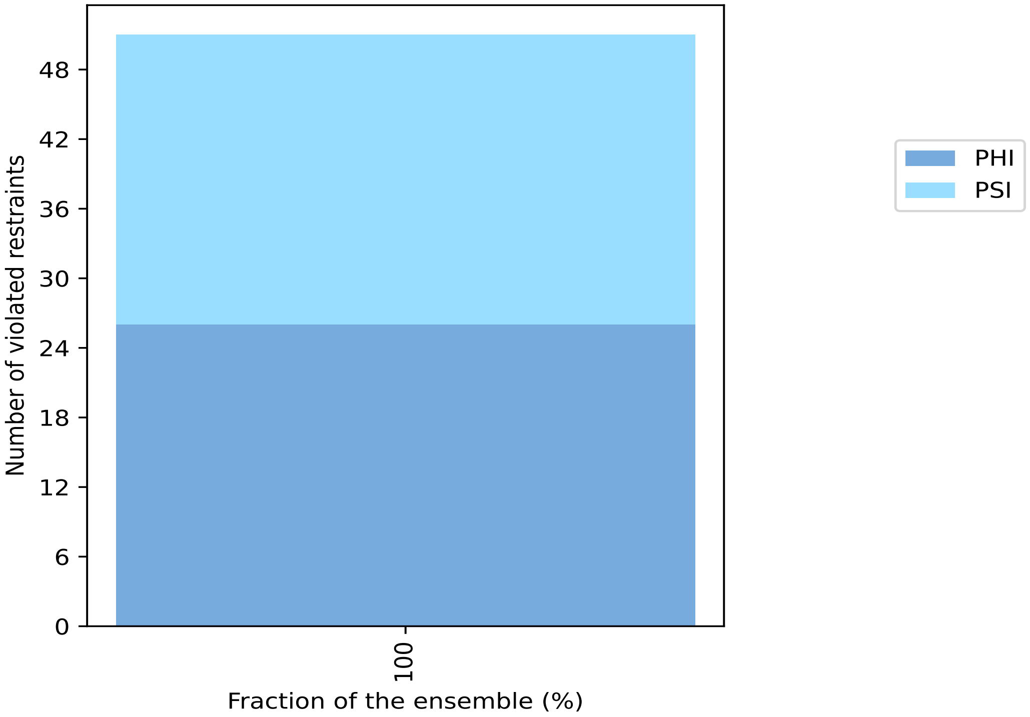
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	
PHI	PSI	Total	Count[1]	%
26	25	51	1	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



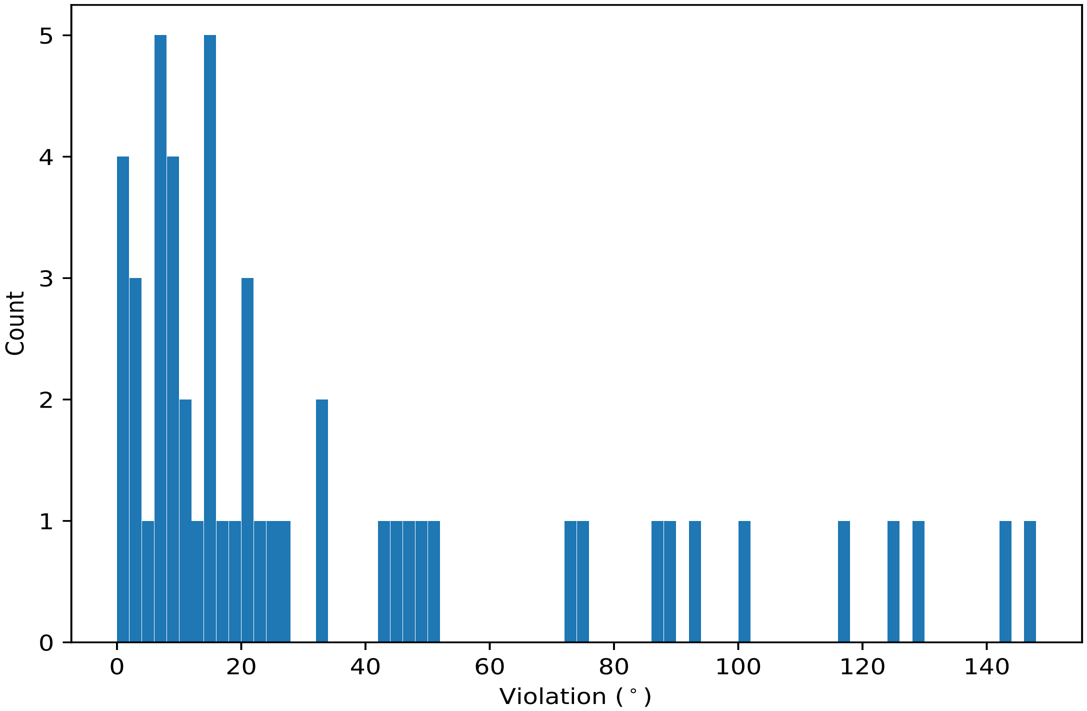
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

No violations found

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 ⓘ

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:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	1:A:9:GLN:N	1	147.8
(1,5)	1:A:3:VAL:C	1:A:4:GLN:N	1:A:4:GLN:CA	1:A:4:GLN:C	1	142.4
(1,153)	1:A:96:MET:C	1:A:97:ARG:N	1:A:97:ARG:CA	1:A:97:ARG:C	1	128.3
(1,152)	1:A:96:MET:N	1:A:96:MET:CA	1:A:96:MET:C	1:A:97:ARG:N	1	125.8
(1,166)	1:A:105:ALA:N	1:A:105:ALA:CA	1:A:105:ALA:C	1:A:106:GLY:N	1	116.2
(1,8)	1:A:5:ASN:N	1:A:5:ASN:CA	1:A:5:ASN:C	1:A:6:LEU:N	1	100.1
(1,377)	1:A:60:GLY:C	1:A:61:GLY:N	1:A:61:GLY:CA	1:A:61:GLY:C	1	93.9
(1,382)	1:A:176:GLN:N	1:A:176:GLN:CA	1:A:176:GLN:C	1:A:177:ALA:N	1	88.1
(1,380)	1:A:175:GLU:N	1:A:175:GLU:CA	1:A:175:GLU:C	1:A:176:GLN:N	1	86.9
(1,104)	1:A:62:HIS:N	1:A:62:HIS:CA	1:A:62:HIS:C	1:A:63:GLN:N	1	74.3
(1,378)	1:A:61:GLY:N	1:A:61:GLY:CA	1:A:61:GLY:C	1:A:62:HIS:N	1	72.5
(1,369)	1:A:145:TYR:C	1:A:146:SER:N	1:A:146:SER:CA	1:A:146:SER:C	1	51.8
(1,7)	1:A:4:GLN:C	1:A:5:ASN:N	1:A:5:ASN:CA	1:A:5:ASN:C	1	48.3
(1,11)	1:A:7:GLN:C	1:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	1	47.2
(1,373)	1:A:176:GLN:C	1:A:177:ALA:N	1:A:177:ALA:CA	1:A:177:ALA:C	1	45.6
(1,364)	1:A:44:SER:N	1:A:44:SER:CA	1:A:44:SER:C	1:A:45:GLU:N	1	42.5
(1,80)	1:A:46:GLY:N	1:A:46:GLY:CA	1:A:46:GLY:C	1:A:47:ALA:N	1	33.1
(1,381)	1:A:175:GLU:C	1:A:176:GLN:N	1:A:176:GLN:CA	1:A:176:GLN:C	1	32.8
(1,81)	1:A:47:ALA:C	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	1	27.9
(1,13)	1:A:9:GLN:C	1:A:10:MET:N	1:A:10:MET:CA	1:A:10:MET:C	1	25.4
(1,56)	1:A:32:PHE:N	1:A:32:PHE:CA	1:A:32:PHE:C	1:A:33:SER:N	1	22.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,321)	1:A:197:ASP:C	1:A:198:CYS:N	1:A:198:CYS:CA	1:A:198:CYS:C	1	21.7
(1,188)	1:A:117:TRP:N	1:A:117:TRP:CA	1:A:117:TRP:C	1:A:118:MET:N	1	21.0
(1,143)	1:A:81:ASP:C	1:A:82:ARG:N	1:A:82:ARG:CA	1:A:82:ARG:C	1	20.4
(1,82)	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	1:A:49:PRO:N	1	19.4
(1,191)	1:A:118:MET:C	1:A:119:THR:N	1:A:119:THR:CA	1:A:119:THR:C	1	16.7
(1,240)	1:A:149:SER:N	1:A:149:SER:CA	1:A:149:SER:C	1:A:150:ILE:N	1	15.3
(1,189)	1:A:117:TRP:C	1:A:118:MET:N	1:A:118:MET:CA	1:A:118:MET:C	1	15.2
(1,79)	1:A:45:GLU:C	1:A:46:GLY:N	1:A:46:GLY:CA	1:A:46:GLY:C	1	15.1
(1,103)	1:A:61:GLY:C	1:A:62:HIS:N	1:A:62:HIS:CA	1:A:62:HIS:C	1	14.1
(1,283)	1:A:173:ARG:C	1:A:174:ALA:N	1:A:174:ALA:CA	1:A:174:ALA:C	1	14.0
(1,361)	1:A:30:LYS:C	1:A:31:ALA:N	1:A:31:ALA:CA	1:A:31:ALA:C	1	12.3
(1,370)	1:A:146:SER:N	1:A:146:SER:CA	1:A:146:SER:C	1:A:147:PRO:N	1	11.5
(1,358)	1:A:220:GLY:N	1:A:220:GLY:CA	1:A:220:GLY:C	1:A:221:VAL:N	1	10.5
(1,77)	1:A:44:SER:C	1:A:45:GLU:N	1:A:45:GLU:CA	1:A:45:GLU:C	1	9.1
(1,51)	1:A:28:GLU:C	1:A:29:GLU:N	1:A:29:GLU:CA	1:A:29:GLU:C	1	8.6
(1,60)	1:A:35:GLU:N	1:A:35:GLU:CA	1:A:35:GLU:C	1:A:36:VAL:N	1	8.2
(1,154)	1:A:97:ARG:N	1:A:97:ARG:CA	1:A:97:ARG:C	1:A:98:GLU:N	1	8.0
(1,383)	1:A:8:GLY:C	1:A:9:GLN:N	1:A:9:GLN:CA	1:A:9:GLN:C	1	6.8
(1,78)	1:A:45:GLU:N	1:A:45:GLU:CA	1:A:45:GLU:C	1:A:46:GLY:N	1	6.7
(1,354)	1:A:218:CYS:N	1:A:218:CYS:CA	1:A:218:CYS:C	1:A:219:GLN:N	1	6.5
(1,387)	1:A:205:LEU:C	1:A:206:GLY:N	1:A:206:GLY:CA	1:A:206:GLY:C	1	6.2
(1,58)	1:A:34:PRO:N	1:A:34:PRO:CA	1:A:34:PRO:C	1:A:35:GLU:N	1	6.1
(1,196)	1:A:122:PRO:N	1:A:122:PRO:CA	1:A:122:PRO:C	1:A:123:PRO:N	1	5.7
(1,55)	1:A:31:ALA:C	1:A:32:PHE:N	1:A:32:PHE:CA	1:A:32:PHE:C	1	2.9
(1,357)	1:A:219:GLN:C	1:A:220:GLY:N	1:A:220:GLY:CA	1:A:220:GLY:C	1	2.2
(1,158)	1:A:100:ARG:N	1:A:100:ARG:CA	1:A:100:ARG:C	1:A:101:GLY:N	1	2.2
(1,285)	1:A:177:ALA:C	1:A:178:SER:N	1:A:178:SER:CA	1:A:178:SER:C	1	1.7
(1,362)	1:A:31:ALA:N	1:A:31:ALA:CA	1:A:31:ALA:C	1:A:32:PHE:N	1	1.6
(1,187)	1:A:116:GLY:C	1:A:117:TRP:N	1:A:117:TRP:CA	1:A:117:TRP:C	1	1.4
(1,322)	1:A:198:CYS:N	1:A:198:CYS:CA	1:A:198:CYS:C	1:A:199:LYS:N	1	1.2