



wwPDB NMR Structure Validation Summary Report i

Jun 4, 2023 – 02:59 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.; Schwitters, C.D.; Perilla, J.R.; Gronenborn, A.M.; Polenova, T.
Deposited on : 2020-05-27

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

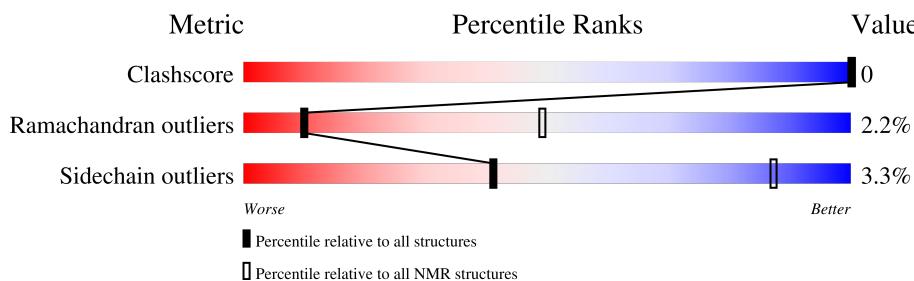
MolProbitiy : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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 $\leq 5\%$.



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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	90% 7% •
1	5D	231	92% 6% •
1	5E	231	91% 8% •
1	6	231	89% 10% •
1	6A	231	92% 7% •
1	6B	231	91% 7% •
1	6C	231	93% 6% •
1	6D	231	93% 6% •
1	6E	231	91% 8%
1	7	231	90% 9% •
1	7A	231	92% 8%
1	7B	231	92% 8%
1	7C	231	89% 10% •
1	7D	231	91% 7% •
1	7E	231	89% 10% •
1	8	231	92% 6% •
1	8A	231	93% 6% •
1	8B	231	91% 8% •
1	8C	231	92% 6% •
1	8D	231	91% 8% •
1	8E	231	89% 10% •
1	9	231	89% 10% •
1	9A	231	90% 8% •
1	9B	231	91% 7% •
1	9C	231	93% 6% •

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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 [\(i\)](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	EE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	FE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	GE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	HE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	IE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	JE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	KE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	LE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	ME	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	NE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	OE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	PE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	QE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	RE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	SE	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
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	

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

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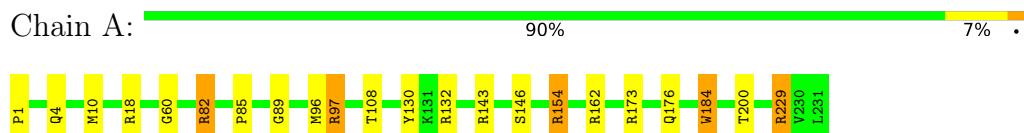
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Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
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1	FF	231	3596	1131	1801	317	334	13	0

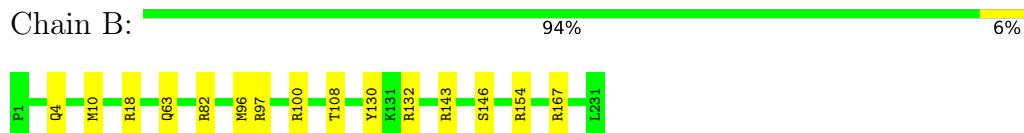
4 Residue-property plots

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.

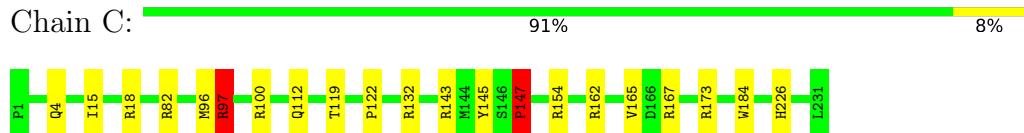
- Molecule 1: HIV-1 capsid protein



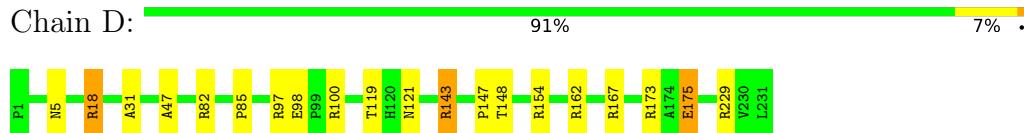
- Molecule 1: HIV-1 capsid protein



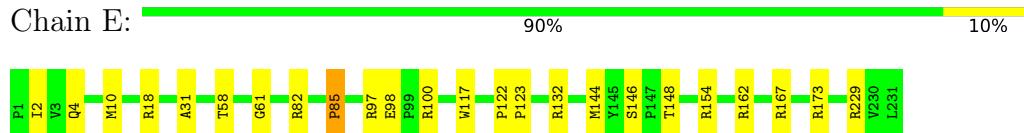
- Molecule 1: HIV-1 capsid protein



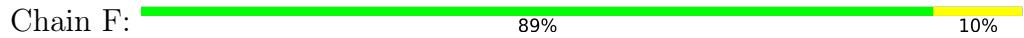
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein





- Molecule 1: HIV-1 capsid protein

Chain 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:  91% •



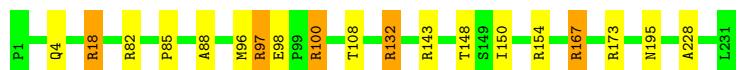
- Molecule 1: HIV-1 capsid protein

Chain O:  90% •



- Molecule 1: HIV-1 capsid protein

Chain P:  92% •



- Molecule 1: HIV-1 capsid protein

Chain Q:  91% •



- Molecule 1: HIV-1 capsid protein

Chain R:  90% •

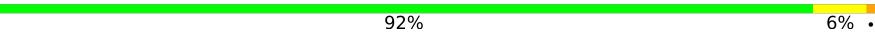


- Molecule 1: HIV-1 capsid protein

Chain S:  90% •



- Molecule 1: HIV-1 capsid protein

Chain T:  92% •



- Molecule 1: HIV-1 capsid protein

Chain U:  6% •

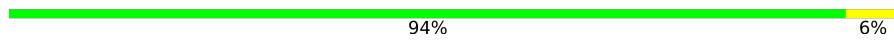


- Molecule 1: HIV-1 capsid protein

Chain V:  10% •

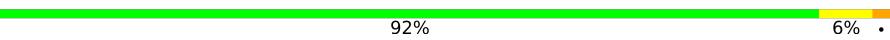


- Molecule 1: HIV-1 capsid protein

Chain W:  6% •



- Molecule 1: HIV-1 capsid protein

Chain X:  6% •



- Molecule 1: HIV-1 capsid protein

Chain Y:  8% •



- Molecule 1: HIV-1 capsid protein

Chain Z:  10% •



- Molecule 1: HIV-1 capsid protein

Chain a:  5% •



- Molecule 1: HIV-1 capsid protein

Chain b:  9% •



- 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:

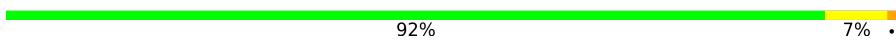


- Molecule 1: HIV-1 capsid protein

Chain i:



- Molecule 1: HIV-1 capsid protein

Chain j:  92% • 7%



- Molecule 1: HIV-1 capsid protein

Chain k:  91% • 8%

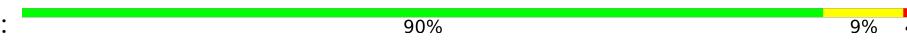


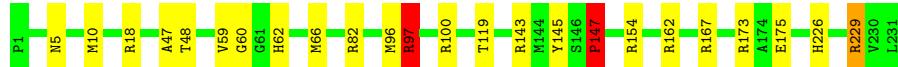
- Molecule 1: HIV-1 capsid protein

Chain l:  89% • 10%



- Molecule 1: HIV-1 capsid protein

Chain m:  90% • 9%

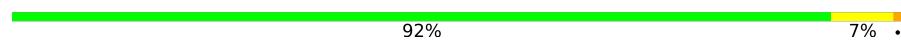


- Molecule 1: HIV-1 capsid protein

Chain n:  91% • 8%



- Molecule 1: HIV-1 capsid protein

Chain o:  92% • 7%



- Molecule 1: HIV-1 capsid protein

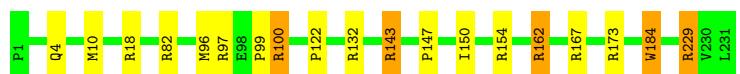
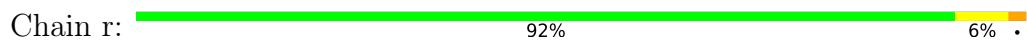
Chain p:  91% • 6%



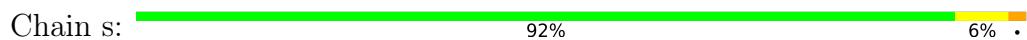
- Molecule 1: HIV-1 capsid protein



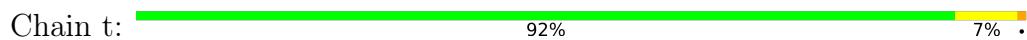
- Molecule 1: HIV-1 capsid protein



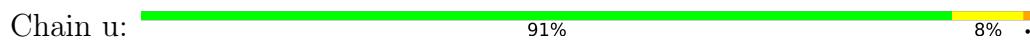
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein





- Molecule 1: HIV-1 capsid protein

Chain y: 90% 8%



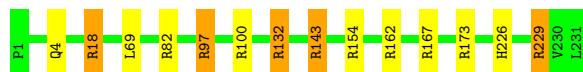
- Molecule 1: HIV-1 capsid protein

Chain z: 92% 7%



- Molecule 1: HIV-1 capsid protein

Chain 0: 94% 6%



- Molecule 1: HIV-1 capsid protein

Chain 1: 89% 10%



- Molecule 1: HIV-1 capsid protein

Chain 2: 90% 7%



- Molecule 1: HIV-1 capsid protein

Chain 3: 90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 4: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain 5:  91% • 8%



- Molecule 1: HIV-1 capsid protein

Chain 6:  89% • 10%



- Molecule 1: HIV-1 capsid protein

Chain 7:  90% • 9%



- Molecule 1: HIV-1 capsid protein

Chain 8:  92% • 6%



- Molecule 1: HIV-1 capsid protein

Chain 9:  89% • 10%



- Molecule 1: HIV-1 capsid protein

Chain AA:  93% • 6%



- Molecule 1: HIV-1 capsid protein

Chain BA:  91% • 8%

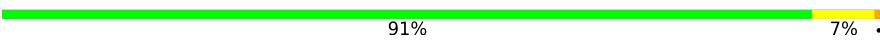


- Molecule 1: HIV-1 capsid protein

Chain CA:  8%



- Molecule 1: HIV-1 capsid protein

Chain DA:  7% •



- Molecule 1: HIV-1 capsid protein

Chain EA:  6% •



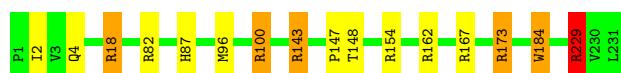
- Molecule 1: HIV-1 capsid protein

Chain FA:  9% •



- Molecule 1: HIV-1 capsid protein

Chain GA:  ..



- Molecule 1: HIV-1 capsid protein

Chain HA:  6% •



- Molecule 1: HIV-1 capsid protein

Chain IA:  7%



- Molecule 1: HIV-1 capsid protein

Chain JA:  6% •



- Molecule 1: HIV-1 capsid protein

Chain KA: 90% 8% •



- Molecule 1: HIV-1 capsid protein

Chain LA: 93% 6% •



- Molecule 1: HIV-1 capsid protein

Chain MA: 91% 7% •



- Molecule 1: HIV-1 capsid protein

Chain NA: 91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain OA: 90% 8% •



- Molecule 1: HIV-1 capsid protein

Chain PA: 92% 6% •

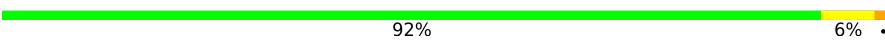


- Molecule 1: HIV-1 capsid protein

Chain QA: 92% 8% •



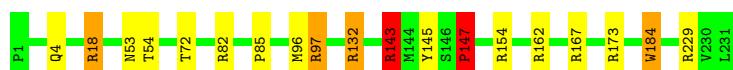
- Molecule 1: HIV-1 capsid protein

Chain RA:  92% •



- Molecule 1: HIV-1 capsid protein

Chain SA:  92% •

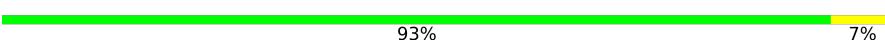


- Molecule 1: HIV-1 capsid protein

Chain TA:  93% •



- Molecule 1: HIV-1 capsid protein

Chain UA:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain VA:  87% •



- Molecule 1: HIV-1 capsid protein

Chain WA:  92% 7%

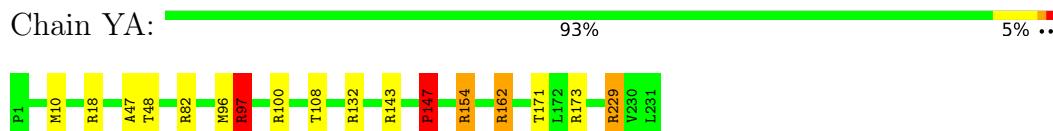


- Molecule 1: HIV-1 capsid protein

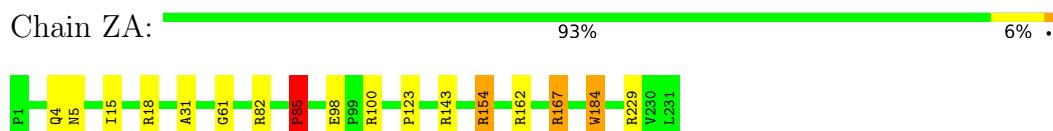
Chain XA:  91% •



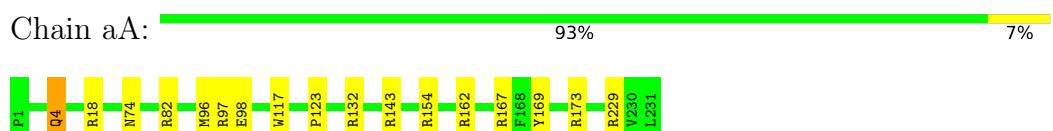
- Molecule 1: HIV-1 capsid protein



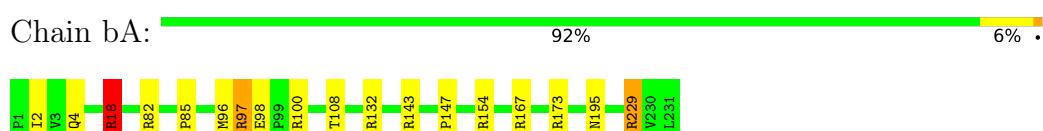
- Molecule 1: HIV-1 capsid protein



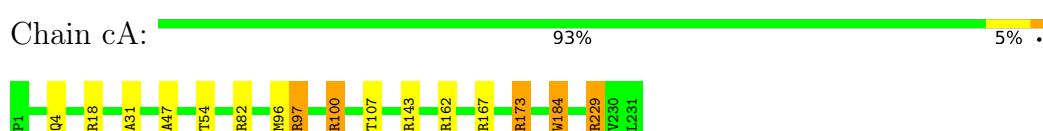
- Molecule 1: HIV-1 capsid protein



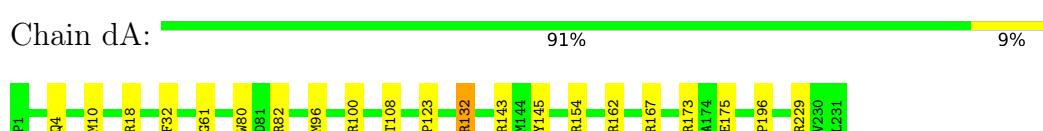
- Molecule 1: HIV-1 capsid protein



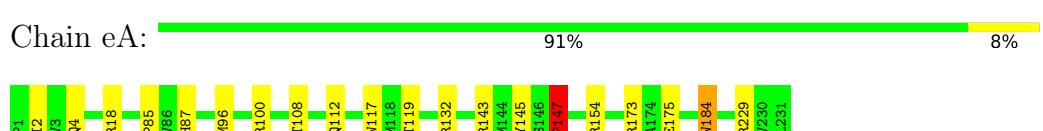
- Molecule 1: HIV-1 capsid protein



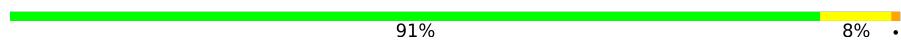
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

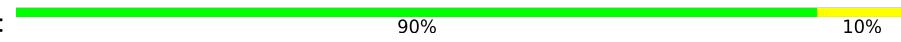


- Molecule 1: HIV-1 capsid protein

Chain fA:  91% 8%

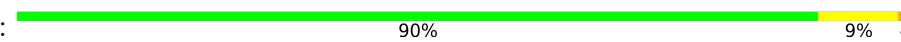


- Molecule 1: HIV-1 capsid protein

Chain gA:  90% 10%

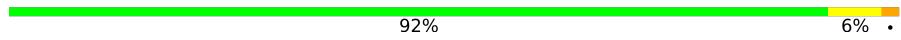


- Molecule 1: HIV-1 capsid protein

Chain hA:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain iA:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain jA:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain kA:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain lA:  92% 7%



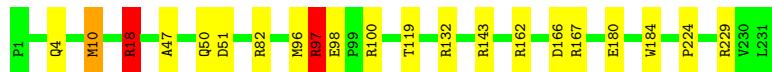
- Molecule 1: HIV-1 capsid protein

Chain mA:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain nA: 91% 8% •



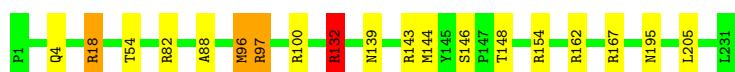
- Molecule 1: HIV-1 capsid protein

Chain oA: 93% 6% •



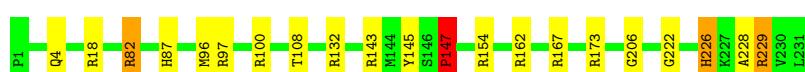
- Molecule 1: HIV-1 capsid protein

Chain pA: 92% 6% •



- Molecule 1: HIV-1 capsid protein

Chain qA: 91% 7% •



- Molecule 1: HIV-1 capsid protein

Chain rA: 90% 9% •



- Molecule 1: HIV-1 capsid protein

Chain sA: 89% 11% •

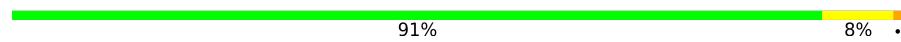


- Molecule 1: HIV-1 capsid protein

Chain tA: 90% 9% •

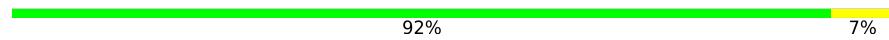


- Molecule 1: HIV-1 capsid protein

Chain uA:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain vA:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain wA:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain xA:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain yA:  91% 8% •



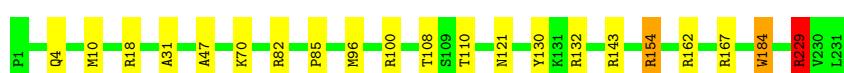
- Molecule 1: HIV-1 capsid protein

Chain zA:  92% 6% •



- Molecule 1: HIV-1 capsid protein

Chain 0A:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain 1A:  10%



- Molecule 1: HIV-1 capsid protein

Chain 2A:  6%

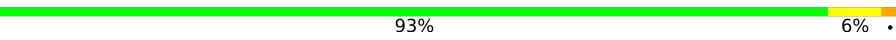


- Molecule 1: HIV-1 capsid protein

Chain 3A:  9%



- Molecule 1: HIV-1 capsid protein

Chain 4A:  6%



- Molecule 1: HIV-1 capsid protein

Chain 5A:  7%



- Molecule 1: HIV-1 capsid protein

Chain 6A:  7%



- Molecule 1: HIV-1 capsid protein

Chain 7A:  8%



- Molecule 1: HIV-1 capsid protein

Chain 8A:  6%



- 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:

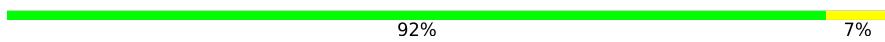


- Molecule 1: HIV-1 capsid protein

Chain FB:

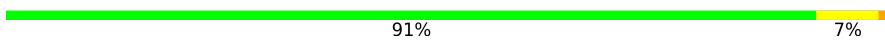


- Molecule 1: HIV-1 capsid protein

Chain GB:  92% • 7%



- Molecule 1: HIV-1 capsid protein

Chain HB:  91% • 7%



- Molecule 1: HIV-1 capsid protein

Chain IB:  91% • 7%

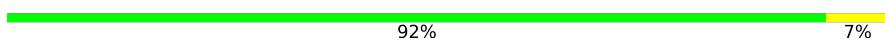


- Molecule 1: HIV-1 capsid protein

Chain JB:  91% • 8%



- Molecule 1: HIV-1 capsid protein

Chain KB:  92% • 7%



- Molecule 1: HIV-1 capsid protein

Chain LB:  90% • 9%



- Molecule 1: HIV-1 capsid protein

Chain MB:  92% • 6%



- Molecule 1: HIV-1 capsid protein

Chain NB:  89%  •



- Molecule 1: HIV-1 capsid protein

Chain OB:  90%  •

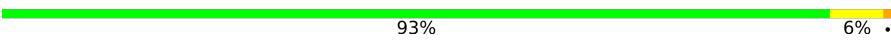


- Molecule 1: HIV-1 capsid protein

Chain PB:  90%  •



- Molecule 1: HIV-1 capsid protein

Chain QB:  93%  •



- Molecule 1: HIV-1 capsid protein

Chain RB:  91%  •



- Molecule 1: HIV-1 capsid protein

Chain SB:  90%  •



- Molecule 1: HIV-1 capsid protein

Chain TB:  91%  •



- Molecule 1: HIV-1 capsid protein

Chain UB:  93%  •



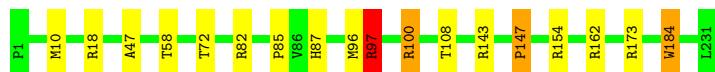
- Molecule 1: HIV-1 capsid protein

Chain VB:



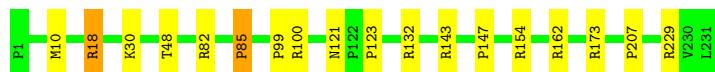
- Molecule 1: HIV-1 capsid protein

Chain WB:



- Molecule 1: HIV-1 capsid protein

Chain XB:



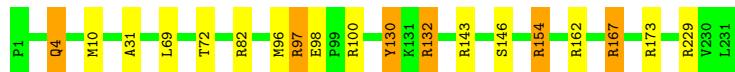
- Molecule 1: HIV-1 capsid protein

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:  92% •



- Molecule 1: HIV-1 capsid protein

Chain dB:  91% •



- Molecule 1: HIV-1 capsid protein

Chain eB:  91% •



- Molecule 1: HIV-1 capsid protein

Chain fB:  92% •



- Molecule 1: HIV-1 capsid protein

Chain gB:  92% •



- Molecule 1: HIV-1 capsid protein

Chain hB:  92% •



- Molecule 1: HIV-1 capsid protein

Chain iB:  90% ••



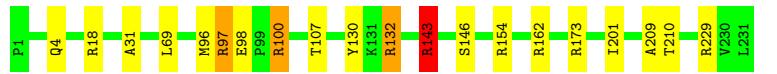
- Molecule 1: HIV-1 capsid protein

Chain jB:  8% •



- Molecule 1: HIV-1 capsid protein

Chain kB:  7% •

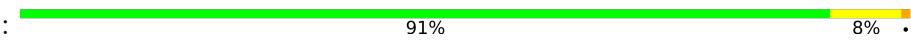


- Molecule 1: HIV-1 capsid protein

Chain lB:  9% •

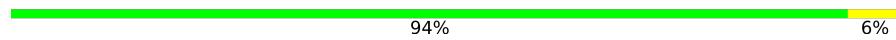


- Molecule 1: HIV-1 capsid protein

Chain mB:  8% •



- Molecule 1: HIV-1 capsid protein

Chain nB:  6%



- Molecule 1: HIV-1 capsid protein

Chain oB:  8% ..



- Molecule 1: HIV-1 capsid protein

Chain pB:  8% •



- Molecule 1: HIV-1 capsid protein

Chain qB:  9% •



- 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:

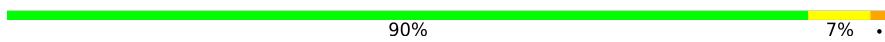


- Molecule 1: HIV-1 capsid protein

Chain xB:

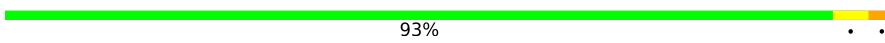


- Molecule 1: HIV-1 capsid protein

Chain yB:  90% 7%



- Molecule 1: HIV-1 capsid protein

Chain zB:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain 0B:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 1B:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 2B:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain 3B:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain 4B:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 5B:
90% 9%



- Molecule 1: HIV-1 capsid protein

Chain 6B:
91% 7%



- Molecule 1: HIV-1 capsid protein

Chain 7B:
92% 8%



- Molecule 1: HIV-1 capsid protein

Chain 8B:
91% 8%



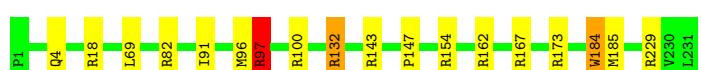
- Molecule 1: HIV-1 capsid protein

Chain 9B:
91% 7%



- Molecule 1: HIV-1 capsid protein

Chain AC:
92% 6%



- Molecule 1: HIV-1 capsid protein

Chain BC:
91% 7%



- Molecule 1: HIV-1 capsid protein

Chain CC:
90% 7%



- Molecule 1: HIV-1 capsid protein

Chain DC: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain EC: 91% 7%



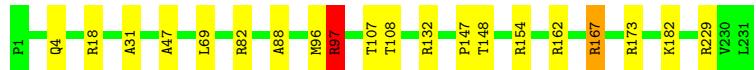
- Molecule 1: HIV-1 capsid protein

Chain FC: 90% 8%



- Molecule 1: HIV-1 capsid protein

Chain GC: 91% 8%



- Molecule 1: HIV-1 capsid protein

Chain HC: 93% 7%



- Molecule 1: HIV-1 capsid protein

Chain IC: 93% 5%

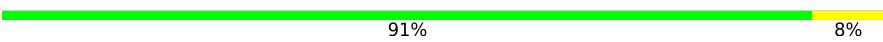


- Molecule 1: HIV-1 capsid protein

Chain JC: 90% 10%



- Molecule 1: HIV-1 capsid protein

Chain KC:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain LC:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain MC:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain NC:  90% 10%



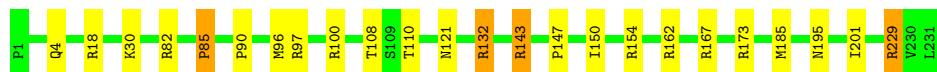
- Molecule 1: HIV-1 capsid protein

Chain OC:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain PC:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain QC:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain RC:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain SC:  92% 7% •



- Molecule 1: HIV-1 capsid protein

Chain TC:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain UC:  91% 6% •



- Molecule 1: HIV-1 capsid protein

Chain VC:  90% 9% •



- Molecule 1: HIV-1 capsid protein

Chain WC:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain XC:  90% 9% •



- Molecule 1: HIV-1 capsid protein

Chain YC:  90% 10%



- 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:

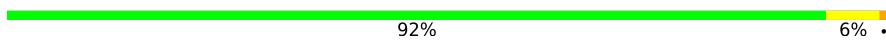


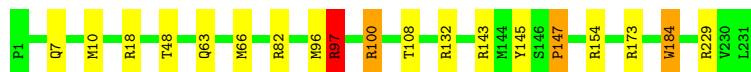
- Molecule 1: HIV-1 capsid protein

Chain fC:

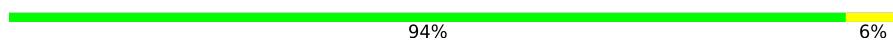


- Molecule 1: HIV-1 capsid protein

Chain gC:  92% •



- Molecule 1: HIV-1 capsid protein

Chain hC:  94% •



- Molecule 1: HIV-1 capsid protein

Chain iC:  92% •

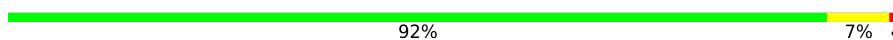


- Molecule 1: HIV-1 capsid protein

Chain jC:  93% •

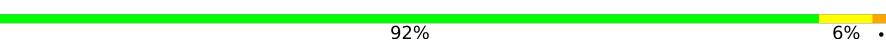


- Molecule 1: HIV-1 capsid protein

Chain kC:  92% •

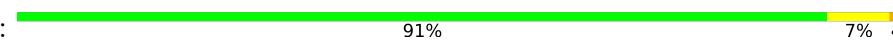


- Molecule 1: HIV-1 capsid protein

Chain lC:  92% •



- Molecule 1: HIV-1 capsid protein

Chain mC:  91% •



- Molecule 1: HIV-1 capsid protein

Chain nC:  91% 6% •



- Molecule 1: HIV-1 capsid protein

Chain oC:  91% 7% •



- Molecule 1: HIV-1 capsid protein

Chain pC:  90% 8% •



- Molecule 1: HIV-1 capsid protein

Chain qC:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain rC:  92% 6% •



- Molecule 1: HIV-1 capsid protein

Chain sC:  92% 6% •

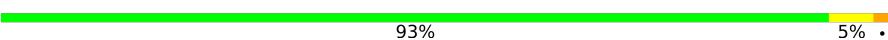


- Molecule 1: HIV-1 capsid protein

Chain tC:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain uC:  93% 5% •



- 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:



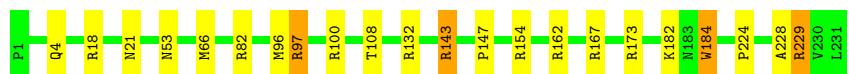
- Molecule 1: HIV-1 capsid protein

Chain 1C:



- Molecule 1: HIV-1 capsid protein

Chain 2C:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain 3C:  93% 7%



- Molecule 1: HIV-1 capsid protein

Chain 4C:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain 5C:  90% 7%



- Molecule 1: HIV-1 capsid protein

Chain 6C:  93% 6%



- Molecule 1: HIV-1 capsid protein

Chain 7C:  89% 10%



- Molecule 1: HIV-1 capsid protein

Chain 8C:  92% 6%

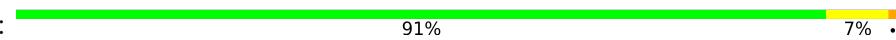


- Molecule 1: HIV-1 capsid protein

Chain 9C:  93% • 6%

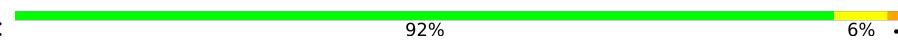


- Molecule 1: HIV-1 capsid protein

Chain AD:  91% • 7%

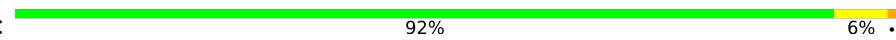


- Molecule 1: HIV-1 capsid protein

Chain BD:  92% • 6%

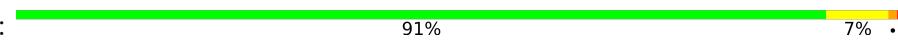


- Molecule 1: HIV-1 capsid protein

Chain CD:  92% • 6%



- Molecule 1: HIV-1 capsid protein

Chain DD:  91% • 7%



- Molecule 1: HIV-1 capsid protein

Chain ED:  90% • 7%



- Molecule 1: HIV-1 capsid protein

Chain FD:  93% • 7%

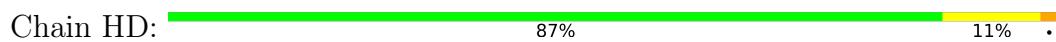


- Molecule 1: HIV-1 capsid protein

Chain GD:  90% • 7%



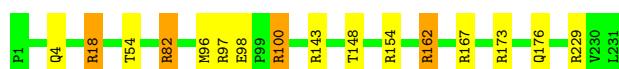
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



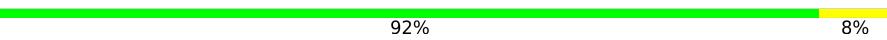
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain OD:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain PD:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain QD:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain RD:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain SD:  91% 6%



- Molecule 1: HIV-1 capsid protein

Chain TD:  91% 8%



- Molecule 1: HIV-1 capsid protein

Chain UD:  89% 9%

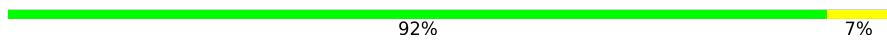


- Molecule 1: HIV-1 capsid protein

Chain VD:  90% 8% •



- Molecule 1: HIV-1 capsid protein

Chain WD:  92% 7% •



- Molecule 1: HIV-1 capsid protein

Chain XD:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain YD:  90% 7% •



- Molecule 1: HIV-1 capsid protein

Chain ZD:  91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain aD:  88% 12% •



- Molecule 1: HIV-1 capsid protein

Chain bD:  92% 6% •



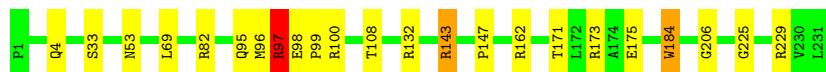
- Molecule 1: HIV-1 capsid protein

Chain cD:  92% 6% •



- Molecule 1: HIV-1 capsid protein

Chain dD: 90% • 9%



- Molecule 1: HIV-1 capsid protein

Chain eD: 93% • 6%



- Molecule 1: HIV-1 capsid protein

Chain fD: 89% • 9%



- Molecule 1: HIV-1 capsid protein

Chain gD: 90% • 9%



- Molecule 1: HIV-1 capsid protein

Chain hD: 92% • 5%



- Molecule 1: HIV-1 capsid protein

Chain iD: 91% • 6%



- Molecule 1: HIV-1 capsid protein

Chain jD: 93% • 7%



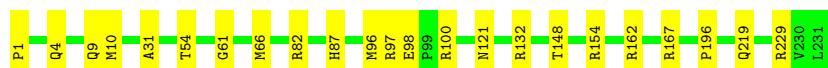
- Molecule 1: HIV-1 capsid protein

Chain kD:  91% 7%

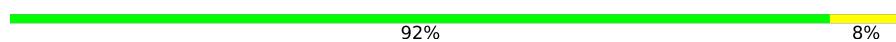


- Molecule 1: HIV-1 capsid protein

Chain lD:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain mD:  92% 8%



- Molecule 1: HIV-1 capsid protein

Chain nD:  91% 7%



- Molecule 1: HIV-1 capsid protein

Chain oD:  92% 6%



- Molecule 1: HIV-1 capsid protein

Chain pD:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain qD:  89% 10%

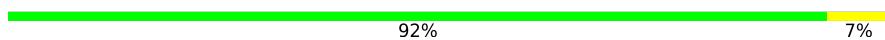


- Molecule 1: HIV-1 capsid protein

Chain rD:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain sD:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain tD:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain uD:  90% 9%



- Molecule 1: HIV-1 capsid protein

Chain vD:  90% 8%



- Molecule 1: HIV-1 capsid protein

Chain wD:  90% 8%

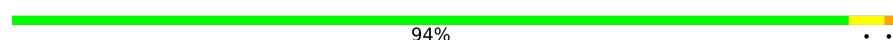


- Molecule 1: HIV-1 capsid protein

Chain xD:  91% 9%

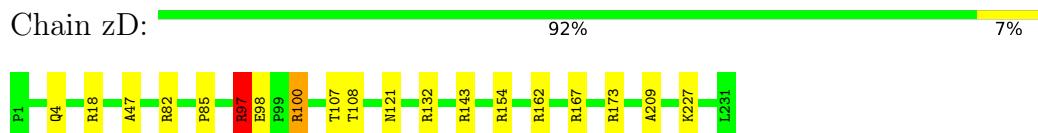


- Molecule 1: HIV-1 capsid protein

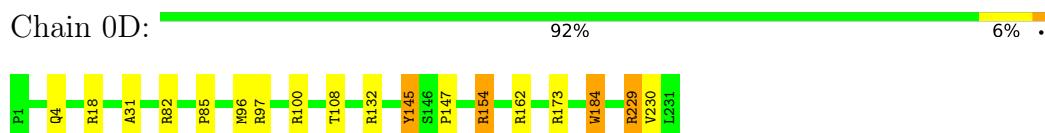
Chain yD:  94% 6%



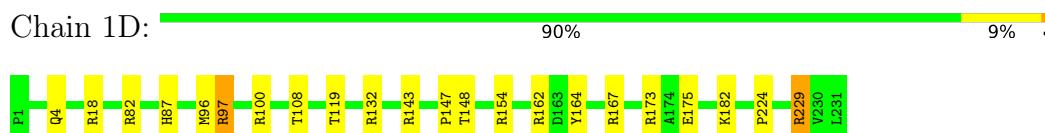
- Molecule 1: HIV-1 capsid protein



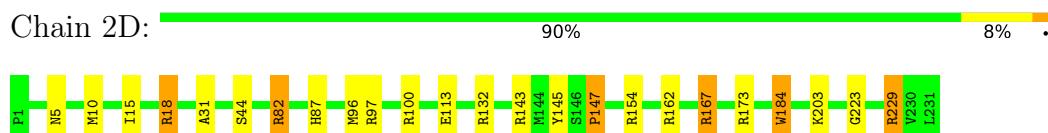
- Molecule 1: HIV-1 capsid protein



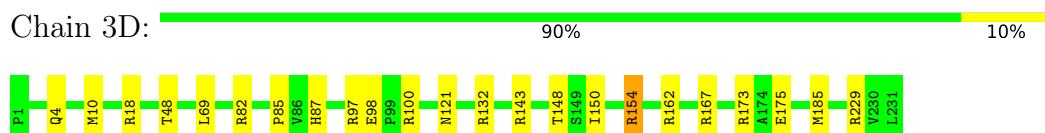
- Molecule 1: HIV-1 capsid protein



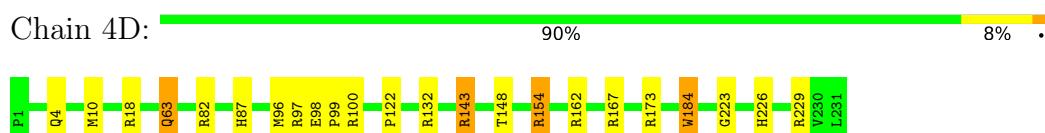
- Molecule 1: HIV-1 capsid protein



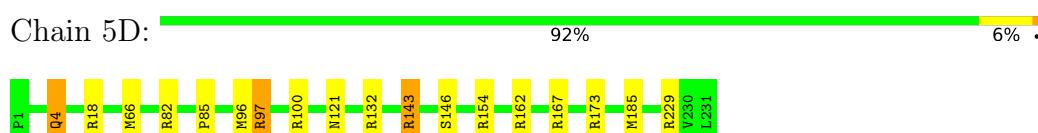
- Molecule 1: HIV-1 capsid protein



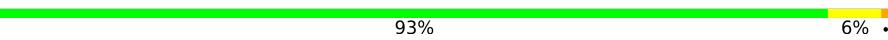
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

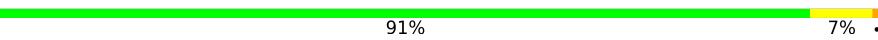


- Molecule 1: HIV-1 capsid protein

Chain 6D:  93% •



- Molecule 1: HIV-1 capsid protein

Chain 7D:  91% •



- Molecule 1: HIV-1 capsid protein

Chain 8D:  91% •



- Molecule 1: HIV-1 capsid protein

Chain 9D:  91% •

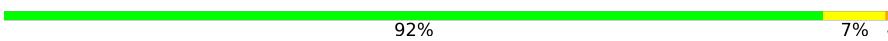


- Molecule 1: HIV-1 capsid protein

Chain AE:  90% 10%



- Molecule 1: HIV-1 capsid protein

Chain BE:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain CE:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain DE: 7% •



- Molecule 1: HIV-1 capsid protein

Chain EE: 7% •



- Molecule 1: HIV-1 capsid protein

Chain FE: 8% •



- Molecule 1: HIV-1 capsid protein

Chain GE: 7%



- Molecule 1: HIV-1 capsid protein

Chain HE: 6% •



- Molecule 1: HIV-1 capsid protein

Chain IE: 5% •



- Molecule 1: HIV-1 capsid protein

Chain JE: 7% •



- Molecule 1: HIV-1 capsid protein

Chain KE: 8% •



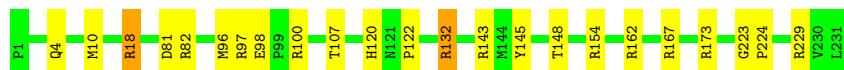
- Molecule 1: HIV-1 capsid protein

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:

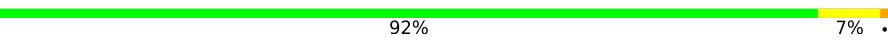


- Molecule 1: HIV-1 capsid protein

Chain RE:

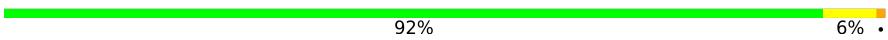


- Molecule 1: HIV-1 capsid protein

Chain SE:  92% •



- Molecule 1: HIV-1 capsid protein

Chain TE:  92% •



- Molecule 1: HIV-1 capsid protein

Chain UE:  93% •

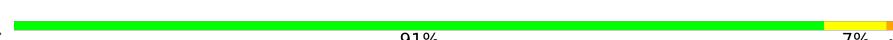


- Molecule 1: HIV-1 capsid protein

Chain VE:  92% •



- Molecule 1: HIV-1 capsid protein

Chain WE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain XE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain YE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain ZE:  10%

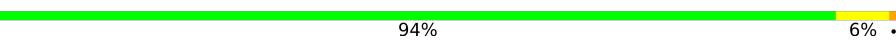


- Molecule 1: HIV-1 capsid protein

Chain aE:  8% •



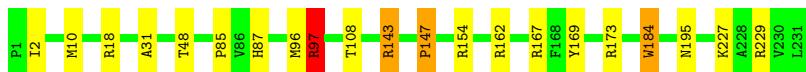
- Molecule 1: HIV-1 capsid protein

Chain bE:  6% •



- Molecule 1: HIV-1 capsid protein

Chain cE:  7% •



- Molecule 1: HIV-1 capsid protein

Chain dE:  8% •

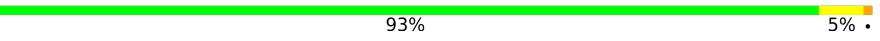


- Molecule 1: HIV-1 capsid protein

Chain eE:  7% •



- Molecule 1: HIV-1 capsid protein

Chain fE:  5% •



- Molecule 1: HIV-1 capsid protein

Chain gE:  7% •



- Molecule 1: HIV-1 capsid protein

Chain hE:



- Molecule 1: HIV-1 capsid protein

Chain iE:



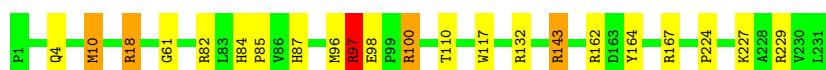
- Molecule 1: HIV-1 capsid protein

Chain jE:



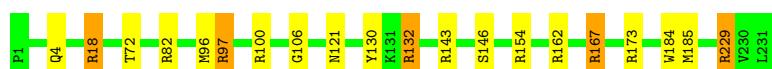
- Molecule 1: HIV-1 capsid protein

Chain kE:



- Molecule 1: HIV-1 capsid protein

Chain lE:



- Molecule 1: HIV-1 capsid protein

Chain mE:

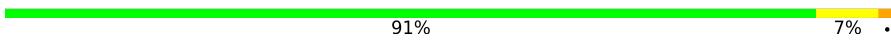


- Molecule 1: HIV-1 capsid protein

Chain nE:



- Molecule 1: HIV-1 capsid protein

Chain oE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain pE:  90% •

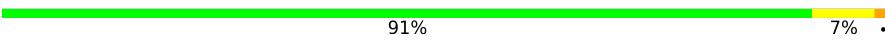


- Molecule 1: HIV-1 capsid protein

Chain qE:  90% •



- Molecule 1: HIV-1 capsid protein

Chain rE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain sE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain tE:  93% •



- Molecule 1: HIV-1 capsid protein

Chain uE:  91% •



- Molecule 1: HIV-1 capsid protein

Chain vE: 91% 7% •



- Molecule 1: HIV-1 capsid protein

Chain wE: 91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain xE: 92% 6% •



- Molecule 1: HIV-1 capsid protein

Chain yE: 92% 7% •



- Molecule 1: HIV-1 capsid protein

Chain zE: 90% 10% •



- Molecule 1: HIV-1 capsid protein

Chain 0E: 90% 7% •



- Molecule 1: HIV-1 capsid protein

Chain 1E: 91% 8% •



- Molecule 1: HIV-1 capsid protein

Chain 2E: 92% 7% •



- Molecule 1: HIV-1 capsid protein

Chain 3E: 94% ..



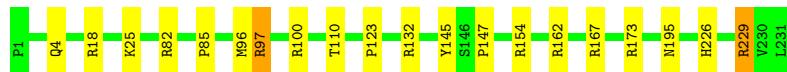
- Molecule 1: HIV-1 capsid protein

Chain 4E: 92% .



- Molecule 1: HIV-1 capsid protein

Chain 5E: 91% .



- Molecule 1: HIV-1 capsid protein

Chain 6E: 91% .



- Molecule 1: HIV-1 capsid protein

Chain 7E: 89% .



- Molecule 1: HIV-1 capsid protein

Chain 8E: 89% .



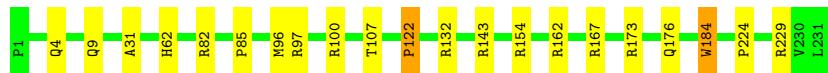
- Molecule 1: HIV-1 capsid protein

Chain 9E: 91% .



- Molecule 1: HIV-1 capsid protein

Chain AF:  91% 8% ..



- Molecule 1: HIV-1 capsid protein

Chain BF:  91% 9%



- Molecule 1: HIV-1 capsid protein

Chain CF:  91% 7% ..



- Molecule 1: HIV-1 capsid protein

Chain DF:  88% 11% ..



- Molecule 1: HIV-1 capsid protein

Chain EF:  92% 7%



- Molecule 1: HIV-1 capsid protein

Chain FF:  89% 9% ..



5 Refinement protocol and experimental data overview i

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 i

6.1 Standard geometry i

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.

5 of 5397 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3E	184	TRP	CB-CG-CD2	-15.41	106.56	126.60
1	jC	173	ARG	NE-CZ-NH1	14.78	127.69	120.30
1	YE	184	TRP	CB-CG-CD2	-14.58	107.64	126.60
1	nA	184	TRP	CB-CG-CD2	-14.01	108.39	126.60
1	DC	162	ARG	NE-CZ-NH1	13.98	127.29	120.30

There are no chirality outliers.

5 of 775 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

6.2 Too-close contacts (i)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
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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 [\(i\)](#)

6.3.1 Protein backbone [\(i\)](#)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

5 of 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

6.3.2 Protein sidechains [\(i\)](#)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

5 of 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

6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping (i)

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

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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

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

7.1.3 Completeness of resonance assignments (i)

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

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

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	Total	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.

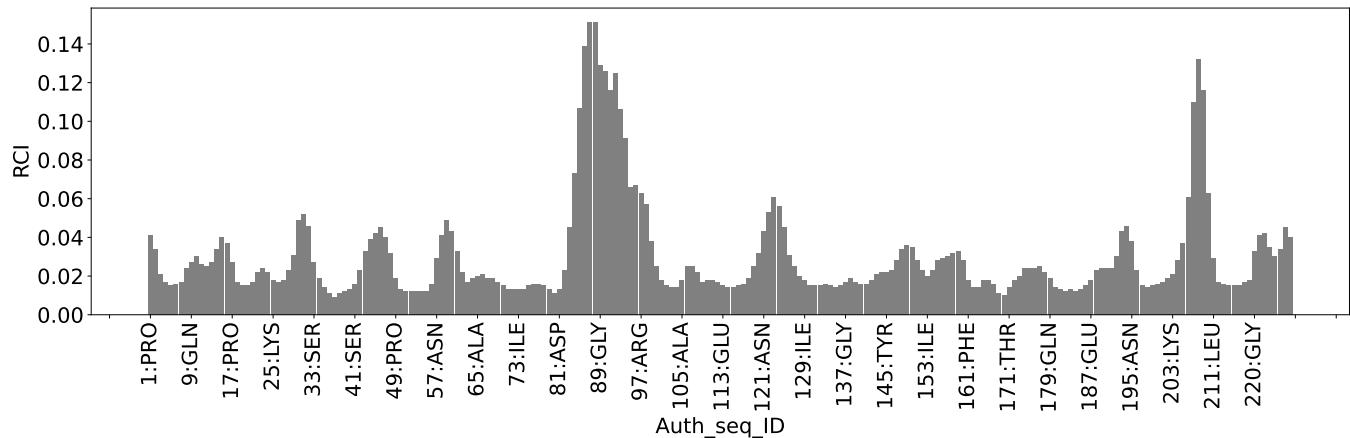
7.1.4 Statistically unusual chemical shifts [\(i\)](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis i

8.1 Conformationally restricting restraints i

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

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

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

8.2 Residual restraint violations i

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 i

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 [\(i\)](#)

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	17.0	9.1
10.0-20.0 (Medium)	10.0	19.4
>20.0 (Large)	24.0	147.8

9 Distance violation analysis i

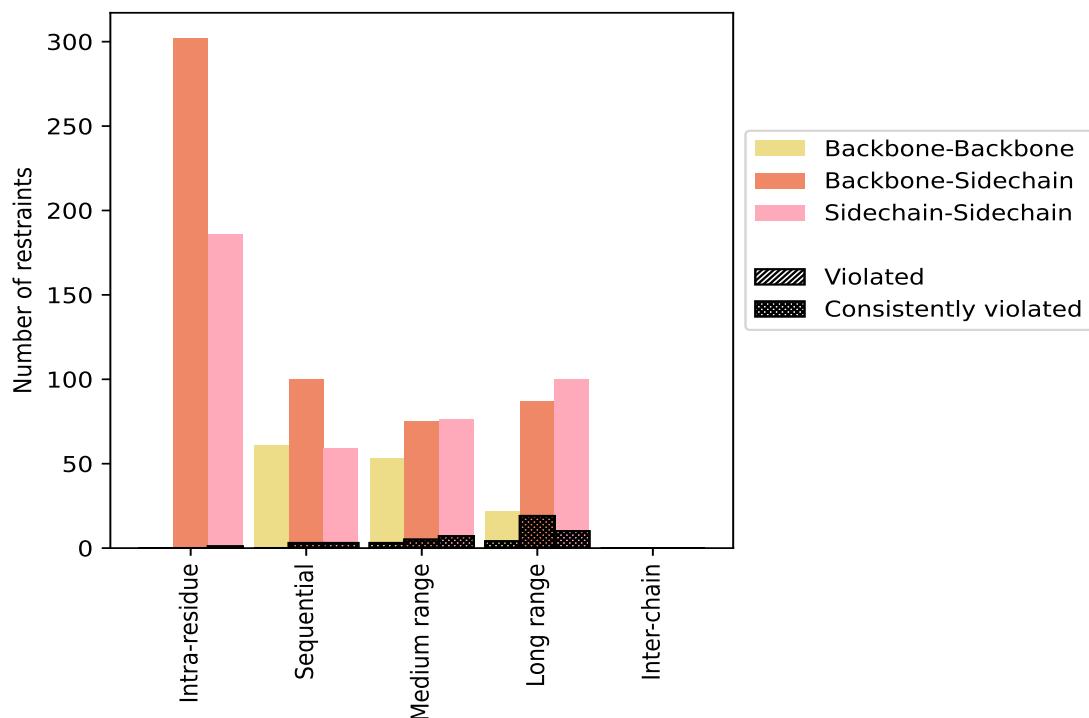
9.1 Summary of distance violations i

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 \text{ & } i-j <5$)	204	18.2	15	7.4	1.3	15	7.4	1.3
Backbone-Backbone	53	4.7	3	5.7	0.3	3	5.7	0.3
Backbone-Sidechain	75	6.7	5	6.7	0.4	5	6.7	0.4
Sidechain-Sidechain	76	6.8	7	9.2	0.6	7	9.2	0.6
Long range ($ i-j \geq 5$)	209	18.6	33	15.8	2.9	33	15.8	2.9
Backbone-Backbone	22	2.0	4	18.2	0.4	4	18.2	0.4
Backbone-Sidechain	87	7.8	19	21.8	1.7	19	21.8	1.7
Sidechain-Sidechain	100	8.9	10	10.0	0.9	10	10.0	0.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1121	100.0	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 [\(i\)](#)



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

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

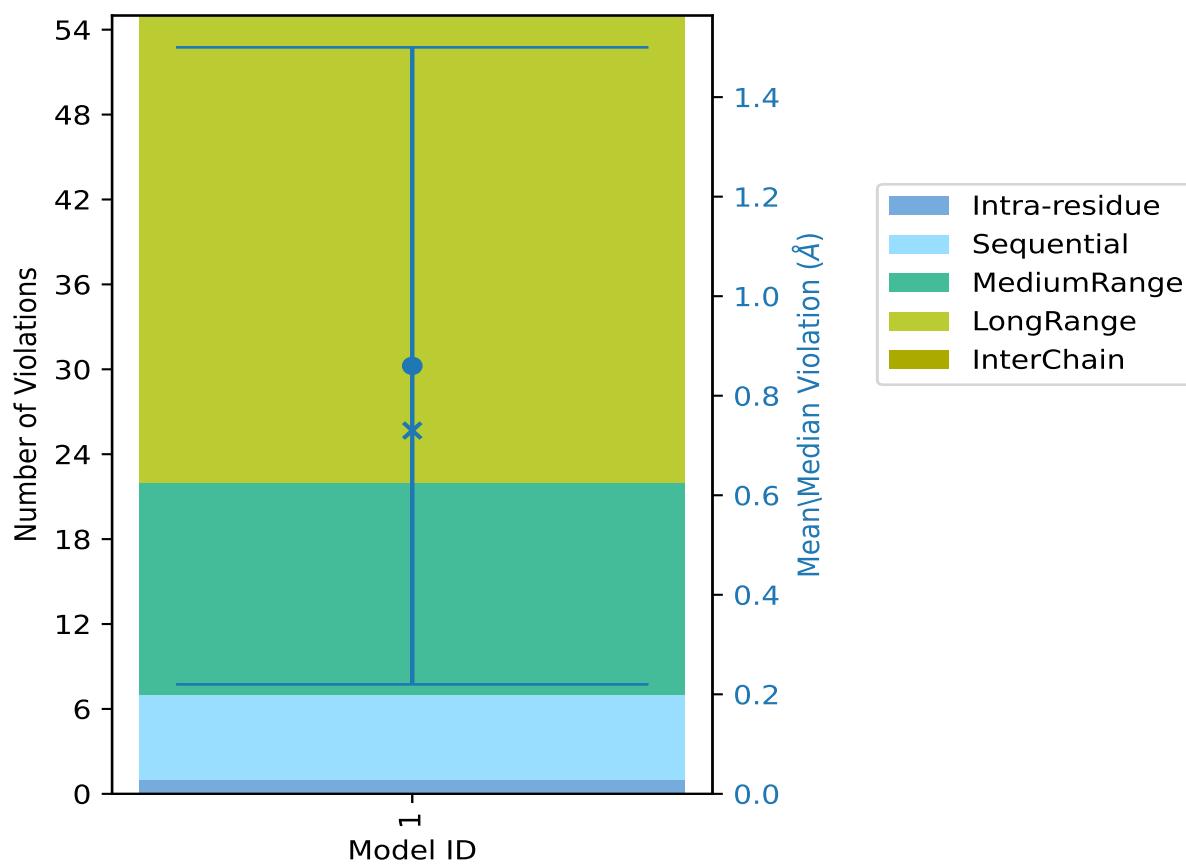
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	6	15	33	0	55	0.86	3.5	0.64	0.73

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

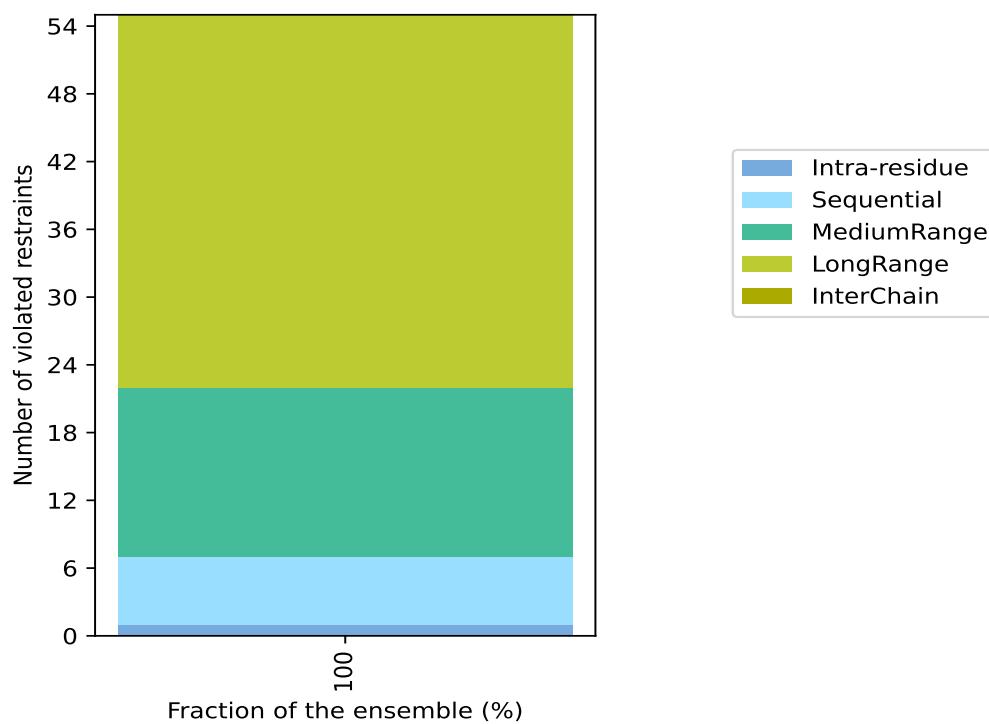
9.3 Distance violation statistics for the ensemble [\(i\)](#)

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

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

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



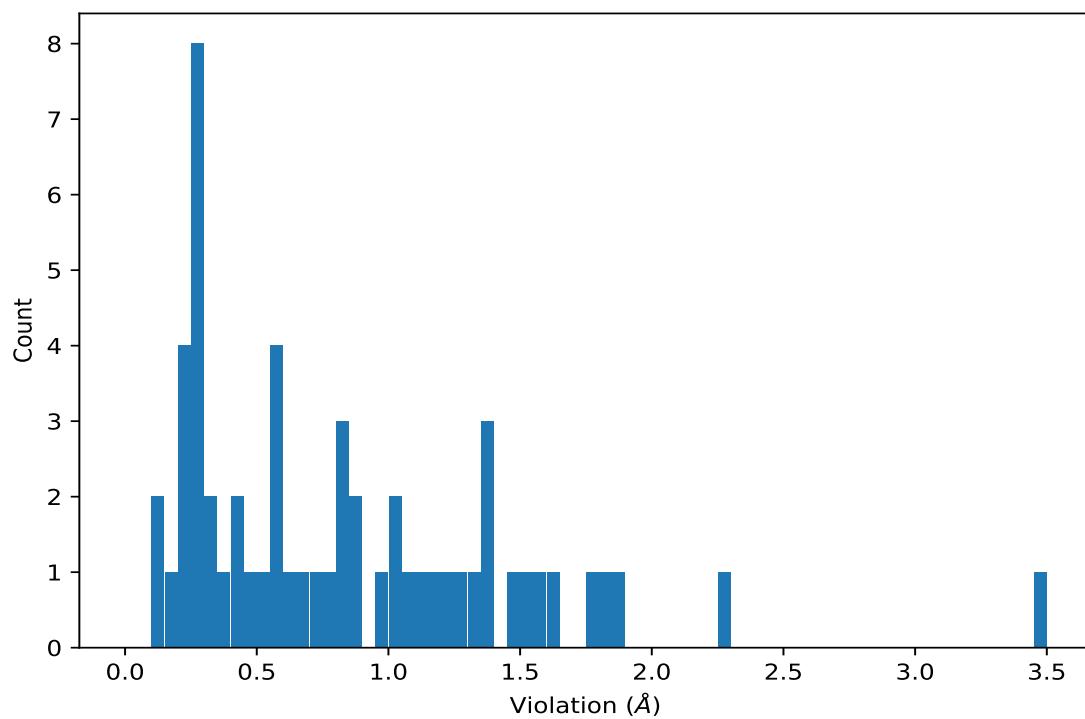
9.4 Most violated distance restraints in the ensemble [\(i\)](#)

No violations found

9.5 All violated distance restraints [\(i\)](#)

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

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



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

The following table provides the 10 worst performing restraints, sorted by the violation 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

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

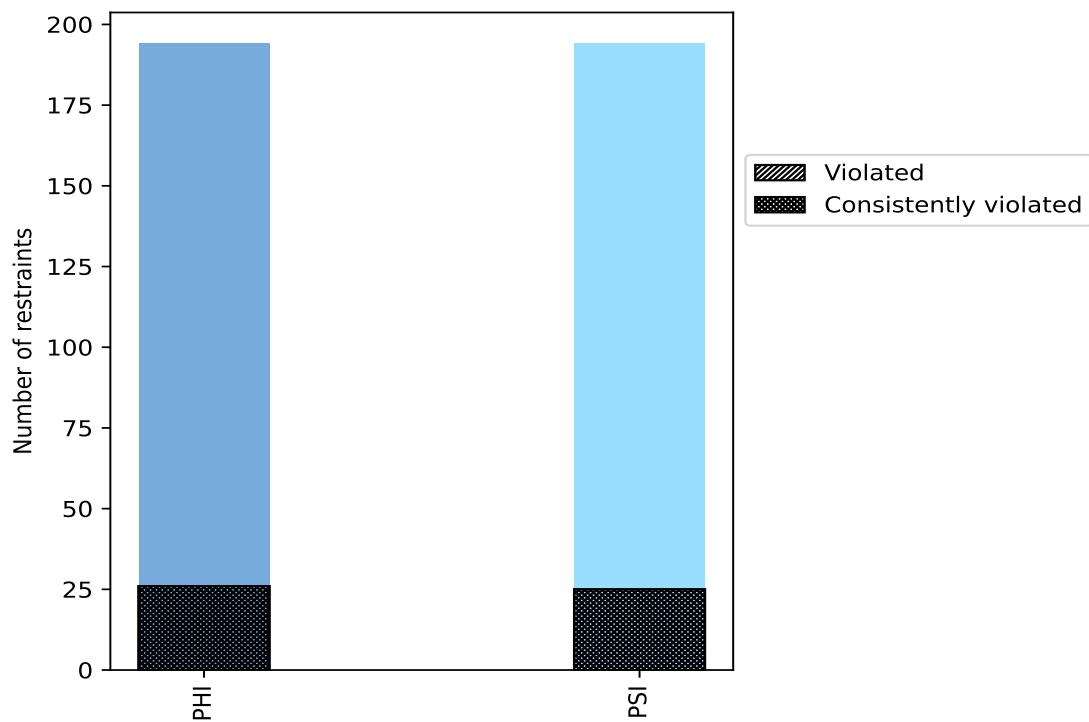
10.1 Summary of dihedral-angle violations [\(i\)](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
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 [\(i\)](#)



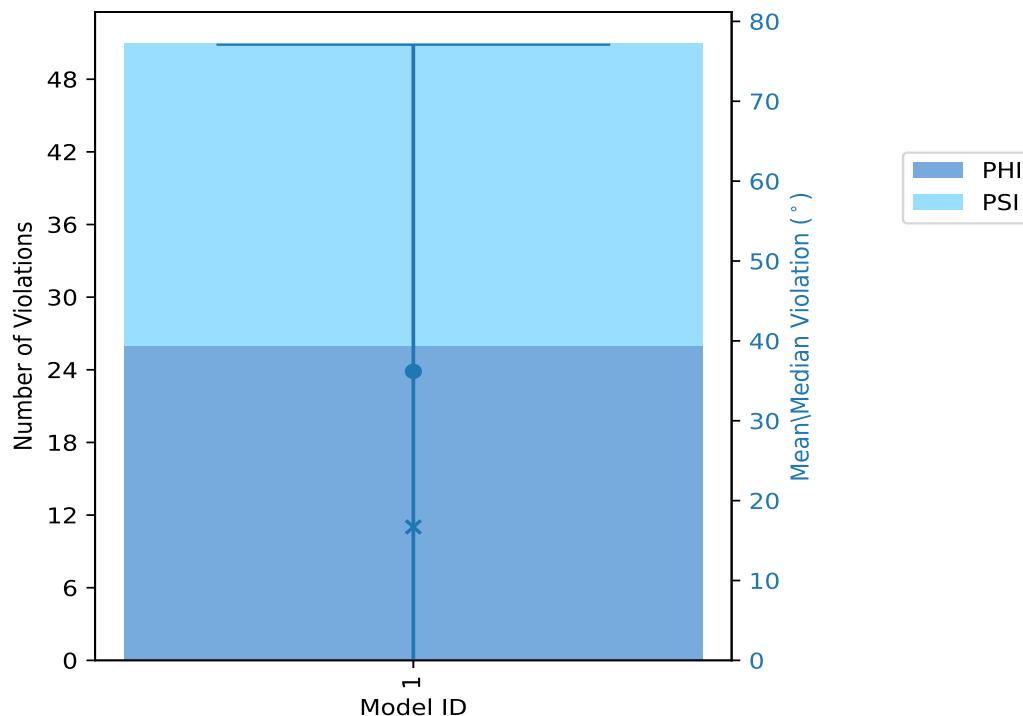
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	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

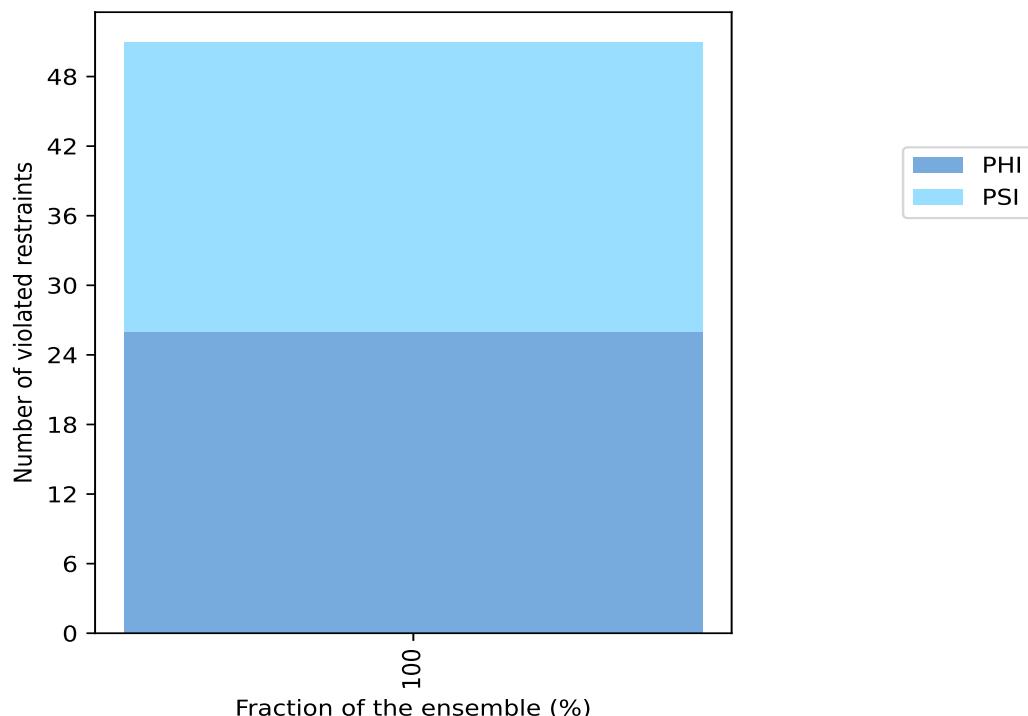
10.3 Dihedral-angle violation statistics for the ensemble [\(i\)](#)

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 [\(i\)](#)



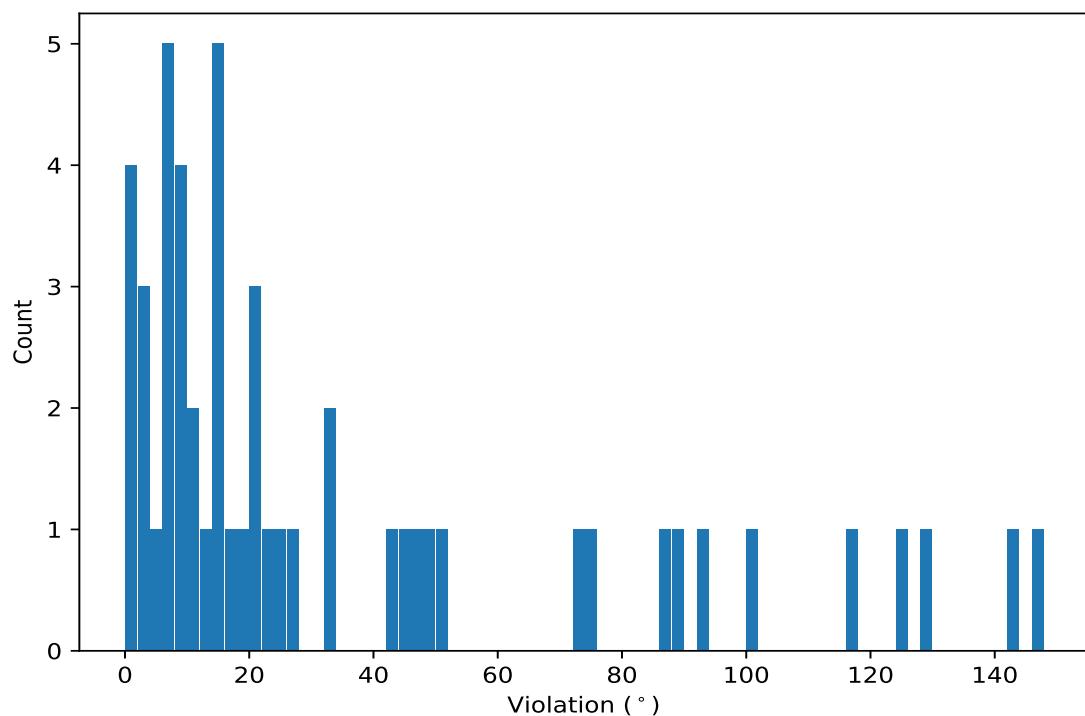
10.4 Most violated dihedral-angle restraints in the ensemble [\(i\)](#)

No violations found

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

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

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



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

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation 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