



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 09:34 am GMT

PDB ID : 8R59
EMDB ID : EMD-18904
Title : Structure of the Co(II) triggered TRAP (S33HK35H) protein cage (levo form)
Authors : Biela, A.P.; Heddle, J.G.
Deposited on : 2023-11-16
Resolution : 2.86 Å(reported)
Based on initial model : 4v4f

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

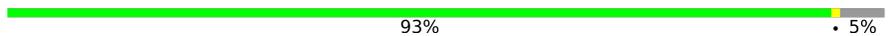
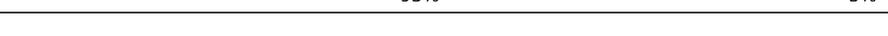
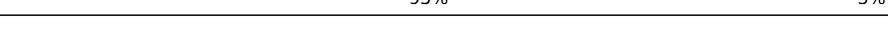
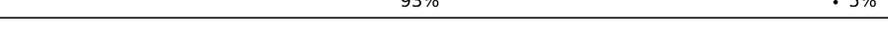
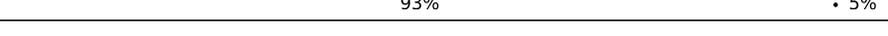
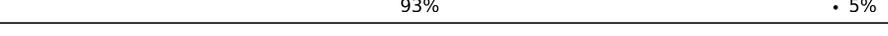
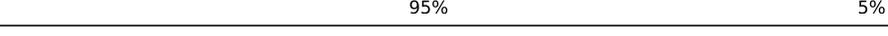
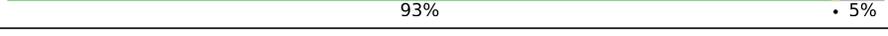
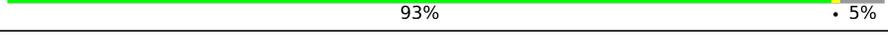
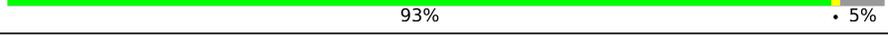
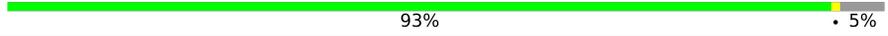
The types of validation reports are described at

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

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

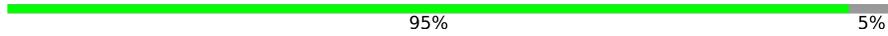
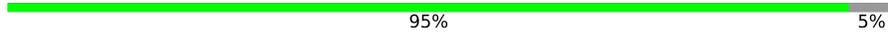
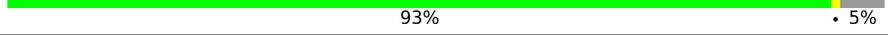
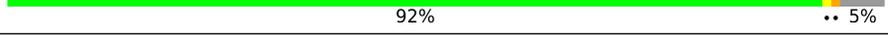
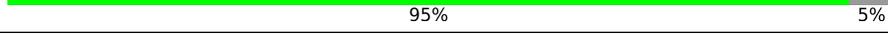
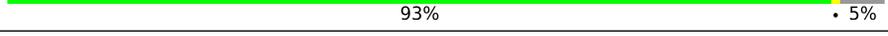
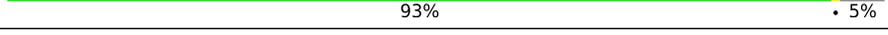
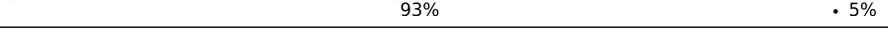
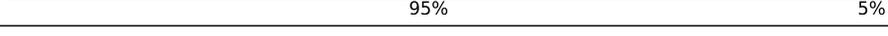
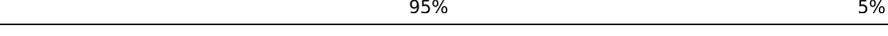
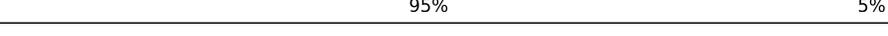
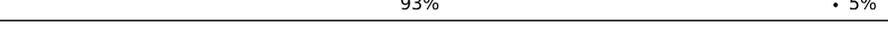
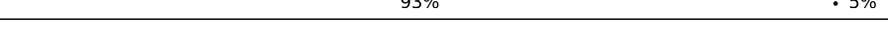
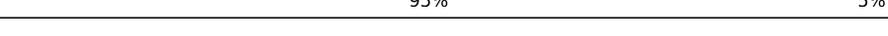
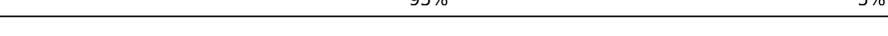
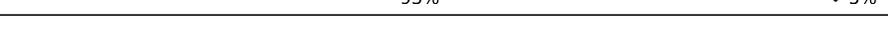
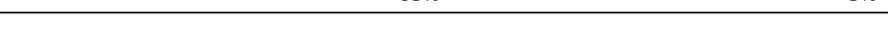
EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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Mol	Chain	Length	Quality of chain
1	2B	74	 93% . 5%
1	2C	74	 93% . 5%
1	3	74	 95% 5%
1	3A	74	 93% . 5%
1	3B	74	 93% . 5%
1	3C	74	 93% . 5%
1	4	74	 95% 5%
1	4A	74	 93% . 5%
1	4B	74	 93% . 5%
1	4C	74	 93% . 5%
1	5	74	 95% 5%
1	5A	74	 95% 5%
1	5B	74	 93% . 5%
1	5C	74	 93% . 5%
1	6	74	 95% 5%
1	6A	74	 93% . 5%
1	6B	74	 93% . 5%
1	6C	74	 93% . 5%
1	7	74	 95% 5%
1	7A	74	 93% . 5%
1	7B	74	 93% . 5%
1	7C	74	 93% . 5%
1	8	74	 95% 5%
1	8A	74	 93% . 5%
1	8B	74	 93% . 5%

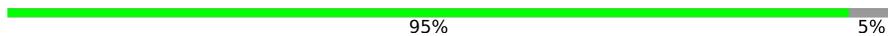
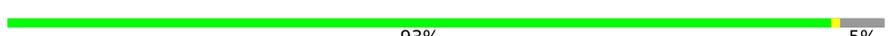
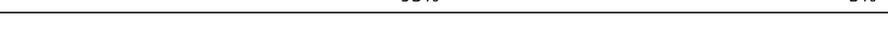
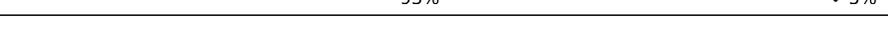
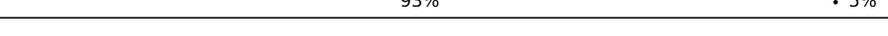
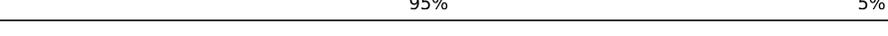
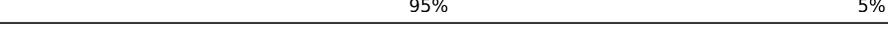
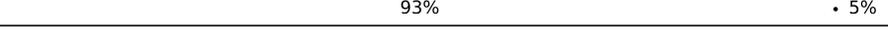
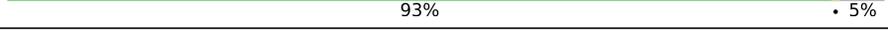
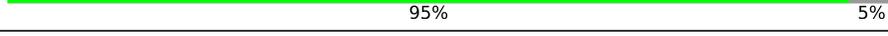
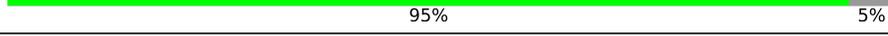
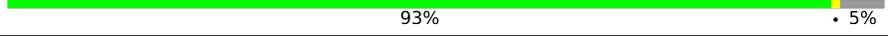
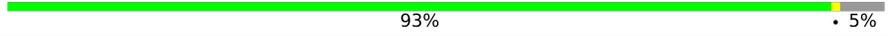
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Mol	Chain	Length	Quality of chain
1	8C	74	 93% . 5%
1	9	74	 95% 5%
1	9A	74	 95% 5%
1	9B	74	 93% . 5%
1	9C	74	 93% . 5%
1	A	74	 92% .. 5%
1	AA	74	 95% 5%
1	AB	74	 93% . 5%
1	AC	74	 93% . 5%
1	AD	74	 93% . 5%
1	B	74	 95% 5%
1	BA	74	 95% 5%
1	BB	74	 95% 5%
1	BC	74	 93% . 5%
1	BD	74	 93% . 5%
1	C	74	 95% 5%
1	CA	74	 95% 5%
1	CB	74	 93% . 5%
1	CC	74	 93% . 5%
1	CD	74	 93% . 5%
1	D	74	 93% . 5%
1	DA	74	 95% 5%
1	DB	74	 93% . 5%
1	DC	74	 93% . 5%
1	DD	74	 92% . 5%

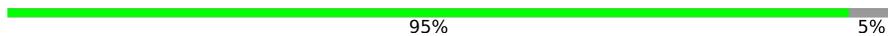
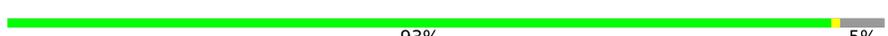
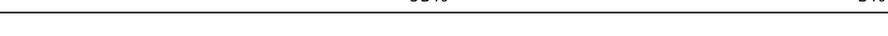
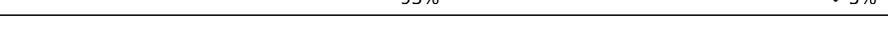
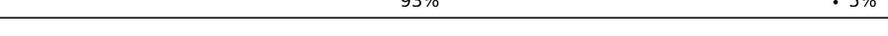
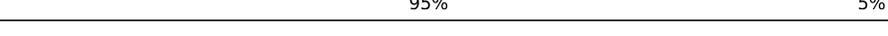
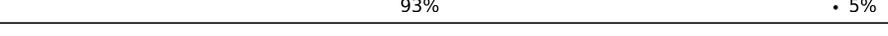
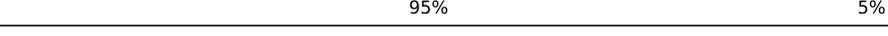
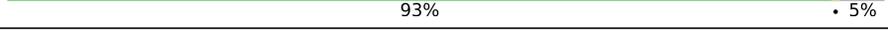
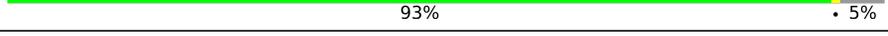
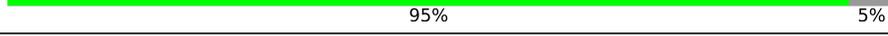
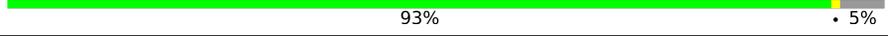
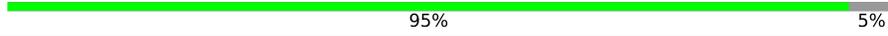
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Mol	Chain	Length	Quality of chain
1	E	74	 93% 5%
1	EA	74	 95% 5%
1	EB	74	 95% 5%
1	EC	74	 93% 5%
1	ED	74	 93% 5%
1	F	74	 93% 5%
1	FA	74	 95% 5%
1	FB	74	 95% 5%
1	FC	74	 93% 5%
1	FD	74	 93% 5%
1	G	74	 95% 5%
1	GA	74	 95% 5%
1	GB	74	 93% 5%
1	GC	74	 93% 5%
1	GD	74	 93% 5%
1	H	74	 93% 5%
1	HA	74	 95% 5%
1	HB	74	 95% 5%
1	HC	74	 93% 5%
1	HD	74	 93% 5%
1	I	74	 95% 5%
1	IA	74	 95% 5%
1	IB	74	 93% 5%
1	IC	74	 93% 5%
1	ID	74	 93% 5%

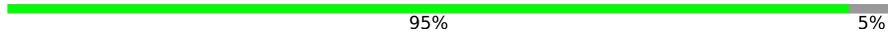
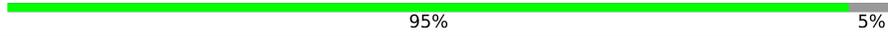
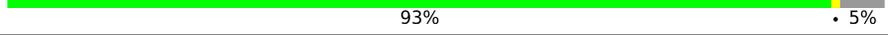
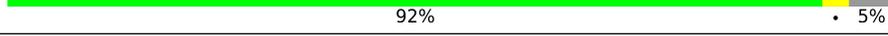
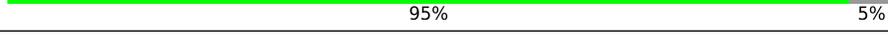
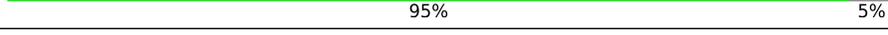
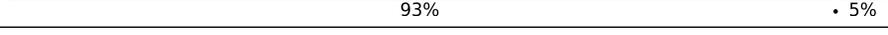
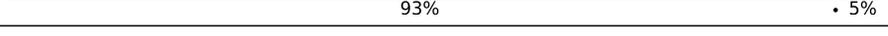
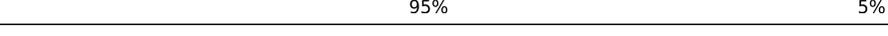
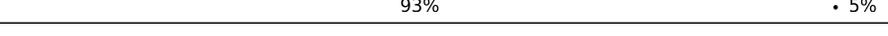
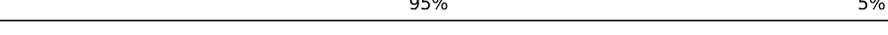
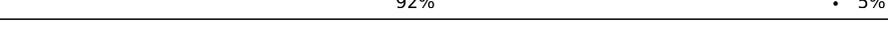
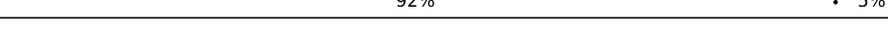
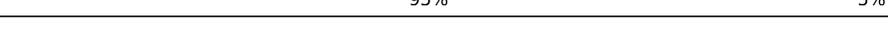
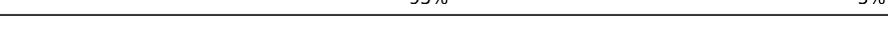
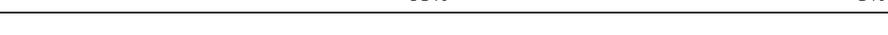
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Mol	Chain	Length	Quality of chain
1	J	74	 93% . 5%
1	JA	74	 95% 5%
1	JB	74	 93% . 5%
1	JC	74	 93% . 5%
1	JD	74	 93% . 5%
1	K	74	 93% . 5%
1	KA	74	 95% 5%
1	KB	74	 93% . 5%
1	KC	74	 95% 5%
1	KD	74	 93% . 5%
1	L	74	 92% . 5%
1	LA	74	 95% 5%
1	LB	74	 93% . 5%
1	LC	74	 95% 5%
1	LD	74	 93% . 5%
1	M	74	 93% . 5%
1	MA	74	 95% 5%
1	MB	74	 93% . 5%
1	MC	74	 95% 5%
1	MD	74	 93% . 5%
1	N	74	 93% . 5%
1	NA	74	 95% 5%
1	NB	74	 93% . 5%
1	NC	74	 95% 5%
1	ND	74	 92% . 5%

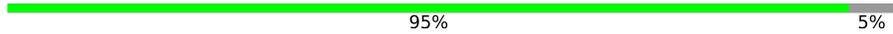
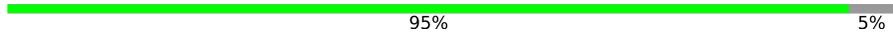
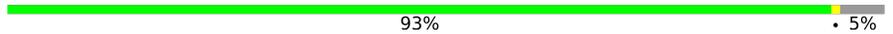
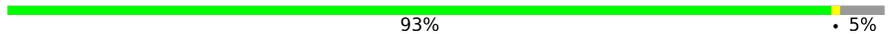
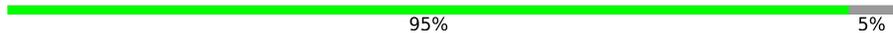
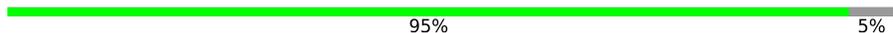
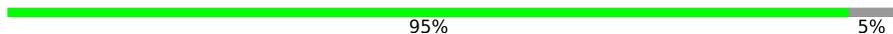
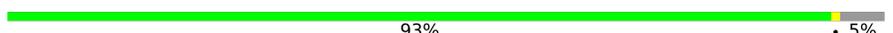
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Mol	Chain	Length	Quality of chain
1	O	74	 93% . 5%
1	OA	74	 95% 5%
1	OB	74	 95% 5%
1	OC	74	 95% 5%
1	OD	74	 93% . 5%
1	P	74	 92% . 5%
1	PA	74	 95% 5%
1	PB	74	 95% 5%
1	PC	74	 95% 5%
1	PD	74	 93% . 5%
1	Q	74	 93% . 5%
1	QA	74	 95% 5%
1	QB	74	 93% . 5%
1	QC	74	 95% 5%
1	QD	74	 92% . 5%
1	R	74	 92% . 5%
1	RA	74	 95% 5%
1	RB	74	 95% 5%
1	RC	74	 95% 5%
1	S	74	 92% . 5%
1	SA	74	 95% 5%
1	SB	74	 93% . 5%
1	SC	74	 95% 5%
1	T	74	 92% . 5%
1	TA	74	 93% . 5%

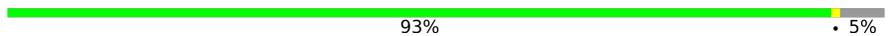
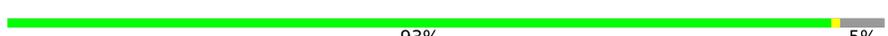
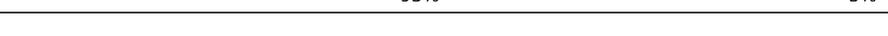
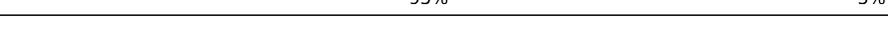
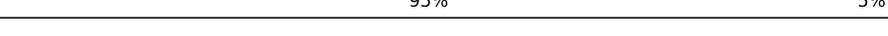
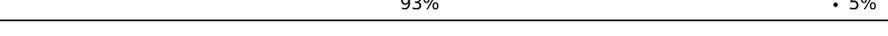
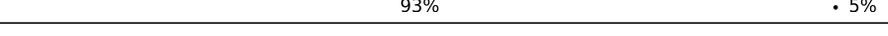
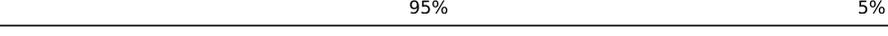
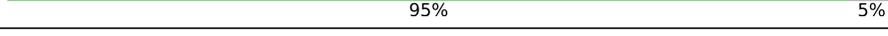
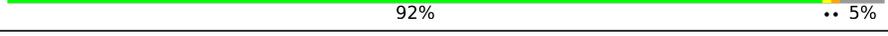
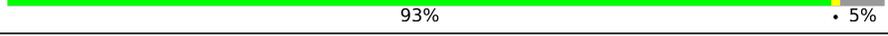
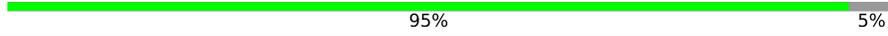
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Mol	Chain	Length	Quality of chain
1	TB	74	 95% 5%
1	TC	74	 95% 5%
1	U	74	 93% 5%
1	UA	74	 93% 5%
1	UB	74	 93% 5%
1	UC	74	 95% 5%
1	V	74	 93% 5%
1	VA	74	 93% 5%
1	VB	74	 95% 5%
1	VC	74	 95% 5%
1	W	74	 92% 5%
1	WA	74	 93% 5%
1	WB	74	 95% 5%
1	WC	74	 95% 5%
1	XA	74	 93% 5%
1	XB	74	 95% 5%
1	XC	74	 95% 5%
1	Y	74	 92% 5%
1	YA	74	 93% 5%
1	YB	74	 95% 5%
1	YC	74	 95% 5%
1	Z	74	 92% 5%
1	ZA	74	 93% 5%
1	ZB	74	 92% 5%
1	ZC	74	 95% 5%

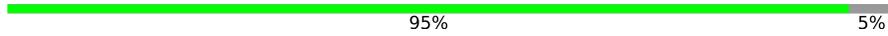
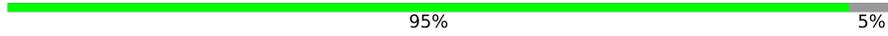
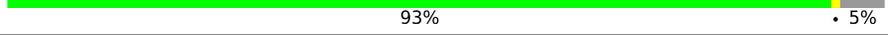
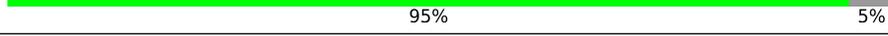
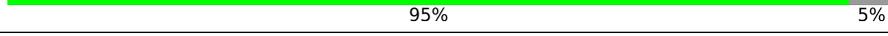
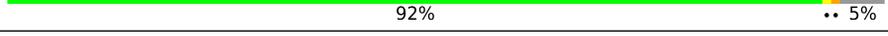
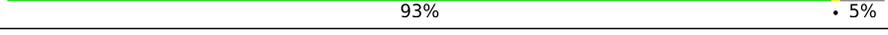
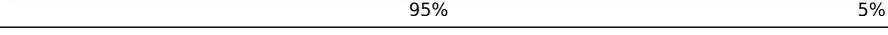
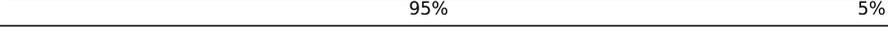
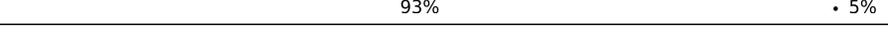
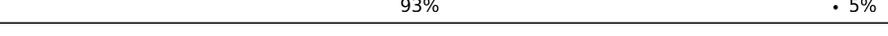
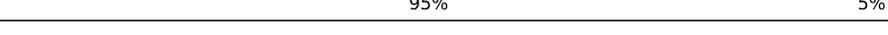
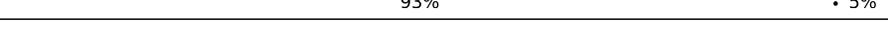
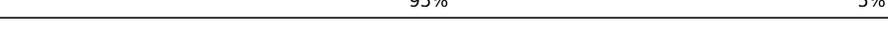
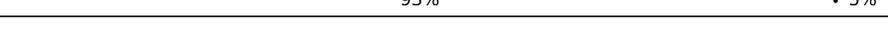
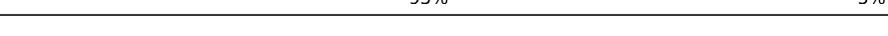
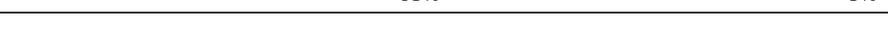
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Mol	Chain	Length	Quality of chain
1	a	74	 92% .. 5%
1	aA	74	 93% . 5%
1	aB	74	 95% 5%
1	aC	74	 95% 5%
1	b	74	 92% . 5%
1	bA	74	 93% . 5%
1	bB	74	 95% 5%
1	bC	74	 95% 5%
1	c	74	 93% . 5%
1	cA	74	 93% . 5%
1	cB	74	 95% 5%
1	cC	74	 95% 5%
1	d	74	 93% . 5%
1	dA	74	 93% . 5%
1	dB	74	 95% 5%
1	dC	74	 95% 5%
1	e	74	 93% . 5%
1	eA	74	 93% . 5%
1	eB	74	 95% 5%
1	eC	74	 95% 5%
1	f	74	 92% .. 5%
1	fA	74	 93% . 5%
1	fB	74	 95% 5%
1	fC	74	 95% 5%
1	g	74	 93% . 5%

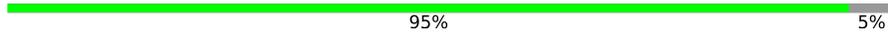
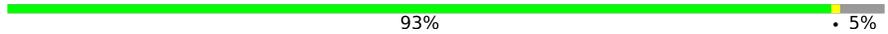
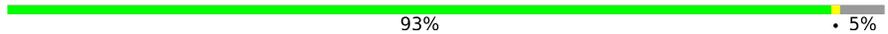
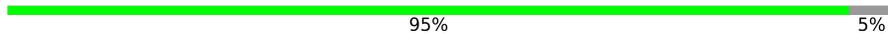
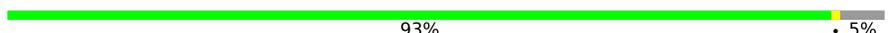
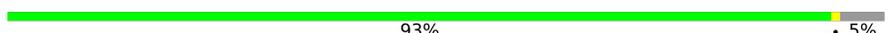
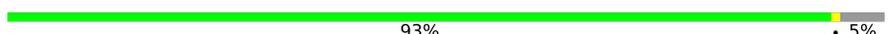
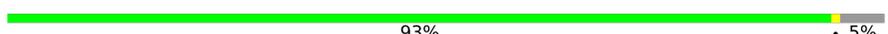
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Mol	Chain	Length	Quality of chain
1	gA	74	 93% . 5%
1	gB	74	 95% 5%
1	gC	74	 95% 5%
1	h	74	 93% . 5%
1	hA	74	 93% . 5%
1	hB	74	 95% 5%
1	hC	74	 95% 5%
1	i	74	 92% .. 5%
1	iA	74	 93% . 5%
1	iB	74	 95% 5%
1	iC	74	 95% 5%
1	j	74	 93% . 5%
1	jA	74	 93% . 5%
1	jB	74	 95% 5%
1	jC	74	 93% . 5%
1	k	74	 95% 5%
1	kA	74	 93% . 5%
1	kB	74	 95% 5%
1	kC	74	 93% . 5%
1	l	74	 93% . 5%
1	lA	74	 93% . 5%
1	lB	74	 95% 5%
1	lC	74	 93% . 5%
1	m	74	 95% 5%
1	mA	74	 93% . 5%

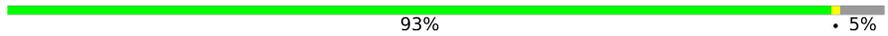
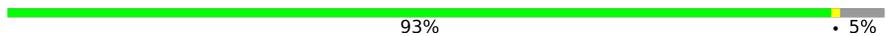
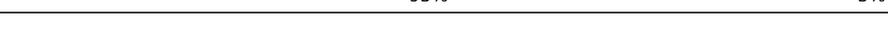
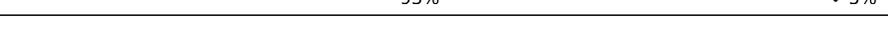
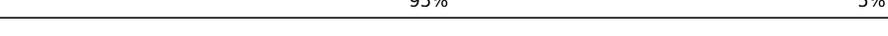
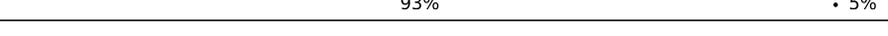
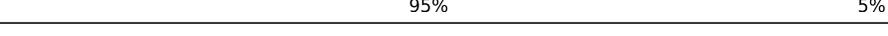
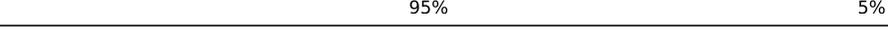
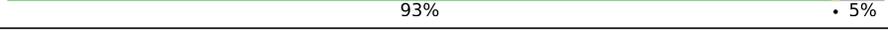
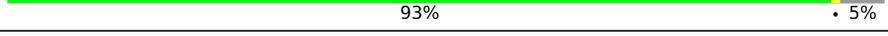
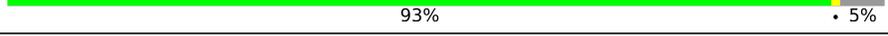
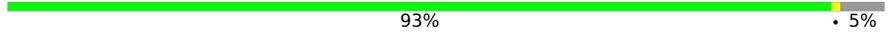
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Mol	Chain	Length	Quality of chain
1	mB	74	 95% 5%
1	mC	74	 93% 5%
1	n	74	 93% 5%
1	nA	74	 93% 5%
1	nB	74	 95% 5%
1	nC	74	 93% 5%
1	o	74	 93% 5%
1	oA	74	 93% 5%
1	oB	74	 95% 5%
1	oC	74	 93% 5%
1	p	74	 93% 5%
1	pA	74	 93% 5%
1	pB	74	 95% 5%
1	pC	74	 93% 5%
1	q	74	 93% 5%
1	qA	74	 93% 5%
1	qB	74	 95% 5%
1	qC	74	 93% 5%
1	r	74	 93% 5%
1	rA	74	 93% 5%
1	rB	74	 95% 5%
1	rC	74	 93% 5%
1	s	74	 95% 5%
1	sA	74	 93% 5%
1	sB	74	 95% 5%

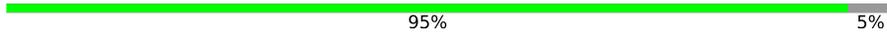
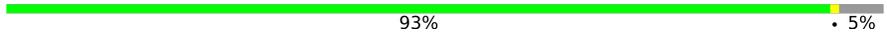
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Mol	Chain	Length	Quality of chain
1	sC	74	 93% . 5%
1	t	74	 93% . 5%
1	tA	74	 95% 5%
1	tB	74	 95% 5%
1	tC	74	 95% 5%
1	u	74	 93% . 5%
1	uA	74	 93% . 5%
1	uB	74	 95% 5%
1	uC	74	 93% . 5%
1	v	74	 95% 5%
1	vA	74	 93% . 5%
1	vB	74	 95% 5%
1	vC	74	 93% . 5%
1	w	74	 95% 5%
1	wA	74	 93% . 5%
1	wB	74	 95% 5%
1	wC	74	 93% . 5%
1	x	74	 95% 5%
1	xA	74	 95% 5%
1	xB	74	 93% . 5%
1	xC	74	 93% . 5%
1	y	74	 93% . 5%
1	yA	74	 95% 5%
1	yB	74	 93% . 5%
1	yC	74	 93% . 5%

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Mol	Chain	Length	Quality of chain
1	z	74	 95% 5%
1	zA	74	 93% 5%
1	zB	74	 93% 5%
1	zC	74	 93% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 144528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription attenuation protein MtrB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	70	547	341	102	104	0	0
1	L	70	547	341	102	104	0	0
1	M	70	547	341	102	104	0	0
1	N	70	547	341	102	104	0	0
1	O	70	547	341	102	104	0	0
1	P	70	547	341	102	104	0	0
1	Q	70	547	341	102	104	0	0
1	R	70	547	341	102	104	0	0
1	S	70	547	341	102	104	0	0
1	T	70	547	341	102	104	0	0
1	U	70	547	341	102	104	0	0
1	V	70	547	341	102	104	0	0
1	W	70	547	341	102	104	0	0
1	Y	70	547	341	102	104	0	0
1	Z	70	547	341	102	104	0	0
1	a	70	547	341	102	104	0	0
1	b	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	c	70	Total 547	C 341	N 102	O 104	0	0
1	d	70	Total 547	C 341	N 102	O 104	0	0
1	e	70	Total 547	C 341	N 102	O 104	0	0
1	f	70	Total 547	C 341	N 102	O 104	0	0
1	g	70	Total 547	C 341	N 102	O 104	0	0
1	h	70	Total 547	C 341	N 102	O 104	0	0
1	i	70	Total 547	C 341	N 102	O 104	0	0
1	B	70	Total 547	C 341	N 102	O 104	0	0
1	j	70	Total 547	C 341	N 102	O 104	0	0
1	k	70	Total 547	C 341	N 102	O 104	0	0
1	l	70	Total 547	C 341	N 102	O 104	0	0
1	m	70	Total 547	C 341	N 102	O 104	0	0
1	n	70	Total 547	C 341	N 102	O 104	0	0
1	o	70	Total 547	C 341	N 102	O 104	0	0
1	p	70	Total 547	C 341	N 102	O 104	0	0
1	q	70	Total 547	C 341	N 102	O 104	0	0
1	r	70	Total 547	C 341	N 102	O 104	0	0
1	s	70	Total 547	C 341	N 102	O 104	0	0
1	t	70	Total 547	C 341	N 102	O 104	0	0
1	u	70	Total 547	C 341	N 102	O 104	0	0
1	v	70	Total 547	C 341	N 102	O 104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	w	70	547	341	102	104	0	0
1	x	70	547	341	102	104	0	0
1	y	70	547	341	102	104	0	0
1	z	70	547	341	102	104	0	0
1	0	70	547	341	102	104	0	0
1	1	70	547	341	102	104	0	0
1	2	70	547	341	102	104	0	0
1	3	70	547	341	102	104	0	0
1	4	70	547	341	102	104	0	0
1	5	70	547	341	102	104	0	0
1	C	70	547	341	102	104	0	0
1	6	70	547	341	102	104	0	0
1	7	70	547	341	102	104	0	0
1	8	70	547	341	102	104	0	0
1	9	70	547	341	102	104	0	0
1	AA	70	547	341	102	104	0	0
1	BA	70	547	341	102	104	0	0
1	CA	70	547	341	102	104	0	0
1	DA	70	547	341	102	104	0	0
1	EA	70	547	341	102	104	0	0
1	FA	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	GA	70	547	341	102	104	0	0
1	HA	70	547	341	102	104	0	0
1	IA	70	547	341	102	104	0	0
1	JA	70	547	341	102	104	0	0
1	KA	70	547	341	102	104	0	0
1	LA	70	547	341	102	104	0	0
1	MA	70	547	341	102	104	0	0
1	NA	70	547	341	102	104	0	0
1	OA	70	547	341	102	104	0	0
1	PA	70	547	341	102	104	0	0
1	QA	70	547	341	102	104	0	0
1	RA	70	547	341	102	104	0	0
1	SA	70	547	341	102	104	0	0
1	D	70	547	341	102	104	0	0
1	TA	70	547	341	102	104	0	0
1	UA	70	547	341	102	104	0	0
1	VA	70	547	341	102	104	0	0
1	WA	70	547	341	102	104	0	0
1	XA	70	547	341	102	104	0	0
1	YA	70	547	341	102	104	0	0
1	ZA	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	aA	70	Total 547	C 341	N 102	O 104	0	0
1	bA	70	Total 547	C 341	N 102	O 104	0	0
1	cA	70	Total 547	C 341	N 102	O 104	0	0
1	dA	70	Total 547	C 341	N 102	O 104	0	0
1	eA	70	Total 547	C 341	N 102	O 104	0	0
1	fA	70	Total 547	C 341	N 102	O 104	0	0
1	gA	70	Total 547	C 341	N 102	O 104	0	0
1	hA	70	Total 547	C 341	N 102	O 104	0	0
1	iA	70	Total 547	C 341	N 102	O 104	0	0
1	jA	70	Total 547	C 341	N 102	O 104	0	0
1	kA	70	Total 547	C 341	N 102	O 104	0	0
1	lA	70	Total 547	C 341	N 102	O 104	0	0
1	mA	70	Total 547	C 341	N 102	O 104	0	0
1	nA	70	Total 547	C 341	N 102	O 104	0	0
1	oA	70	Total 547	C 341	N 102	O 104	0	0
1	pA	70	Total 547	C 341	N 102	O 104	0	0
1	E	70	Total 547	C 341	N 102	O 104	0	0
1	qA	70	Total 547	C 341	N 102	O 104	0	0
1	rA	70	Total 547	C 341	N 102	O 104	0	0
1	sA	70	Total 547	C 341	N 102	O 104	0	0
1	tA	70	Total 547	C 341	N 102	O 104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	uA	70	547	341	102	104	0	0
1	vA	70	547	341	102	104	0	0
1	wA	70	547	341	102	104	0	0
1	xA	70	547	341	102	104	0	0
1	yA	70	547	341	102	104	0	0
1	zA	70	547	341	102	104	0	0
1	0A	70	547	341	102	104	0	0
1	1A	70	547	341	102	104	0	0
1	2A	70	547	341	102	104	0	0
1	3A	70	547	341	102	104	0	0
1	4A	70	547	341	102	104	0	0
1	5A	70	547	341	102	104	0	0
1	6A	70	547	341	102	104	0	0
1	7A	70	547	341	102	104	0	0
1	8A	70	547	341	102	104	0	0
1	9A	70	547	341	102	104	0	0
1	AB	70	547	341	102	104	0	0
1	BB	70	547	341	102	104	0	0
1	CB	70	547	341	102	104	0	0
1	F	70	547	341	102	104	0	0
1	DB	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	EB	70	547	341	102	104	0	0
1	FB	70	547	341	102	104	0	0
1	GB	70	547	341	102	104	0	0
1	HB	70	547	341	102	104	0	0
1	IB	70	547	341	102	104	0	0
1	JB	70	547	341	102	104	0	0
1	KB	70	547	341	102	104	0	0
1	LB	70	547	341	102	104	0	0
1	MB	70	547	341	102	104	0	0
1	NB	70	547	341	102	104	0	0
1	OB	70	547	341	102	104	0	0
1	PB	70	547	341	102	104	0	0
1	QB	70	547	341	102	104	0	0
1	RB	70	547	341	102	104	0	0
1	SB	70	547	341	102	104	0	0
1	TB	70	547	341	102	104	0	0
1	UB	70	547	341	102	104	0	0
1	VB	70	547	341	102	104	0	0
1	WB	70	547	341	102	104	0	0
1	XB	70	547	341	102	104	0	0
1	YB	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	ZB	70	547	341	102	104	0	0
1	G	70	547	341	102	104	0	0
1	aB	70	547	341	102	104	0	0
1	bB	70	547	341	102	104	0	0
1	cB	70	547	341	102	104	0	0
1	dB	70	547	341	102	104	0	0
1	eB	70	547	341	102	104	0	0
1	fB	70	547	341	102	104	0	0
1	gB	70	547	341	102	104	0	0
1	hB	70	547	341	102	104	0	0
1	iB	70	547	341	102	104	0	0
1	jB	70	547	341	102	104	0	0
1	kB	70	547	341	102	104	0	0
1	lB	70	547	341	102	104	0	0
1	mB	70	547	341	102	104	0	0
1	nB	70	547	341	102	104	0	0
1	oB	70	547	341	102	104	0	0
1	pB	70	547	341	102	104	0	0
1	qB	70	547	341	102	104	0	0
1	rB	70	547	341	102	104	0	0
1	sB	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	tB	70	547	341	102	104	0	0
1	uB	70	547	341	102	104	0	0
1	vB	70	547	341	102	104	0	0
1	wB	70	547	341	102	104	0	0
1	H	70	547	341	102	104	0	0
1	xB	70	547	341	102	104	0	0
1	yB	70	547	341	102	104	0	0
1	zB	70	547	341	102	104	0	0
1	0B	70	547	341	102	104	0	0
1	1B	70	547	341	102	104	0	0
1	2B	70	547	341	102	104	0	0
1	3B	70	547	341	102	104	0	0
1	4B	70	547	341	102	104	0	0
1	5B	70	547	341	102	104	0	0
1	6B	70	547	341	102	104	0	0
1	7B	70	547	341	102	104	0	0
1	8B	70	547	341	102	104	0	0
1	9B	70	547	341	102	104	0	0
1	AC	70	547	341	102	104	0	0
1	BC	70	547	341	102	104	0	0
1	CC	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	DC	70	547	341	102	104	0	0
1	EC	70	547	341	102	104	0	0
1	FC	70	547	341	102	104	0	0
1	GC	70	547	341	102	104	0	0
1	HC	70	547	341	102	104	0	0
1	IC	70	547	341	102	104	0	0
1	JC	70	547	341	102	104	0	0
1	I	70	547	341	102	104	0	0
1	KC	70	547	341	102	104	0	0
1	LC	70	547	341	102	104	0	0
1	MC	70	547	341	102	104	0	0
1	NC	70	547	341	102	104	0	0
1	OC	70	547	341	102	104	0	0
1	PC	70	547	341	102	104	0	0
1	QC	70	547	341	102	104	0	0
1	RC	70	547	341	102	104	0	0
1	SC	70	547	341	102	104	0	0
1	TC	70	547	341	102	104	0	0
1	UC	70	547	341	102	104	0	0
1	VC	70	547	341	102	104	0	0
1	WC	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	XC	70	Total 547	C 341	N 102	O 104	0	0
1	YC	70	Total 547	C 341	N 102	O 104	0	0
1	ZC	70	Total 547	C 341	N 102	O 104	0	0
1	aC	70	Total 547	C 341	N 102	O 104	0	0
1	bC	70	Total 547	C 341	N 102	O 104	0	0
1	cC	70	Total 547	C 341	N 102	O 104	0	0
1	dC	70	Total 547	C 341	N 102	O 104	0	0
1	eC	70	Total 547	C 341	N 102	O 104	0	0
1	fC	70	Total 547	C 341	N 102	O 104	0	0
1	gC	70	Total 547	C 341	N 102	O 104	0	0
1	J	70	Total 547	C 341	N 102	O 104	0	0
1	hC	70	Total 547	C 341	N 102	O 104	0	0
1	iC	70	Total 547	C 341	N 102	O 104	0	0
1	jC	70	Total 547	C 341	N 102	O 104	0	0
1	kC	70	Total 547	C 341	N 102	O 104	0	0
1	lC	70	Total 547	C 341	N 102	O 104	0	0
1	mC	70	Total 547	C 341	N 102	O 104	0	0
1	nC	70	Total 547	C 341	N 102	O 104	0	0
1	oC	70	Total 547	C 341	N 102	O 104	0	0
1	pC	70	Total 547	C 341	N 102	O 104	0	0
1	qC	70	Total 547	C 341	N 102	O 104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	rC	70	547	341	102	104	0	0
1	sC	70	547	341	102	104	0	0
1	tC	70	547	341	102	104	0	0
1	uC	70	547	341	102	104	0	0
1	vC	70	547	341	102	104	0	0
1	wC	70	547	341	102	104	0	0
1	xC	70	547	341	102	104	0	0
1	yC	70	547	341	102	104	0	0
1	zC	70	547	341	102	104	0	0
1	0C	70	547	341	102	104	0	0
1	1C	70	547	341	102	104	0	0
1	2C	70	547	341	102	104	0	0
1	3C	70	547	341	102	104	0	0
1	K	70	547	341	102	104	0	0
1	4C	70	547	341	102	104	0	0
1	5C	70	547	341	102	104	0	0
1	6C	70	547	341	102	104	0	0
1	7C	70	547	341	102	104	0	0
1	8C	70	547	341	102	104	0	0
1	9C	70	547	341	102	104	0	0
1	AD	70	547	341	102	104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	BD	70	Total 547	C 341	N 102	O 104	0	0
1	CD	70	Total 547	C 341	N 102	O 104	0	0
1	DD	70	Total 547	C 341	N 102	O 104	0	0
1	ED	70	Total 547	C 341	N 102	O 104	0	0
1	FD	70	Total 547	C 341	N 102	O 104	0	0
1	GD	70	Total 547	C 341	N 102	O 104	0	0
1	HD	70	Total 547	C 341	N 102	O 104	0	0
1	ID	70	Total 547	C 341	N 102	O 104	0	0
1	JD	70	Total 547	C 341	N 102	O 104	0	0
1	KD	70	Total 547	C 341	N 102	O 104	0	0
1	LD	70	Total 547	C 341	N 102	O 104	0	0
1	MD	70	Total 547	C 341	N 102	O 104	0	0
1	ND	70	Total 547	C 341	N 102	O 104	0	0
1	OD	70	Total 547	C 341	N 102	O 104	0	0
1	PD	70	Total 547	C 341	N 102	O 104	0	0
1	QD	70	Total 547	C 341	N 102	O 104	0	0

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	SER	engineered mutation	UNP Q9X6J6
A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
L	33	HIS	SER	engineered mutation	UNP Q9X6J6
L	35	HIS	LYS	engineered mutation	UNP Q9X6J6
M	33	HIS	SER	engineered mutation	UNP Q9X6J6
M	35	HIS	LYS	engineered mutation	UNP Q9X6J6
N	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	35	HIS	LYS	engineered mutation	UNP Q9X6J6
O	33	HIS	SER	engineered mutation	UNP Q9X6J6
O	35	HIS	LYS	engineered mutation	UNP Q9X6J6
P	33	HIS	SER	engineered mutation	UNP Q9X6J6
P	35	HIS	LYS	engineered mutation	UNP Q9X6J6
Q	33	HIS	SER	engineered mutation	UNP Q9X6J6
Q	35	HIS	LYS	engineered mutation	UNP Q9X6J6
R	33	HIS	SER	engineered mutation	UNP Q9X6J6
R	35	HIS	LYS	engineered mutation	UNP Q9X6J6
S	33	HIS	SER	engineered mutation	UNP Q9X6J6
S	35	HIS	LYS	engineered mutation	UNP Q9X6J6
T	33	HIS	SER	engineered mutation	UNP Q9X6J6
T	35	HIS	LYS	engineered mutation	UNP Q9X6J6
U	33	HIS	SER	engineered mutation	UNP Q9X6J6
U	35	HIS	LYS	engineered mutation	UNP Q9X6J6
V	33	HIS	SER	engineered mutation	UNP Q9X6J6
V	35	HIS	LYS	engineered mutation	UNP Q9X6J6
W	33	HIS	SER	engineered mutation	UNP Q9X6J6
W	35	HIS	LYS	engineered mutation	UNP Q9X6J6
Y	33	HIS	SER	engineered mutation	UNP Q9X6J6
Y	35	HIS	LYS	engineered mutation	UNP Q9X6J6
Z	33	HIS	SER	engineered mutation	UNP Q9X6J6
Z	35	HIS	LYS	engineered mutation	UNP Q9X6J6
a	33	HIS	SER	engineered mutation	UNP Q9X6J6
a	35	HIS	LYS	engineered mutation	UNP Q9X6J6
b	33	HIS	SER	engineered mutation	UNP Q9X6J6
b	35	HIS	LYS	engineered mutation	UNP Q9X6J6
c	33	HIS	SER	engineered mutation	UNP Q9X6J6
c	35	HIS	LYS	engineered mutation	UNP Q9X6J6
d	33	HIS	SER	engineered mutation	UNP Q9X6J6
d	35	HIS	LYS	engineered mutation	UNP Q9X6J6
e	33	HIS	SER	engineered mutation	UNP Q9X6J6
e	35	HIS	LYS	engineered mutation	UNP Q9X6J6
f	33	HIS	SER	engineered mutation	UNP Q9X6J6
f	35	HIS	LYS	engineered mutation	UNP Q9X6J6
g	33	HIS	SER	engineered mutation	UNP Q9X6J6
g	35	HIS	LYS	engineered mutation	UNP Q9X6J6
h	33	HIS	SER	engineered mutation	UNP Q9X6J6
h	35	HIS	LYS	engineered mutation	UNP Q9X6J6
i	33	HIS	SER	engineered mutation	UNP Q9X6J6
i	35	HIS	LYS	engineered mutation	UNP Q9X6J6
B	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
j	33	HIS	SER	engineered mutation	UNP Q9X6J6
j	35	HIS	LYS	engineered mutation	UNP Q9X6J6
k	33	HIS	SER	engineered mutation	UNP Q9X6J6
k	35	HIS	LYS	engineered mutation	UNP Q9X6J6
l	33	HIS	SER	engineered mutation	UNP Q9X6J6
l	35	HIS	LYS	engineered mutation	UNP Q9X6J6
m	33	HIS	SER	engineered mutation	UNP Q9X6J6
m	35	HIS	LYS	engineered mutation	UNP Q9X6J6
n	33	HIS	SER	engineered mutation	UNP Q9X6J6
n	35	HIS	LYS	engineered mutation	UNP Q9X6J6
o	33	HIS	SER	engineered mutation	UNP Q9X6J6
o	35	HIS	LYS	engineered mutation	UNP Q9X6J6
p	33	HIS	SER	engineered mutation	UNP Q9X6J6
p	35	HIS	LYS	engineered mutation	UNP Q9X6J6
q	33	HIS	SER	engineered mutation	UNP Q9X6J6
q	35	HIS	LYS	engineered mutation	UNP Q9X6J6
r	33	HIS	SER	engineered mutation	UNP Q9X6J6
r	35	HIS	LYS	engineered mutation	UNP Q9X6J6
s	33	HIS	SER	engineered mutation	UNP Q9X6J6
s	35	HIS	LYS	engineered mutation	UNP Q9X6J6
t	33	HIS	SER	engineered mutation	UNP Q9X6J6
t	35	HIS	LYS	engineered mutation	UNP Q9X6J6
u	33	HIS	SER	engineered mutation	UNP Q9X6J6
u	35	HIS	LYS	engineered mutation	UNP Q9X6J6
v	33	HIS	SER	engineered mutation	UNP Q9X6J6
v	35	HIS	LYS	engineered mutation	UNP Q9X6J6
w	33	HIS	SER	engineered mutation	UNP Q9X6J6
w	35	HIS	LYS	engineered mutation	UNP Q9X6J6
x	33	HIS	SER	engineered mutation	UNP Q9X6J6
x	35	HIS	LYS	engineered mutation	UNP Q9X6J6
y	33	HIS	SER	engineered mutation	UNP Q9X6J6
y	35	HIS	LYS	engineered mutation	UNP Q9X6J6
z	33	HIS	SER	engineered mutation	UNP Q9X6J6
z	35	HIS	LYS	engineered mutation	UNP Q9X6J6
0	33	HIS	SER	engineered mutation	UNP Q9X6J6
0	35	HIS	LYS	engineered mutation	UNP Q9X6J6
1	33	HIS	SER	engineered mutation	UNP Q9X6J6
1	35	HIS	LYS	engineered mutation	UNP Q9X6J6
2	33	HIS	SER	engineered mutation	UNP Q9X6J6
2	35	HIS	LYS	engineered mutation	UNP Q9X6J6
3	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
3	35	HIS	LYS	engineered mutation	UNP Q9X6J6
4	33	HIS	SER	engineered mutation	UNP Q9X6J6
4	35	HIS	LYS	engineered mutation	UNP Q9X6J6
5	33	HIS	SER	engineered mutation	UNP Q9X6J6
5	35	HIS	LYS	engineered mutation	UNP Q9X6J6
C	33	HIS	SER	engineered mutation	UNP Q9X6J6
C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
6	33	HIS	SER	engineered mutation	UNP Q9X6J6
6	35	HIS	LYS	engineered mutation	UNP Q9X6J6
7	33	HIS	SER	engineered mutation	UNP Q9X6J6
7	35	HIS	LYS	engineered mutation	UNP Q9X6J6
8	33	HIS	SER	engineered mutation	UNP Q9X6J6
8	35	HIS	LYS	engineered mutation	UNP Q9X6J6
9	33	HIS	SER	engineered mutation	UNP Q9X6J6
9	35	HIS	LYS	engineered mutation	UNP Q9X6J6
AA	33	HIS	SER	engineered mutation	UNP Q9X6J6
AA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
BA	33	HIS	SER	engineered mutation	UNP Q9X6J6
BA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
CA	33	HIS	SER	engineered mutation	UNP Q9X6J6
CA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
DA	33	HIS	SER	engineered mutation	UNP Q9X6J6
DA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
EA	33	HIS	SER	engineered mutation	UNP Q9X6J6
EA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
FA	33	HIS	SER	engineered mutation	UNP Q9X6J6
FA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
GA	33	HIS	SER	engineered mutation	UNP Q9X6J6
GA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
HA	33	HIS	SER	engineered mutation	UNP Q9X6J6
HA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
IA	33	HIS	SER	engineered mutation	UNP Q9X6J6
IA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
JA	33	HIS	SER	engineered mutation	UNP Q9X6J6
JA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
KA	33	HIS	SER	engineered mutation	UNP Q9X6J6
KA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
LA	33	HIS	SER	engineered mutation	UNP Q9X6J6
LA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
MA	33	HIS	SER	engineered mutation	UNP Q9X6J6
MA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
NA	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
NA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
OA	33	HIS	SER	engineered mutation	UNP Q9X6J6
OA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
PA	33	HIS	SER	engineered mutation	UNP Q9X6J6
PA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
QA	33	HIS	SER	engineered mutation	UNP Q9X6J6
QA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
RA	33	HIS	SER	engineered mutation	UNP Q9X6J6
RA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
SA	33	HIS	SER	engineered mutation	UNP Q9X6J6
SA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
D	33	HIS	SER	engineered mutation	UNP Q9X6J6
D	35	HIS	LYS	engineered mutation	UNP Q9X6J6
TA	33	HIS	SER	engineered mutation	UNP Q9X6J6
TA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
UA	33	HIS	SER	engineered mutation	UNP Q9X6J6
UA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
VA	33	HIS	SER	engineered mutation	UNP Q9X6J6
VA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
WA	33	HIS	SER	engineered mutation	UNP Q9X6J6
WA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
XA	33	HIS	SER	engineered mutation	UNP Q9X6J6
XA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
YA	33	HIS	SER	engineered mutation	UNP Q9X6J6
YA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ZA	33	HIS	SER	engineered mutation	UNP Q9X6J6
ZA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
aA	33	HIS	SER	engineered mutation	UNP Q9X6J6
aA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
bA	33	HIS	SER	engineered mutation	UNP Q9X6J6
bA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
cA	33	HIS	SER	engineered mutation	UNP Q9X6J6
cA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
dA	33	HIS	SER	engineered mutation	UNP Q9X6J6
dA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
eA	33	HIS	SER	engineered mutation	UNP Q9X6J6
eA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
fA	33	HIS	SER	engineered mutation	UNP Q9X6J6
fA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
gA	33	HIS	SER	engineered mutation	UNP Q9X6J6
gA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
hA	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
hA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
iA	33	HIS	SER	engineered mutation	UNP Q9X6J6
iA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
jA	33	HIS	SER	engineered mutation	UNP Q9X6J6
jA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
kA	33	HIS	SER	engineered mutation	UNP Q9X6J6
kA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
lA	33	HIS	SER	engineered mutation	UNP Q9X6J6
lA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
mA	33	HIS	SER	engineered mutation	UNP Q9X6J6
mA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
nA	33	HIS	SER	engineered mutation	UNP Q9X6J6
nA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
oA	33	HIS	SER	engineered mutation	UNP Q9X6J6
oA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
pA	33	HIS	SER	engineered mutation	UNP Q9X6J6
pA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
E	33	HIS	SER	engineered mutation	UNP Q9X6J6
E	35	HIS	LYS	engineered mutation	UNP Q9X6J6
qA	33	HIS	SER	engineered mutation	UNP Q9X6J6
qA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
rA	33	HIS	SER	engineered mutation	UNP Q9X6J6
rA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
sA	33	HIS	SER	engineered mutation	UNP Q9X6J6
sA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
tA	33	HIS	SER	engineered mutation	UNP Q9X6J6
tA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
uA	33	HIS	SER	engineered mutation	UNP Q9X6J6
uA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
vA	33	HIS	SER	engineered mutation	UNP Q9X6J6
vA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
wA	33	HIS	SER	engineered mutation	UNP Q9X6J6
wA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
xA	33	HIS	SER	engineered mutation	UNP Q9X6J6
xA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
yA	33	HIS	SER	engineered mutation	UNP Q9X6J6
yA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
zA	33	HIS	SER	engineered mutation	UNP Q9X6J6
zA	35	HIS	LYS	engineered mutation	UNP Q9X6J6
0A	33	HIS	SER	engineered mutation	UNP Q9X6J6
0A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
1A	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
1A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
2A	33	HIS	SER	engineered mutation	UNP Q9X6J6
2A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
3A	33	HIS	SER	engineered mutation	UNP Q9X6J6
3A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
4A	33	HIS	SER	engineered mutation	UNP Q9X6J6
4A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
5A	33	HIS	SER	engineered mutation	UNP Q9X6J6
5A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
6A	33	HIS	SER	engineered mutation	UNP Q9X6J6
6A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
7A	33	HIS	SER	engineered mutation	UNP Q9X6J6
7A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
8A	33	HIS	SER	engineered mutation	UNP Q9X6J6
8A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
9A	33	HIS	SER	engineered mutation	UNP Q9X6J6
9A	35	HIS	LYS	engineered mutation	UNP Q9X6J6
AB	33	HIS	SER	engineered mutation	UNP Q9X6J6
AB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
BB	33	HIS	SER	engineered mutation	UNP Q9X6J6
BB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
CB	33	HIS	SER	engineered mutation	UNP Q9X6J6
CB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
F	33	HIS	SER	engineered mutation	UNP Q9X6J6
F	35	HIS	LYS	engineered mutation	UNP Q9X6J6
DB	33	HIS	SER	engineered mutation	UNP Q9X6J6
DB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
EB	33	HIS	SER	engineered mutation	UNP Q9X6J6
EB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
FB	33	HIS	SER	engineered mutation	UNP Q9X6J6
FB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
GB	33	HIS	SER	engineered mutation	UNP Q9X6J6
GB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
HB	33	HIS	SER	engineered mutation	UNP Q9X6J6
HB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
IB	33	HIS	SER	engineered mutation	UNP Q9X6J6
IB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
JB	33	HIS	SER	engineered mutation	UNP Q9X6J6
JB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
KB	33	HIS	SER	engineered mutation	UNP Q9X6J6
KB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
LB	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
LB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
MB	33	HIS	SER	engineered mutation	UNP Q9X6J6
MB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
NB	33	HIS	SER	engineered mutation	UNP Q9X6J6
NB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
OB	33	HIS	SER	engineered mutation	UNP Q9X6J6
OB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
PB	33	HIS	SER	engineered mutation	UNP Q9X6J6
PB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
QB	33	HIS	SER	engineered mutation	UNP Q9X6J6
QB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
RB	33	HIS	SER	engineered mutation	UNP Q9X6J6
RB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
SB	33	HIS	SER	engineered mutation	UNP Q9X6J6
SB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
TB	33	HIS	SER	engineered mutation	UNP Q9X6J6
TB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
UB	33	HIS	SER	engineered mutation	UNP Q9X6J6
UB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
VB	33	HIS	SER	engineered mutation	UNP Q9X6J6
VB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
WB	33	HIS	SER	engineered mutation	UNP Q9X6J6
WB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
XB	33	HIS	SER	engineered mutation	UNP Q9X6J6
XB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
YB	33	HIS	SER	engineered mutation	UNP Q9X6J6
YB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ZB	33	HIS	SER	engineered mutation	UNP Q9X6J6
ZB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
G	33	HIS	SER	engineered mutation	UNP Q9X6J6
G	35	HIS	LYS	engineered mutation	UNP Q9X6J6
aB	33	HIS	SER	engineered mutation	UNP Q9X6J6
aB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
bB	33	HIS	SER	engineered mutation	UNP Q9X6J6
bB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
cB	33	HIS	SER	engineered mutation	UNP Q9X6J6
cB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
dB	33	HIS	SER	engineered mutation	UNP Q9X6J6
dB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
eB	33	HIS	SER	engineered mutation	UNP Q9X6J6
eB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
fB	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
fB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
gB	33	HIS	SER	engineered mutation	UNP Q9X6J6
gB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
hB	33	HIS	SER	engineered mutation	UNP Q9X6J6
hB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
iB	33	HIS	SER	engineered mutation	UNP Q9X6J6
iB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
jB	33	HIS	SER	engineered mutation	UNP Q9X6J6
jB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
kB	33	HIS	SER	engineered mutation	UNP Q9X6J6
kB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
lB	33	HIS	SER	engineered mutation	UNP Q9X6J6
lB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
mB	33	HIS	SER	engineered mutation	UNP Q9X6J6
mB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
nB	33	HIS	SER	engineered mutation	UNP Q9X6J6
nB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
oB	33	HIS	SER	engineered mutation	UNP Q9X6J6
oB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
pB	33	HIS	SER	engineered mutation	UNP Q9X6J6
pB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
qB	33	HIS	SER	engineered mutation	UNP Q9X6J6
qB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
rB	33	HIS	SER	engineered mutation	UNP Q9X6J6
rB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
sB	33	HIS	SER	engineered mutation	UNP Q9X6J6
sB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
tB	33	HIS	SER	engineered mutation	UNP Q9X6J6
tB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
uB	33	HIS	SER	engineered mutation	UNP Q9X6J6
uB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
vB	33	HIS	SER	engineered mutation	UNP Q9X6J6
vB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
wB	33	HIS	SER	engineered mutation	UNP Q9X6J6
wB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
H	33	HIS	SER	engineered mutation	UNP Q9X6J6
H	35	HIS	LYS	engineered mutation	UNP Q9X6J6
xB	33	HIS	SER	engineered mutation	UNP Q9X6J6
xB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
yB	33	HIS	SER	engineered mutation	UNP Q9X6J6
yB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
zB	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
zB	35	HIS	LYS	engineered mutation	UNP Q9X6J6
0B	33	HIS	SER	engineered mutation	UNP Q9X6J6
0B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
1B	33	HIS	SER	engineered mutation	UNP Q9X6J6
1B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
2B	33	HIS	SER	engineered mutation	UNP Q9X6J6
2B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
3B	33	HIS	SER	engineered mutation	UNP Q9X6J6
3B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
4B	33	HIS	SER	engineered mutation	UNP Q9X6J6
4B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
5B	33	HIS	SER	engineered mutation	UNP Q9X6J6
5B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
6B	33	HIS	SER	engineered mutation	UNP Q9X6J6
6B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
7B	33	HIS	SER	engineered mutation	UNP Q9X6J6
7B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
8B	33	HIS	SER	engineered mutation	UNP Q9X6J6
8B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
9B	33	HIS	SER	engineered mutation	UNP Q9X6J6
9B	35	HIS	LYS	engineered mutation	UNP Q9X6J6
AC	33	HIS	SER	engineered mutation	UNP Q9X6J6
AC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
BC	33	HIS	SER	engineered mutation	UNP Q9X6J6
BC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
CC	33	HIS	SER	engineered mutation	UNP Q9X6J6
CC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
DC	33	HIS	SER	engineered mutation	UNP Q9X6J6
DC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
EC	33	HIS	SER	engineered mutation	UNP Q9X6J6
EC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
FC	33	HIS	SER	engineered mutation	UNP Q9X6J6
FC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
GC	33	HIS	SER	engineered mutation	UNP Q9X6J6
GC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
HC	33	HIS	SER	engineered mutation	UNP Q9X6J6
HC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
IC	33	HIS	SER	engineered mutation	UNP Q9X6J6
IC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
JC	33	HIS	SER	engineered mutation	UNP Q9X6J6
JC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
I	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	35	HIS	LYS	engineered mutation	UNP Q9X6J6
KC	33	HIS	SER	engineered mutation	UNP Q9X6J6
KC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
LC	33	HIS	SER	engineered mutation	UNP Q9X6J6
LC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
MC	33	HIS	SER	engineered mutation	UNP Q9X6J6
MC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
NC	33	HIS	SER	engineered mutation	UNP Q9X6J6
NC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
OC	33	HIS	SER	engineered mutation	UNP Q9X6J6
OC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
PC	33	HIS	SER	engineered mutation	UNP Q9X6J6
PC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
QC	33	HIS	SER	engineered mutation	UNP Q9X6J6
QC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
RC	33	HIS	SER	engineered mutation	UNP Q9X6J6
RC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
SC	33	HIS	SER	engineered mutation	UNP Q9X6J6
SC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
TC	33	HIS	SER	engineered mutation	UNP Q9X6J6
TC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
UC	33	HIS	SER	engineered mutation	UNP Q9X6J6
UC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
VC	33	HIS	SER	engineered mutation	UNP Q9X6J6
VC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
WC	33	HIS	SER	engineered mutation	UNP Q9X6J6
WC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
XC	33	HIS	SER	engineered mutation	UNP Q9X6J6
XC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
YC	33	HIS	SER	engineered mutation	UNP Q9X6J6
YC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ZC	33	HIS	SER	engineered mutation	UNP Q9X6J6
ZC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
aC	33	HIS	SER	engineered mutation	UNP Q9X6J6
aC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
bC	33	HIS	SER	engineered mutation	UNP Q9X6J6
bC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
cC	33	HIS	SER	engineered mutation	UNP Q9X6J6
cC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
dC	33	HIS	SER	engineered mutation	UNP Q9X6J6
dC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
eC	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
eC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
fC	33	HIS	SER	engineered mutation	UNP Q9X6J6
fC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
gC	33	HIS	SER	engineered mutation	UNP Q9X6J6
gC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
J	33	HIS	SER	engineered mutation	UNP Q9X6J6
J	35	HIS	LYS	engineered mutation	UNP Q9X6J6
hC	33	HIS	SER	engineered mutation	UNP Q9X6J6
hC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
iC	33	HIS	SER	engineered mutation	UNP Q9X6J6
iC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
jC	33	HIS	SER	engineered mutation	UNP Q9X6J6
jC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
kC	33	HIS	SER	engineered mutation	UNP Q9X6J6
kC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
lC	33	HIS	SER	engineered mutation	UNP Q9X6J6
lC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
mC	33	HIS	SER	engineered mutation	UNP Q9X6J6
mC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
nC	33	HIS	SER	engineered mutation	UNP Q9X6J6
nC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
oC	33	HIS	SER	engineered mutation	UNP Q9X6J6
oC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
pC	33	HIS	SER	engineered mutation	UNP Q9X6J6
pC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
qC	33	HIS	SER	engineered mutation	UNP Q9X6J6
qC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
rC	33	HIS	SER	engineered mutation	UNP Q9X6J6
rC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
sC	33	HIS	SER	engineered mutation	UNP Q9X6J6
sC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
tC	33	HIS	SER	engineered mutation	UNP Q9X6J6
tC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
uC	33	HIS	SER	engineered mutation	UNP Q9X6J6
uC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
vC	33	HIS	SER	engineered mutation	UNP Q9X6J6
vC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
wC	33	HIS	SER	engineered mutation	UNP Q9X6J6
wC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
xC	33	HIS	SER	engineered mutation	UNP Q9X6J6
xC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
yC	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
yC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
zC	33	HIS	SER	engineered mutation	UNP Q9X6J6
zC	35	HIS	LYS	engineered mutation	UNP Q9X6J6
0C	33	HIS	SER	engineered mutation	UNP Q9X6J6
0C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
1C	33	HIS	SER	engineered mutation	UNP Q9X6J6
1C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
2C	33	HIS	SER	engineered mutation	UNP Q9X6J6
2C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
3C	33	HIS	SER	engineered mutation	UNP Q9X6J6
3C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
K	33	HIS	SER	engineered mutation	UNP Q9X6J6
K	35	HIS	LYS	engineered mutation	UNP Q9X6J6
4C	33	HIS	SER	engineered mutation	UNP Q9X6J6
4C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
5C	33	HIS	SER	engineered mutation	UNP Q9X6J6
5C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
6C	33	HIS	SER	engineered mutation	UNP Q9X6J6
6C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
7C	33	HIS	SER	engineered mutation	UNP Q9X6J6
7C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
8C	33	HIS	SER	engineered mutation	UNP Q9X6J6
8C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
9C	33	HIS	SER	engineered mutation	UNP Q9X6J6
9C	35	HIS	LYS	engineered mutation	UNP Q9X6J6
AD	33	HIS	SER	engineered mutation	UNP Q9X6J6
AD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
BD	33	HIS	SER	engineered mutation	UNP Q9X6J6
BD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
CD	33	HIS	SER	engineered mutation	UNP Q9X6J6
CD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
DD	33	HIS	SER	engineered mutation	UNP Q9X6J6
DD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ED	33	HIS	SER	engineered mutation	UNP Q9X6J6
ED	35	HIS	LYS	engineered mutation	UNP Q9X6J6
FD	33	HIS	SER	engineered mutation	UNP Q9X6J6
FD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
GD	33	HIS	SER	engineered mutation	UNP Q9X6J6
GD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
HD	33	HIS	SER	engineered mutation	UNP Q9X6J6
HD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ID	33	HIS	SER	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
ID	35	HIS	LYS	engineered mutation	UNP Q9X6J6
JD	33	HIS	SER	engineered mutation	UNP Q9X6J6
JD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
KD	33	HIS	SER	engineered mutation	UNP Q9X6J6
KD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
LD	33	HIS	SER	engineered mutation	UNP Q9X6J6
LD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
MD	33	HIS	SER	engineered mutation	UNP Q9X6J6
MD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
ND	33	HIS	SER	engineered mutation	UNP Q9X6J6
ND	35	HIS	LYS	engineered mutation	UNP Q9X6J6
OD	33	HIS	SER	engineered mutation	UNP Q9X6J6
OD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
PD	33	HIS	SER	engineered mutation	UNP Q9X6J6
PD	35	HIS	LYS	engineered mutation	UNP Q9X6J6
QD	33	HIS	SER	engineered mutation	UNP Q9X6J6
QD	35	HIS	LYS	engineered mutation	UNP Q9X6J6

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total Co 1 1	0
2	DB	1	Total Co 1 1	0
2	EB	1	Total Co 1 1	0
2	FB	1	Total Co 1 1	0
2	GB	1	Total Co 1 1	0
2	HB	1	Total Co 1 1	0
2	IB	1	Total Co 1 1	0
2	JB	1	Total Co 1 1	0
2	KB	1	Total Co 1 1	0
2	LB	1	Total Co 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Co	
2	MB	1	1	1	0
2	NB	1	1	1	0
2	OB	1	1	1	0
2	PB	1	1	1	0
2	QB	1	1	1	0
2	RB	1	1	1	0
2	SB	1	1	1	0
2	TB	1	1	1	0
2	UB	1	1	1	0
2	VB	1	1	1	0
2	WB	1	1	1	0
2	XB	1	1	1	0
2	YB	1	1	1	0
2	ZB	1	1	1	0
2	G	1	1	1	0
2	aB	1	1	1	0
2	bB	1	1	1	0
2	cB	1	1	1	0
2	dB	1	1	1	0
2	eB	1	1	1	0
2	fB	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
2	gB	1	Total 1	Co 1	0
2	hB	1	Total 1	Co 1	0
2	iB	1	Total 1	Co 1	0
2	jB	1	Total 1	Co 1	0
2	kB	1	Total 1	Co 1	0
2	lB	1	Total 1	Co 1	0
2	mB	1	Total 1	Co 1	0
2	nB	1	Total 1	Co 1	0
2	oB	1	Total 1	Co 1	0
2	pB	1	Total 1	Co 1	0
2	qB	1	Total 1	Co 1	0
2	rB	1	Total 1	Co 1	0
2	sB	1	Total 1	Co 1	0
2	tB	1	Total 1	Co 1	0
2	uB	1	Total 1	Co 1	0
2	vB	1	Total 1	Co 1	0
2	wB	1	Total 1	Co 1	0
2	I	1	Total 1	Co 1	0
2	KC	1	Total 1	Co 1	0
2	LC	1	Total 1	Co 1	0
2	MC	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Co	
2	NC	1	1	1	0
2	OC	1	1	1	0
2	PC	1	1	1	0
2	QC	1	1	1	0
2	RC	1	1	1	0
2	SC	1	1	1	0
2	TC	1	1	1	0
2	UC	1	1	1	0
2	VC	1	1	1	0
2	WC	1	1	1	0
2	XC	1	1	1	0
2	YC	1	1	1	0
2	ZC	1	1	1	0
2	aC	1	1	1	0
2	bC	1	1	1	0
2	cC	1	1	1	0
2	dC	1	1	1	0
2	eC	1	1	1	0
2	fC	1	1	1	0
2	gC	1	1	1	0
2	J	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
2	hC	1	Total 1	Co 1	0
2	iC	1	Total 1	Co 1	0
2	jC	1	Total 1	Co 1	0
2	kC	1	Total 1	Co 1	0
2	lC	1	Total 1	Co 1	0
2	mC	1	Total 1	Co 1	0
2	nC	1	Total 1	Co 1	0
2	oC	1	Total 1	Co 1	0
2	pC	1	Total 1	Co 1	0
2	qC	1	Total 1	Co 1	0
2	rC	1	Total 1	Co 1	0
2	sC	1	Total 1	Co 1	0
2	tC	1	Total 1	Co 1	0
2	uC	1	Total 1	Co 1	0
2	vC	1	Total 1	Co 1	0
2	wC	1	Total 1	Co 1	0
2	xC	1	Total 1	Co 1	0
2	yC	1	Total 1	Co 1	0
2	zC	1	Total 1	Co 1	0
2	0C	1	Total 1	Co 1	0
2	1C	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	2C	1	Total 1	Co 1	0
2	3C	1	Total 1	Co 1	0
2	K	1	Total 1	Co 1	0
2	4C	1	Total 1	Co 1	0
2	5C	1	Total 1	Co 1	0
2	6C	1	Total 1	Co 1	0
2	7C	1	Total 1	Co 1	0
2	8C	1	Total 1	Co 1	0
2	9C	1	Total 1	Co 1	0
2	AD	1	Total 1	Co 1	0
2	BD	1	Total 1	Co 1	0
2	CD	1	Total 1	Co 1	0
2	DD	1	Total 1	Co 1	0
2	ED	1	Total 1	Co 1	0
2	FD	1	Total 1	Co 1	0
2	GD	1	Total 1	Co 1	0
2	HD	1	Total 1	Co 1	0
2	ID	1	Total 1	Co 1	0
2	JD	1	Total 1	Co 1	0
2	KD	1	Total 1	Co 1	0
2	LD	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	MD	1	Total 1	Co 1	0
2	ND	1	Total 1	Co 1	0
2	OD	1	Total 1	Co 1	0
2	PD	1	Total 1	Co 1	0
2	QD	1	Total 1	Co 1	0

3 Residue-property plots [i](#)

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

- Molecule 1: Transcription attenuation protein MtrB

Chain A:  92% •• 5%

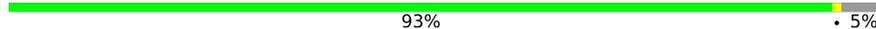


- Molecule 1: Transcription attenuation protein MtrB

Chain L:  92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain M:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain N:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain O:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain P:  92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain Q: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain R: 92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain S: 92% • 5%



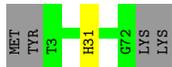
- Molecule 1: Transcription attenuation protein MtrB

Chain T: 92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain U: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain V: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain W: 92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain Y: 92% .. 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain Z: 92% .. 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain a: 92% .. 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain b: 92% . 5%



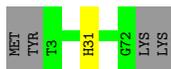
- Molecule 1: Transcription attenuation protein MtrB

Chain c: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain d: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

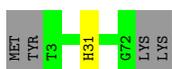
Chain e: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain l: 93% . 5%



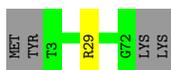
- Molecule 1: Transcription attenuation protein MtrB

Chain m: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain n: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain o: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain p: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain q: 93% . 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain r: 93% . 5%



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



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- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

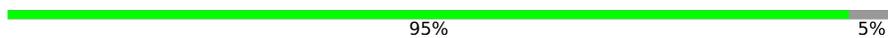


- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain JA:  95% 5%

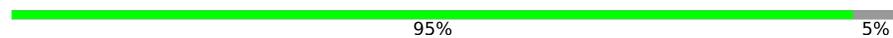


- Molecule 1: Transcription attenuation protein MtrB

Chain KA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain LA:  95% 5%

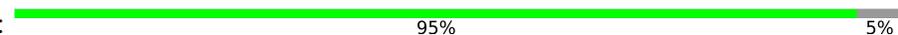


- Molecule 1: Transcription attenuation protein MtrB

Chain MA:  95% 5%

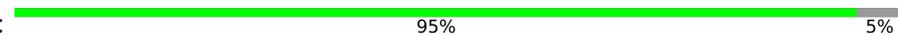


- Molecule 1: Transcription attenuation protein MtrB

Chain NA:  95% 5%

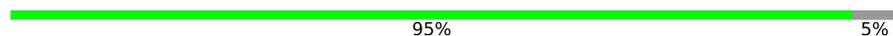


- Molecule 1: Transcription attenuation protein MtrB

Chain OA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain PA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain WA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain XA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain YA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ZA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain aA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain bA: 93% • 5%

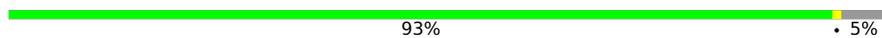


- Molecule 1: Transcription attenuation protein MtrB

Chain cA: 93% • 5%

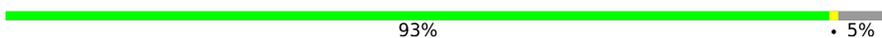


- Molecule 1: Transcription attenuation protein MtrB

Chain dA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain eA:  93% • 5%

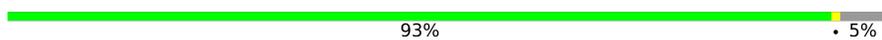


- Molecule 1: Transcription attenuation protein MtrB

Chain fA:  93% • 5%

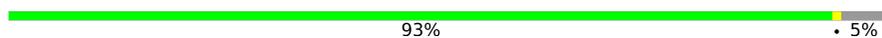


- Molecule 1: Transcription attenuation protein MtrB

Chain gA:  93% • 5%



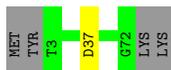
- Molecule 1: Transcription attenuation protein MtrB

Chain hA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain iA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain jA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain kA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain lA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain mA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain nA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain oA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain pA: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain E: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





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• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain 4A: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 5A: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 6A: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 7A: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 8A: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 9A: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain AB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain BB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain CB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain F: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain DB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain EB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain FB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain GB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain HB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain IB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain JB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain KB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain LB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain MB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain NB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain OB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain PB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain QB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain RB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain SB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain TB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain UB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain VB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain WB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain XB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain YB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ZB: 92% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain G: 95% 5%

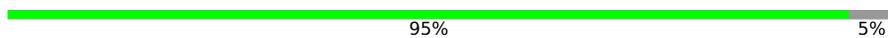


- Molecule 1: Transcription attenuation protein MtrB

Chain aB: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain bB:  95% 5%

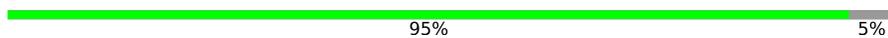


- Molecule 1: Transcription attenuation protein MtrB

Chain cB:  95% 5%

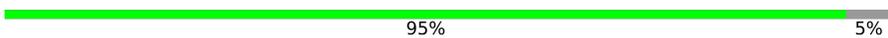


- Molecule 1: Transcription attenuation protein MtrB

Chain dB:  95% 5%

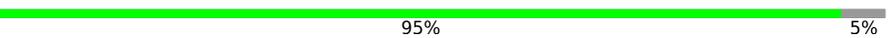


- Molecule 1: Transcription attenuation protein MtrB

Chain eB:  95% 5%

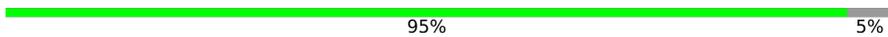


- Molecule 1: Transcription attenuation protein MtrB

Chain fB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain gB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain hB:  95% 5%

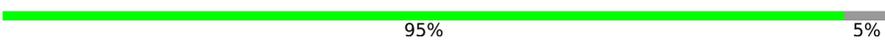


- Molecule 1: Transcription attenuation protein MtrB

Chain iB:  95% 5%

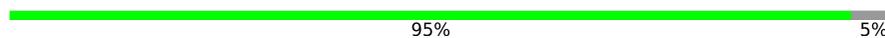


- Molecule 1: Transcription attenuation protein MtrB

Chain jB:  95% 5%

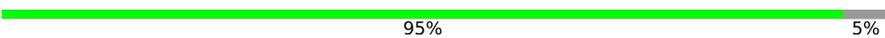


- Molecule 1: Transcription attenuation protein MtrB

Chain kB:  95% 5%

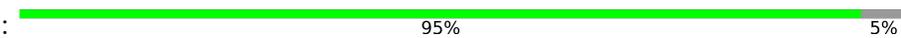


- Molecule 1: Transcription attenuation protein MtrB

Chain lB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain mB:  95% 5%

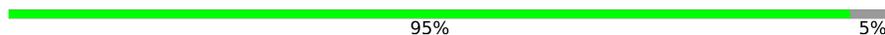


- Molecule 1: Transcription attenuation protein MtrB

Chain nB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain oB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

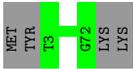


- Molecule 1: Transcription attenuation protein MtrB



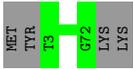
- Molecule 1: Transcription attenuation protein MtrB





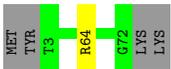
- Molecule 1: Transcription attenuation protein MtrB

Chain wB: 95% 5%



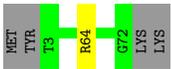
- Molecule 1: Transcription attenuation protein MtrB

Chain H: 93% 5%



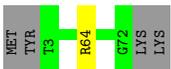
- Molecule 1: Transcription attenuation protein MtrB

Chain xB: 93% 5%



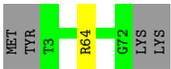
- Molecule 1: Transcription attenuation protein MtrB

Chain yB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain zB: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 0B: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 1B: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 2B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 3B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 4B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 5B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 6B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 7B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 8B: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain MC:  95% 5%

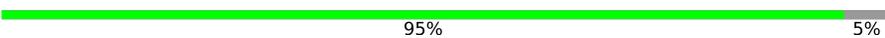


- Molecule 1: Transcription attenuation protein MtrB

Chain NC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain OC:  95% 5%

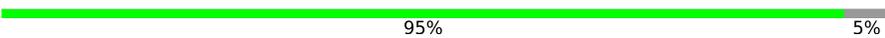


- Molecule 1: Transcription attenuation protein MtrB

Chain PC:  95% 5%

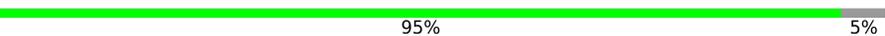


- Molecule 1: Transcription attenuation protein MtrB

Chain QC:  95% 5%

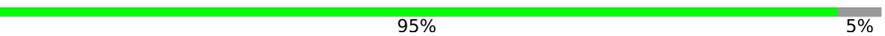


- Molecule 1: Transcription attenuation protein MtrB

Chain RC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain SC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain TC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain UC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain VC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain WC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain XC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain YC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ZC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain aC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain bC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain cC:  95% 5%

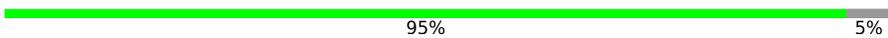


- Molecule 1: Transcription attenuation protein MtrB

Chain dC:  95% 5%

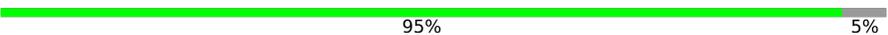


- Molecule 1: Transcription attenuation protein MtrB

Chain eC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain fC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain gC:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain J: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain hC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain iC: 95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain jC: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain kC: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain lC: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain mC: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain uC: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain vC: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain wC: 93% 5%



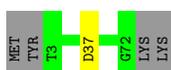
- Molecule 1: Transcription attenuation protein MtrB

Chain xC: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain yC: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain zC: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 0C: 93% 5%



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB



• Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain LD: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain MD: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ND: 92% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain OD: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain PD: 93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain QD: 92% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	157100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.31	0/556	0.55	0/749
1	0A	0.30	0/556	0.54	0/749
1	0B	0.31	0/556	0.55	0/749
1	0C	0.30	0/556	0.55	0/749
1	1	0.31	0/556	0.55	0/749
1	1A	0.30	0/556	0.54	0/749
1	1B	0.30	0/556	0.55	0/749
1	1C	0.30	0/556	0.54	0/749
1	2	0.30	0/556	0.55	0/749
1	2A	0.31	0/556	0.54	0/749
1	2B	0.30	0/556	0.55	0/749
1	2C	0.30	0/556	0.54	0/749
1	3	0.31	0/556	0.55	0/749
1	3A	0.30	0/556	0.55	0/749
1	3B	0.31	0/556	0.55	0/749
1	3C	0.30	0/556	0.55	0/749
1	4	0.31	0/556	0.55	0/749
1	4A	0.30	0/556	0.54	0/749
1	4B	0.30	0/556	0.55	0/749
1	4C	0.30	0/556	0.55	0/749
1	5	0.30	0/556	0.55	0/749
1	5A	0.30	0/556	0.54	0/749
1	5B	0.30	0/556	0.56	0/749
1	5C	0.32	0/556	0.54	0/749
1	6	0.30	0/556	0.55	0/749
1	6A	0.30	0/556	0.54	0/749
1	6B	0.30	0/556	0.55	0/749
1	6C	0.30	0/556	0.54	0/749
1	7	0.31	0/556	0.55	0/749
1	7A	0.30	0/556	0.54	0/749
1	7B	0.30	0/556	0.56	0/749
1	7C	0.31	0/556	0.55	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	8	0.30	0/556	0.55	0/749
1	8A	0.30	0/556	0.54	0/749
1	8B	0.30	0/556	0.56	0/749
1	8C	0.31	0/556	0.55	0/749
1	9	0.31	0/556	0.55	0/749
1	9A	0.30	0/556	0.55	0/749
1	9B	0.30	0/556	0.56	0/749
1	9C	0.31	0/556	0.55	0/749
1	A	0.30	0/556	0.59	1/749 (0.1%)
1	AA	0.31	0/556	0.55	0/749
1	AB	0.30	0/556	0.54	0/749
1	AC	0.30	0/556	0.56	0/749
1	AD	0.31	0/556	0.55	0/749
1	B	0.30	0/556	0.55	0/749
1	BA	0.31	0/556	0.56	0/749
1	BB	0.30	0/556	0.54	0/749
1	BC	0.30	0/556	0.55	0/749
1	BD	0.30	0/556	0.54	0/749
1	C	0.31	0/556	0.55	0/749
1	CA	0.31	0/556	0.56	0/749
1	CB	0.30	0/556	0.54	0/749
1	CC	0.30	0/556	0.56	0/749
1	CD	0.30	0/556	0.54	0/749
1	D	0.30	0/556	0.55	0/749
1	DA	0.31	0/556	0.56	0/749
1	DB	0.31	0/556	0.54	0/749
1	DC	0.30	0/556	0.56	0/749
1	DD	0.31	0/556	0.55	0/749
1	E	0.30	0/556	0.54	0/749
1	EA	0.31	0/556	0.55	0/749
1	EB	0.31	0/556	0.54	0/749
1	EC	0.30	0/556	0.56	0/749
1	ED	0.30	0/556	0.54	0/749
1	F	0.31	0/556	0.54	0/749
1	FA	0.31	0/556	0.56	0/749
1	FB	0.31	0/556	0.54	0/749
1	FC	0.30	0/556	0.56	0/749
1	FD	0.31	0/556	0.55	0/749
1	G	0.31	0/556	0.55	0/749
1	GA	0.31	0/556	0.55	0/749
1	GB	0.31	0/556	0.54	0/749
1	GC	0.31	0/556	0.56	0/749
1	GD	0.31	0/556	0.55	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.30	0/556	0.56	0/749
1	HA	0.31	0/556	0.55	0/749
1	HB	0.31	0/556	0.54	0/749
1	HC	0.30	0/556	0.55	0/749
1	HD	0.31	0/556	0.55	0/749
1	I	0.30	0/556	0.56	0/749
1	IA	0.31	0/556	0.55	0/749
1	IB	0.31	0/556	0.54	0/749
1	IC	0.30	0/556	0.55	0/749
1	ID	0.31	0/556	0.55	0/749
1	J	0.30	0/556	0.55	0/749
1	JA	0.31	0/556	0.55	0/749
1	JB	0.31	0/556	0.54	0/749
1	JC	0.31	0/556	0.56	0/749
1	JD	0.31	0/556	0.55	0/749
1	K	0.31	0/556	0.54	0/749
1	KA	0.31	0/556	0.55	0/749
1	KB	0.31	0/556	0.55	0/749
1	KC	0.30	0/556	0.55	0/749
1	KD	0.32	0/556	0.54	0/749
1	L	0.30	0/556	0.58	1/749 (0.1%)
1	LA	0.31	0/556	0.55	0/749
1	LB	0.31	0/556	0.54	0/749
1	LC	0.30	0/556	0.55	0/749
1	LD	0.31	0/556	0.55	0/749
1	M	0.30	0/556	0.54	0/749
1	MA	0.30	0/556	0.55	0/749
1	MB	0.31	0/556	0.54	0/749
1	MC	0.31	0/556	0.56	0/749
1	MD	0.30	0/556	0.54	0/749
1	N	0.30	0/556	0.57	0/749
1	NA	0.31	0/556	0.55	0/749
1	NB	0.31	0/556	0.54	0/749
1	NC	0.30	0/556	0.56	0/749
1	ND	0.31	0/556	0.54	0/749
1	O	0.30	0/556	0.54	0/749
1	OA	0.30	0/556	0.55	0/749
1	OB	0.31	0/556	0.54	0/749
1	OC	0.30	0/556	0.55	0/749
1	OD	0.31	0/556	0.55	0/749
1	P	0.30	0/556	0.58	1/749 (0.1%)
1	PA	0.31	0/556	0.55	0/749
1	PB	0.31	0/556	0.54	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	PC	0.30	0/556	0.55	0/749
1	PD	0.31	0/556	0.55	0/749
1	Q	0.30	0/556	0.57	0/749
1	QA	0.31	0/556	0.55	0/749
1	QB	0.31	0/556	0.54	0/749
1	QC	0.31	0/556	0.56	0/749
1	QD	0.31	0/556	0.54	0/749
1	R	0.30	0/556	0.58	1/749 (0.1%)
1	RA	0.31	0/556	0.55	0/749
1	RB	0.31	0/556	0.54	0/749
1	RC	0.30	0/556	0.55	0/749
1	S	0.31	0/556	0.58	1/749 (0.1%)
1	SA	0.30	0/556	0.55	0/749
1	SB	0.31	0/556	0.54	0/749
1	SC	0.30	0/556	0.56	0/749
1	T	0.30	0/556	0.58	1/749 (0.1%)
1	TA	0.30	0/556	0.55	0/749
1	TB	0.31	0/556	0.54	0/749
1	TC	0.30	0/556	0.56	0/749
1	U	0.30	0/556	0.54	0/749
1	UA	0.30	0/556	0.55	0/749
1	UB	0.31	0/556	0.54	0/749
1	UC	0.31	0/556	0.55	0/749
1	V	0.30	0/556	0.57	0/749
1	VA	0.30	0/556	0.55	0/749
1	VB	0.31	0/556	0.54	0/749
1	VC	0.31	0/556	0.56	0/749
1	W	0.30	0/556	0.58	1/749 (0.1%)
1	WA	0.30	0/556	0.55	0/749
1	WB	0.31	0/556	0.54	0/749
1	WC	0.30	0/556	0.55	0/749
1	XA	0.30	0/556	0.55	0/749
1	XB	0.31	0/556	0.54	0/749
1	XC	0.30	0/556	0.56	0/749
1	Y	0.30	0/556	0.58	1/749 (0.1%)
1	YA	0.30	0/556	0.55	0/749
1	YB	0.31	0/556	0.54	0/749
1	YC	0.30	0/556	0.56	0/749
1	Z	0.30	0/556	0.58	1/749 (0.1%)
1	ZA	0.30	0/556	0.55	0/749
1	ZB	0.31	0/556	0.54	0/749
1	ZC	0.30	0/556	0.55	0/749
1	a	0.30	0/556	0.59	1/749 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	aA	0.30	0/556	0.55	0/749
1	aB	0.31	0/556	0.54	0/749
1	aC	0.30	0/556	0.55	0/749
1	b	0.30	0/556	0.58	1/749 (0.1%)
1	bA	0.30	0/556	0.55	0/749
1	bB	0.30	0/556	0.55	0/749
1	bC	0.30	0/556	0.56	0/749
1	c	0.30	0/556	0.54	0/749
1	cA	0.30	0/556	0.55	0/749
1	cB	0.31	0/556	0.55	0/749
1	cC	0.30	0/556	0.55	0/749
1	d	0.30	0/556	0.54	0/749
1	dA	0.30	0/556	0.55	0/749
1	dB	0.31	0/556	0.55	0/749
1	dC	0.30	0/556	0.56	0/749
1	e	0.30	0/556	0.54	0/749
1	eA	0.30	0/556	0.55	0/749
1	eB	0.31	0/556	0.55	0/749
1	eC	0.30	0/556	0.56	0/749
1	f	0.30	0/556	0.59	1/749 (0.1%)
1	fA	0.30	0/556	0.55	0/749
1	fB	0.31	0/556	0.55	0/749
1	fC	0.30	0/556	0.56	0/749
1	g	0.30	0/556	0.54	0/749
1	gA	0.30	0/556	0.55	0/749
1	gB	0.31	0/556	0.55	0/749
1	gC	0.31	0/556	0.56	0/749
1	h	0.30	0/556	0.54	0/749
1	hA	0.30	0/556	0.55	0/749
1	hB	0.30	0/556	0.55	0/749
1	hC	0.30	0/556	0.54	0/749
1	i	0.30	0/556	0.59	1/749 (0.1%)
1	iA	0.30	0/556	0.55	0/749
1	iB	0.31	0/556	0.55	0/749
1	iC	0.30	0/556	0.55	0/749
1	j	0.30	0/556	0.56	0/749
1	jA	0.30	0/556	0.55	0/749
1	jB	0.31	0/556	0.54	0/749
1	jC	0.30	0/556	0.54	0/749
1	k	0.30	0/556	0.55	0/749
1	kA	0.30	0/556	0.55	0/749
1	kB	0.31	0/556	0.55	0/749
1	kC	0.30	0/556	0.54	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l	0.30	0/556	0.56	0/749
1	lA	0.30	0/556	0.55	0/749
1	lB	0.31	0/556	0.55	0/749
1	lC	0.30	0/556	0.54	0/749
1	m	0.30	0/556	0.55	0/749
1	mA	0.30	0/556	0.55	0/749
1	mB	0.31	0/556	0.55	0/749
1	mC	0.30	0/556	0.54	0/749
1	n	0.30	0/556	0.56	0/749
1	nA	0.30	0/556	0.55	0/749
1	nB	0.31	0/556	0.55	0/749
1	nC	0.30	0/556	0.54	0/749
1	o	0.30	0/556	0.56	0/749
1	oA	0.30	0/556	0.55	0/749
1	oB	0.31	0/556	0.55	0/749
1	oC	0.30	0/556	0.55	0/749
1	p	0.30	0/556	0.55	0/749
1	pA	0.30	0/556	0.55	0/749
1	pB	0.31	0/556	0.55	0/749
1	pC	0.30	0/556	0.54	0/749
1	q	0.30	0/556	0.55	0/749
1	qA	0.30	0/556	0.54	0/749
1	qB	0.30	0/556	0.55	0/749
1	qC	0.30	0/556	0.55	0/749
1	r	0.30	0/556	0.56	0/749
1	rA	0.30	0/556	0.54	0/749
1	rB	0.31	0/556	0.55	0/749
1	rC	0.30	0/556	0.54	0/749
1	s	0.31	0/556	0.55	0/749
1	sA	0.30	0/556	0.54	0/749
1	sB	0.31	0/556	0.55	0/749
1	sC	0.30	0/556	0.54	0/749
1	t	0.30	0/556	0.55	0/749
1	tA	0.30	0/556	0.54	0/749
1	tB	0.30	0/556	0.55	0/749
1	tC	0.30	0/556	0.54	0/749
1	u	0.30	0/556	0.55	0/749
1	uA	0.31	0/556	0.55	0/749
1	uB	0.31	0/556	0.55	0/749
1	uC	0.30	0/556	0.54	0/749
1	v	0.31	0/556	0.56	0/749
1	vA	0.30	0/556	0.54	0/749
1	vB	0.31	0/556	0.55	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	vC	0.30	0/556	0.53	0/749
1	w	0.31	0/556	0.55	0/749
1	wA	0.30	0/556	0.54	0/749
1	wB	0.31	0/556	0.54	0/749
1	wC	0.30	0/556	0.54	0/749
1	x	0.30	0/556	0.55	0/749
1	xA	0.31	0/556	0.55	0/749
1	xB	0.30	0/556	0.55	0/749
1	xC	0.30	0/556	0.55	0/749
1	y	0.31	0/556	0.56	0/749
1	yA	0.31	0/556	0.55	0/749
1	yB	0.30	0/556	0.56	0/749
1	yC	0.30	0/556	0.54	0/749
1	z	0.30	0/556	0.55	0/749
1	zA	0.30	0/556	0.54	0/749
1	zB	0.30	0/556	0.55	0/749
1	zC	0.30	0/556	0.54	0/749
All	All	0.30	0/146784	0.55	13/197736 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	Z	27	ASP	CB-CG-OD1	5.68	123.41	118.30
1	f	27	ASP	CB-CG-OD1	5.67	123.40	118.30
1	i	27	ASP	CB-CG-OD1	5.65	123.39	118.30
1	a	27	ASP	CB-CG-OD1	5.64	123.38	118.30
1	T	27	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	27	ASP	CB-CG-OD1	5.63	123.36	118.30
1	S	27	ASP	CB-CG-OD1	5.59	123.33	118.30
1	Y	27	ASP	CB-CG-OD1	5.59	123.33	118.30
1	P	27	ASP	CB-CG-OD1	5.57	123.31	118.30
1	L	27	ASP	CB-CG-OD1	5.57	123.31	118.30
1	b	27	ASP	CB-CG-OD1	5.56	123.31	118.30
1	W	27	ASP	CB-CG-OD1	5.55	123.29	118.30
1	R	27	ASP	CB-CG-OD1	5.45	123.21	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	0A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	0B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	0C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	1	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	1A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	1B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	1C	68/74 (92%)	68 (100%)	0	0	100	100
1	2	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	2A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	2B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	2C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	3	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	3A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	3B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	3C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	4	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	4A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	4B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	4C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	5	68/74 (92%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	5B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	5C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	6	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	6A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	6B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	6C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	7	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	7A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	7B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	7C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	8	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	8A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	8B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	8C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	9	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	9A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	9B	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	9C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	A	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	AA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	AB	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	AC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	AD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	BA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	BB	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	BC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	BD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	C	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	CA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CB	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	CC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	CD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	D	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	DA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	DB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	DC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	DD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	E	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	EA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	EB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	EC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ED	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	F	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	FA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	FB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	FC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	FD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	G	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	GA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	GB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	GC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	GD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	H	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	HA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	HB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	HC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	HD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	I	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	IA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	IB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ID	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	J	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	JA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	JB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	JC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	JD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	K	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	KA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	KB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	KC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	KD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	L	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	M	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	MA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	MB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	MC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	MD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	N	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	NA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	NB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	NC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ND	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	O	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	OA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	OB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	OC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	P	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	PA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	PB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	PC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	PD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	Q	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	QA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	QB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	QC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	QD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	R	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	RA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	RB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	RC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	S	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	SA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	SB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	SC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	T	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	TA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	TB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	TC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	U	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	UA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	UB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	UC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	V	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	VA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	VB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	VC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	WA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	WB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	WC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	XA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	XB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	XC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	Y	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	YA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	YB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	YC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	Z	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ZA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	ZB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ZC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	a	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	aA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	aB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	aC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	b	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	bA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	bB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	bC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	c	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	cA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	cB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	cC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	d	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	dA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	dB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	dC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	eA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	eB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	eC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	f	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	fA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	fB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	fC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	g	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	gA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	gB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	gC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	h	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	hA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	hB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	hC	68/74 (92%)	68 (100%)	0	0	100	100
1	i	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	iA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	iB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	iC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	j	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	jA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	jB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	jC	68/74 (92%)	68 (100%)	0	0	100	100
1	k	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	kA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	kB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	kC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	l	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	lA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	lB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	lC	68/74 (92%)	68 (100%)	0	0	100	100
1	m	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	mA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	mB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	mC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	n	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	nA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	nB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	nC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	o	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	oA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	oB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	oC	68/74 (92%)	68 (100%)	0	0	100	100
1	p	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	pA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	pB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	pC	68/74 (92%)	68 (100%)	0	0	100	100
1	q	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	qA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	qB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	qC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	r	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	rA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	rB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	rC	68/74 (92%)	68 (100%)	0	0	100	100
1	s	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	sA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	sB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	sC	68/74 (92%)	68 (100%)	0	0	100	100
1	t	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	tA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	tB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	tC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	u	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	uA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	uB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	uC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	v	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	vA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	vB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	vC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	w	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	wA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	wB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	wC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	x	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	xA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	xB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	xC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	y	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	yA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	yB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	yC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	z	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	zA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	zB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	zC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
All	All	17952/19536 (92%)	17507 (98%)	445 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	58/62 (94%)	58 (100%)	0	100	100
1	0A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	0B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	0C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	1	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	1A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	1B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	1C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	2	58/62 (94%)	58 (100%)	0	100	100
1	2A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	2B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	2C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	3	58/62 (94%)	58 (100%)	0	100	100
1	3A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	3B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	3C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	4	58/62 (94%)	58 (100%)	0	100	100
1	4A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	4B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	4C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	5	58/62 (94%)	58 (100%)	0	100	100
1	5A	58/62 (94%)	58 (100%)	0	100	100
1	5B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	5C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	6	58/62 (94%)	58 (100%)	0	100	100
1	6A	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	6C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	7	58/62 (94%)	58 (100%)	0	100	100
1	7A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	7B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	7C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	8	58/62 (94%)	58 (100%)	0	100	100
1	8A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	8B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	8C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	9	58/62 (94%)	58 (100%)	0	100	100
1	9A	58/62 (94%)	58 (100%)	0	100	100
1	9B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	9C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	A	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	AA	58/62 (94%)	58 (100%)	0	100	100
1	AB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	AC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	AD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	B	58/62 (94%)	58 (100%)	0	100	100
1	BA	58/62 (94%)	58 (100%)	0	100	100
1	BB	58/62 (94%)	58 (100%)	0	100	100
1	BC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	BD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	C	58/62 (94%)	58 (100%)	0	100	100
1	CA	58/62 (94%)	58 (100%)	0	100	100
1	CB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	CC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	CD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	D	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	DA	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	DC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	DD	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	E	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	EA	58/62 (94%)	58 (100%)	0	100	100
1	EB	58/62 (94%)	58 (100%)	0	100	100
1	EC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	ED	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	F	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	FA	58/62 (94%)	58 (100%)	0	100	100
1	FB	58/62 (94%)	58 (100%)	0	100	100
1	FC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	FD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	G	58/62 (94%)	58 (100%)	0	100	100
1	GA	58/62 (94%)	58 (100%)	0	100	100
1	GB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	GC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	GD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	H	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	HA	58/62 (94%)	58 (100%)	0	100	100
1	HB	58/62 (94%)	58 (100%)	0	100	100
1	HC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	HD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	I	58/62 (94%)	58 (100%)	0	100	100
1	IA	58/62 (94%)	58 (100%)	0	100	100
1	IB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	IC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	ID	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	J	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	JA	58/62 (94%)	58 (100%)	0	100	100
1	JB	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	JD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	K	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	KA	58/62 (94%)	58 (100%)	0	100	100
1	KB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	KC	58/62 (94%)	58 (100%)	0	100	100
1	KD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	L	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	LA	58/62 (94%)	58 (100%)	0	100	100
1	LB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	LC	58/62 (94%)	58 (100%)	0	100	100
1	LD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	M	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	MA	58/62 (94%)	58 (100%)	0	100	100
1	MB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	MC	58/62 (94%)	58 (100%)	0	100	100
1	MD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	N	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	NA	58/62 (94%)	58 (100%)	0	100	100
1	NB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	NC	58/62 (94%)	58 (100%)	0	100	100
1	ND	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	O	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	OA	58/62 (94%)	58 (100%)	0	100	100
1	OB	58/62 (94%)	58 (100%)	0	100	100
1	OC	58/62 (94%)	58 (100%)	0	100	100
1	OD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	P	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	PA	58/62 (94%)	58 (100%)	0	100	100
1	PB	58/62 (94%)	58 (100%)	0	100	100
1	PC	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	Q	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	QA	58/62 (94%)	58 (100%)	0	100	100
1	QB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	QC	58/62 (94%)	58 (100%)	0	100	100
1	QD	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	R	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	RA	58/62 (94%)	58 (100%)	0	100	100
1	RB	58/62 (94%)	58 (100%)	0	100	100
1	RC	58/62 (94%)	58 (100%)	0	100	100
1	S	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	SA	58/62 (94%)	58 (100%)	0	100	100
1	SB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	SC	58/62 (94%)	58 (100%)	0	100	100
1	T	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	TA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	TB	58/62 (94%)	58 (100%)	0	100	100
1	TC	58/62 (94%)	58 (100%)	0	100	100
1	U	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	UA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	UB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	UC	58/62 (94%)	58 (100%)	0	100	100
1	V	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	VA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	VB	58/62 (94%)	58 (100%)	0	100	100
1	VC	58/62 (94%)	58 (100%)	0	100	100
1	W	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	WA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	WB	58/62 (94%)	58 (100%)	0	100	100
1	WC	58/62 (94%)	58 (100%)	0	100	100
1	XA	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XB	58/62 (94%)	58 (100%)	0	100	100
1	XC	58/62 (94%)	58 (100%)	0	100	100
1	Y	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	YA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	YB	58/62 (94%)	58 (100%)	0	100	100
1	YC	58/62 (94%)	58 (100%)	0	100	100
1	Z	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	ZA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	ZB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	ZC	58/62 (94%)	58 (100%)	0	100	100
1	a	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	aA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	aB	58/62 (94%)	58 (100%)	0	100	100
1	aC	58/62 (94%)	58 (100%)	0	100	100
1	b	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	bA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	bB	58/62 (94%)	58 (100%)	0	100	100
1	bC	58/62 (94%)	58 (100%)	0	100	100
1	c	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	cA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	cB	58/62 (94%)	58 (100%)	0	100	100
1	cC	58/62 (94%)	58 (100%)	0	100	100
1	d	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	dA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	dB	58/62 (94%)	58 (100%)	0	100	100
1	dC	58/62 (94%)	58 (100%)	0	100	100
1	e	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	eA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	eB	58/62 (94%)	58 (100%)	0	100	100
1	eC	58/62 (94%)	58 (100%)	0	100	100
1	f	58/62 (94%)	56 (97%)	2 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	fA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	fB	58/62 (94%)	58 (100%)	0	100	100
1	fC	58/62 (94%)	58 (100%)	0	100	100
1	g	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	gA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	gB	58/62 (94%)	58 (100%)	0	100	100
1	gC	58/62 (94%)	58 (100%)	0	100	100
1	h	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	hA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	hB	58/62 (94%)	58 (100%)	0	100	100
1	hC	58/62 (94%)	58 (100%)	0	100	100
1	i	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	iA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	iB	58/62 (94%)	58 (100%)	0	100	100
1	iC	58/62 (94%)	58 (100%)	0	100	100
1	j	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	jA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	jB	58/62 (94%)	58 (100%)	0	100	100
1	jC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	k	58/62 (94%)	58 (100%)	0	100	100
1	kA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	kB	58/62 (94%)	58 (100%)	0	100	100
1	kC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	l	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	lA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	lB	58/62 (94%)	58 (100%)	0	100	100
1	lC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	m	58/62 (94%)	58 (100%)	0	100	100
1	mA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	mB	58/62 (94%)	58 (100%)	0	100	100
1	mC	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	nA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	nB	58/62 (94%)	58 (100%)	0	100	100
1	nC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	o	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	oA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	oB	58/62 (94%)	58 (100%)	0	100	100
1	oC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	p	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	pA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	pB	58/62 (94%)	58 (100%)	0	100	100
1	pC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	q	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	qA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	qB	58/62 (94%)	58 (100%)	0	100	100
1	qC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	r	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	rA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	rB	58/62 (94%)	58 (100%)	0	100	100
1	rC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	s	58/62 (94%)	58 (100%)	0	100	100
1	sA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	sB	58/62 (94%)	58 (100%)	0	100	100
1	sC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	t	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	tA	58/62 (94%)	58 (100%)	0	100	100
1	tB	58/62 (94%)	58 (100%)	0	100	100
1	tC	58/62 (94%)	58 (100%)	0	100	100
1	u	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	uA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	uB	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	uC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	v	58/62 (94%)	58 (100%)	0	100	100
1	vA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	vB	58/62 (94%)	58 (100%)	0	100	100
1	vC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	w	58/62 (94%)	58 (100%)	0	100	100
1	wA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	wB	58/62 (94%)	58 (100%)	0	100	100
1	wC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	x	58/62 (94%)	58 (100%)	0	100	100
1	xA	58/62 (94%)	58 (100%)	0	100	100
1	xB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	xC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	y	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	yA	58/62 (94%)	58 (100%)	0	100	100
1	yB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	yC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	z	58/62 (94%)	58 (100%)	0	100	100
1	zA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	zB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	zC	58/62 (94%)	57 (98%)	1 (2%)	56	78
All	All	15312/16368 (94%)	15143 (99%)	169 (1%)	69	85

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	31	HIS
1	L	31	HIS
1	M	31	HIS
1	N	31	HIS
1	O	31	HIS
1	P	31	HIS
1	Q	31	HIS
1	R	31	HIS

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Mol	Chain	Res	Type
1	S	31	HIS
1	T	31	HIS
1	U	31	HIS
1	V	31	HIS
1	W	31	HIS
1	Y	27	ASP
1	Y	31	HIS
1	Z	27	ASP
1	Z	31	HIS
1	a	27	ASP
1	a	31	HIS
1	b	31	HIS
1	c	31	HIS
1	d	31	HIS
1	e	31	HIS
1	f	27	ASP
1	f	31	HIS
1	g	31	HIS
1	h	31	HIS
1	i	27	ASP
1	i	31	HIS
1	j	29	ARG
1	l	29	ARG
1	n	29	ARG
1	o	29	ARG
1	p	29	ARG
1	q	29	ARG
1	r	29	ARG
1	t	29	ARG
1	u	29	ARG
1	y	29	ARG
1	1	29	ARG
1	D	37	ASP
1	TA	37	ASP
1	UA	37	ASP
1	VA	37	ASP
1	WA	37	ASP
1	XA	37	ASP
1	YA	37	ASP
1	ZA	37	ASP
1	aA	37	ASP
1	bA	37	ASP

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Mol	Chain	Res	Type
1	cA	37	ASP
1	dA	37	ASP
1	eA	37	ASP
1	fA	37	ASP
1	gA	37	ASP
1	hA	37	ASP
1	iA	37	ASP
1	jA	37	ASP
1	kA	37	ASP
1	lA	37	ASP
1	mA	37	ASP
1	nA	37	ASP
1	oA	37	ASP
1	pA	37	ASP
1	E	15	ASP
1	qA	37	ASP
1	rA	37	ASP
1	sA	37	ASP
1	uA	15	ASP
1	vA	37	ASP
1	wA	15	ASP
1	zA	37	ASP
1	0A	37	ASP
1	1A	15	ASP
1	2A	15	ASP
1	3A	15	ASP
1	4A	37	ASP
1	6A	37	ASP
1	7A	37	ASP
1	8A	15	ASP
1	AB	15	ASP
1	CB	37	ASP
1	F	31	HIS
1	DB	31	HIS
1	GB	37	ASP
1	IB	37	ASP
1	JB	37	ASP
1	KB	31	HIS
1	LB	31	HIS
1	MB	31	HIS
1	NB	37	ASP
1	QB	37	ASP

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Mol	Chain	Res	Type
1	SB	37	ASP
1	UB	37	ASP
1	ZB	31	HIS
1	ZB	37	ASP
1	H	64	ARG
1	xB	64	ARG
1	yB	64	ARG
1	zB	64	ARG
1	0B	64	ARG
1	1B	64	ARG
1	2B	64	ARG
1	3B	64	ARG
1	4B	64	ARG
1	5B	64	ARG
1	6B	64	ARG
1	7B	64	ARG
1	8B	64	ARG
1	9B	64	ARG
1	AC	64	ARG
1	BC	64	ARG
1	CC	64	ARG
1	DC	64	ARG
1	EC	64	ARG
1	FC	64	ARG
1	GC	64	ARG
1	HC	64	ARG
1	IC	64	ARG
1	JC	64	ARG
1	J	37	ASP
1	jC	37	ASP
1	kC	37	ASP
1	lC	37	ASP
1	mC	37	ASP
1	nC	37	ASP
1	oC	37	ASP
1	pC	37	ASP
1	qC	37	ASP
1	rC	37	ASP
1	sC	37	ASP
1	uC	37	ASP
1	vC	37	ASP
1	wC	37	ASP

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Mol	Chain	Res	Type
1	xC	37	ASP
1	yC	37	ASP
1	zC	37	ASP
1	0C	37	ASP
1	1C	37	ASP
1	2C	37	ASP
1	3C	37	ASP
1	K	37	ASP
1	4C	37	ASP
1	5C	37	ASP
1	6C	37	ASP
1	7C	37	ASP
1	8C	37	ASP
1	9C	37	ASP
1	AD	37	ASP
1	BD	37	ASP
1	CD	37	ASP
1	DD	37	ASP
1	DD	40	GLU
1	ED	37	ASP
1	FD	37	ASP
1	GD	37	ASP
1	HD	37	ASP
1	ID	37	ASP
1	JD	37	ASP
1	KD	37	ASP
1	LD	37	ASP
1	MD	37	ASP
1	ND	37	ASP
1	ND	40	GLU
1	OD	37	ASP
1	PD	37	ASP
1	QD	37	ASP
1	QD	40	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	L	31	HIS
1	M	31	HIS
1	N	31	HIS

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Mol	Chain	Res	Type
1	O	31	HIS
1	P	31	HIS
1	Q	31	HIS
1	R	31	HIS
1	S	31	HIS
1	T	31	HIS
1	U	31	HIS
1	V	31	HIS
1	W	31	HIS
1	Y	31	HIS
1	Z	31	HIS
1	a	31	HIS
1	b	31	HIS
1	c	31	HIS
1	d	31	HIS
1	e	31	HIS
1	f	31	HIS
1	g	31	HIS
1	h	31	HIS
1	i	31	HIS
1	D	31	HIS
1	TA	31	HIS
1	UA	31	HIS
1	VA	31	HIS
1	WA	31	HIS
1	XA	4	ASN
1	XA	31	HIS
1	YA	4	ASN
1	YA	31	HIS
1	ZA	31	HIS
1	aA	31	HIS
1	bA	31	HIS
1	cA	31	HIS
1	dA	31	HIS
1	eA	31	HIS
1	fA	4	ASN
1	fA	31	HIS
1	gA	31	HIS
1	hA	31	HIS
1	iA	31	HIS
1	jA	4	ASN
1	jA	31	HIS

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Mol	Chain	Res	Type
1	kA	31	HIS
1	lA	31	HIS
1	mA	31	HIS
1	nA	31	HIS
1	oA	31	HIS
1	pA	31	HIS
1	rA	31	HIS
1	sA	31	HIS
1	zA	31	HIS
1	0A	31	HIS
1	2A	31	HIS
1	5A	31	HIS
1	6A	31	HIS
1	7A	31	HIS
1	8A	31	HIS
1	AB	31	HIS
1	CB	31	HIS
1	F	31	HIS
1	DB	31	HIS
1	EB	31	HIS
1	FB	31	HIS
1	GB	31	HIS
1	HB	31	HIS
1	IB	31	HIS
1	JB	31	HIS
1	KB	31	HIS
1	LB	31	HIS
1	MB	31	HIS
1	NB	31	HIS
1	OB	31	HIS
1	PB	31	HIS
1	QB	31	HIS
1	RB	31	HIS
1	SB	31	HIS
1	TB	31	HIS
1	UB	31	HIS
1	VB	31	HIS
1	WB	31	HIS
1	XB	31	HIS
1	YB	31	HIS
1	ZB	31	HIS
1	fB	32	HIS

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Mol	Chain	Res	Type
1	uB	4	ASN
1	oC	31	HIS
1	rC	31	HIS
1	wC	31	HIS
1	3C	31	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.