



Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 02:41 pm 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:

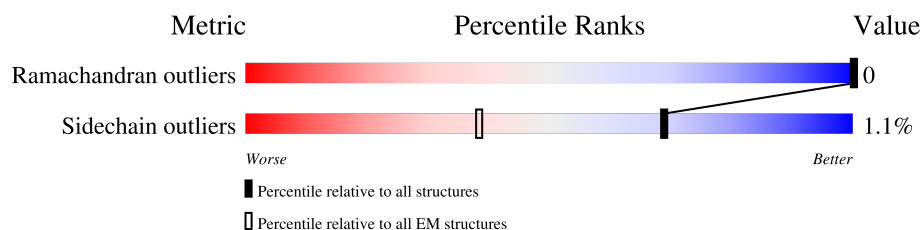
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.5

1 Overall quality at a glance

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

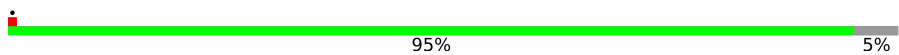
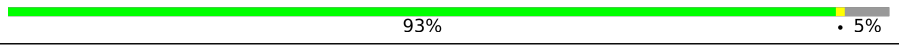
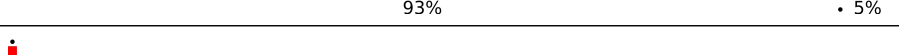
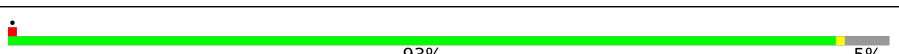
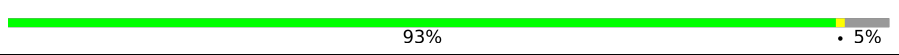
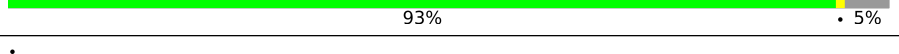
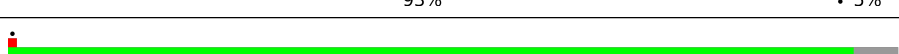


The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



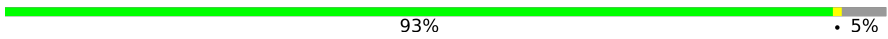
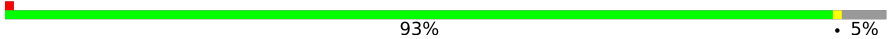
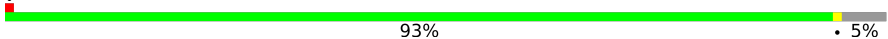
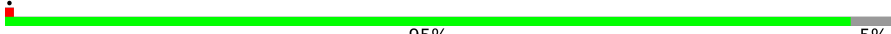


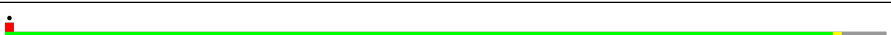
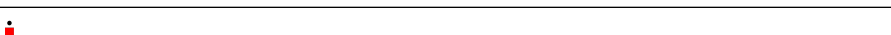
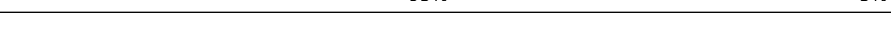
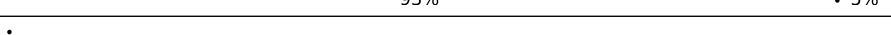
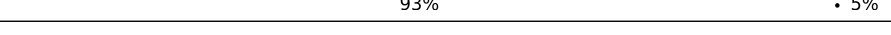
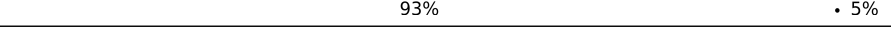

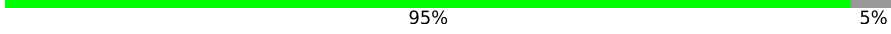
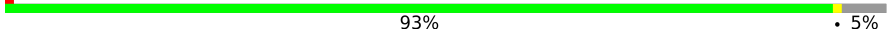
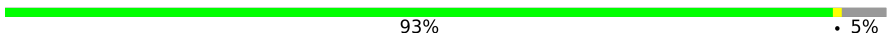
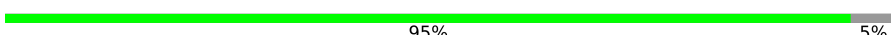
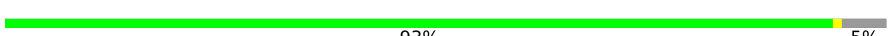





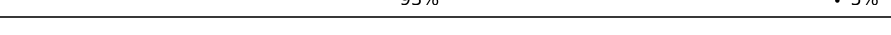
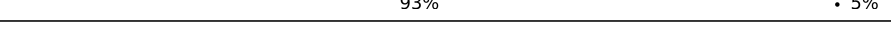
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	74	
1	0A	74	
1	0B	74	
1	0C	74	
1	1	74	
1	1A	74	
1	1B	74	
1	1C	74	
1	2	74	

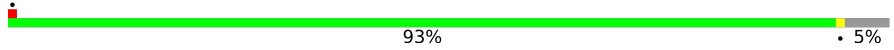
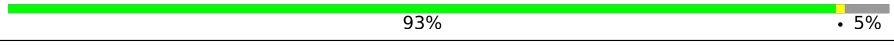
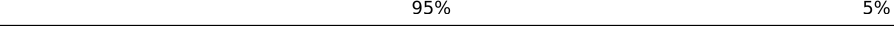
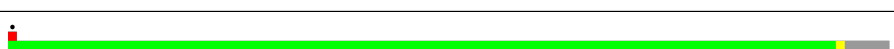

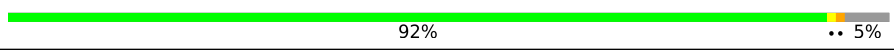
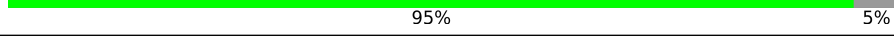
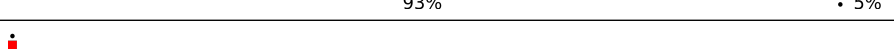
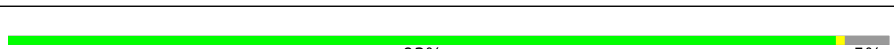
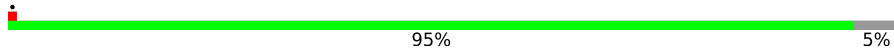
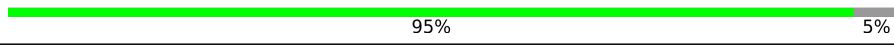
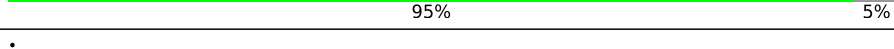
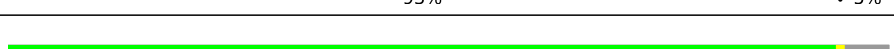
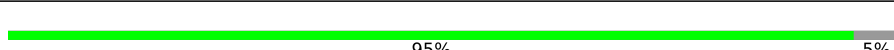
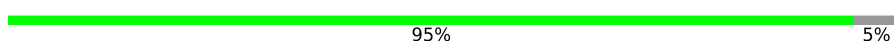
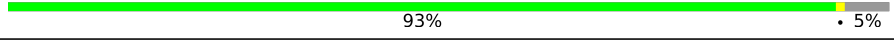
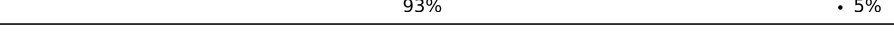

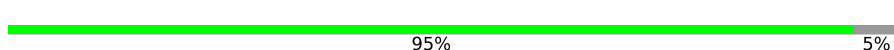
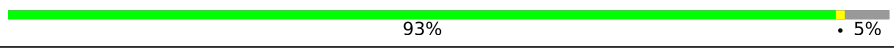
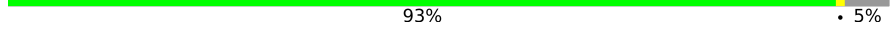



Continued on next page...

Continued from previous page...

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


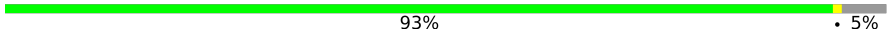
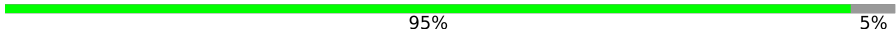
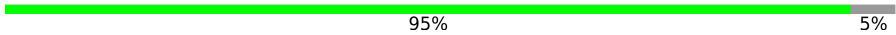
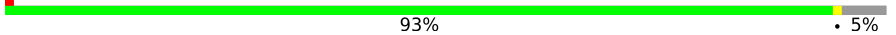
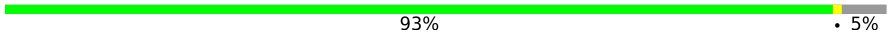
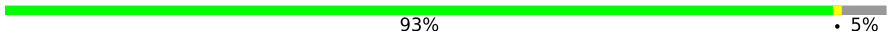
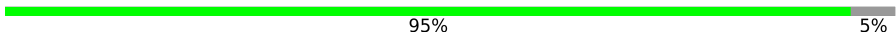
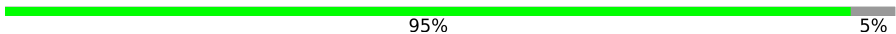
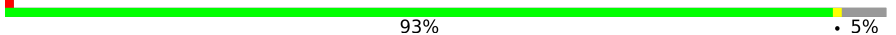

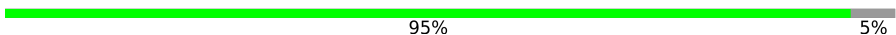
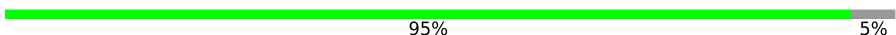



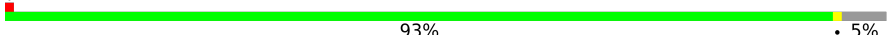
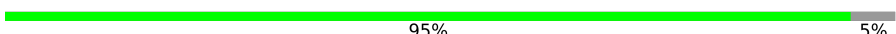
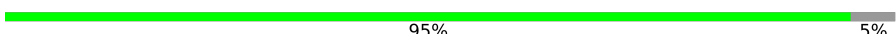
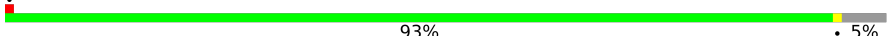
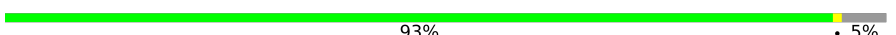
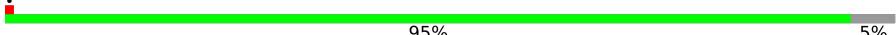
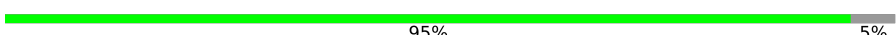


Continued on next page...

Continued from previous page...

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

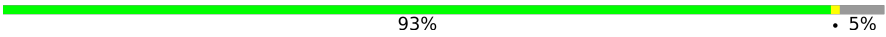
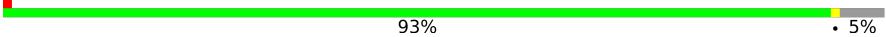
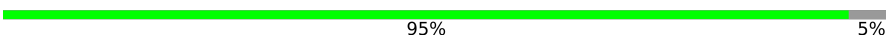
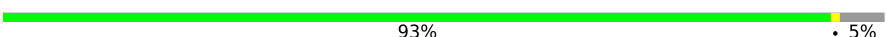
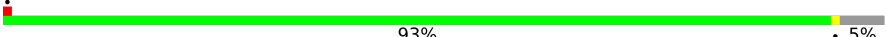
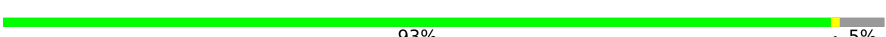
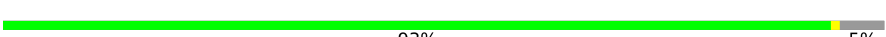



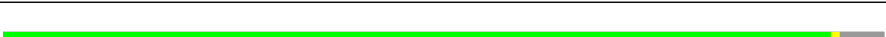


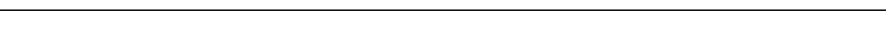
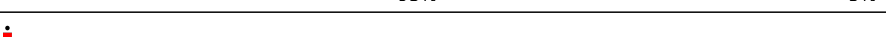
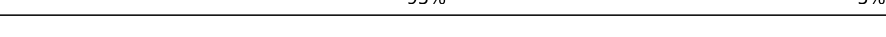
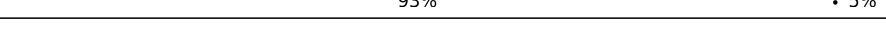
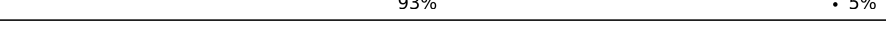
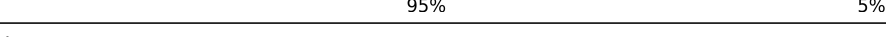
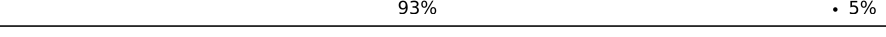
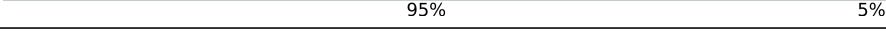
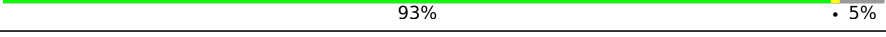
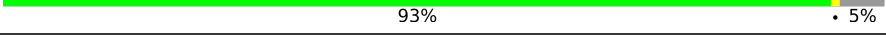
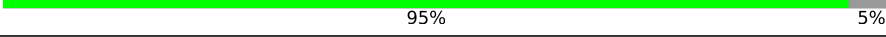
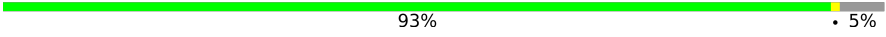
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DD	74	 92% • 5%
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%


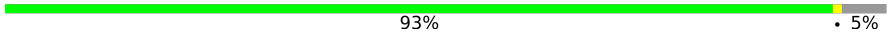
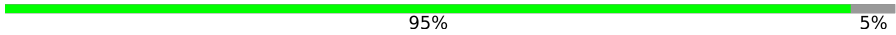
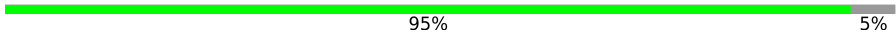
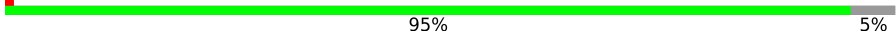
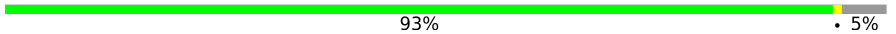

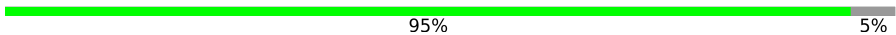
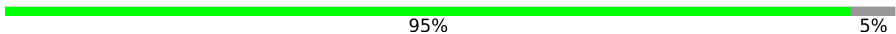
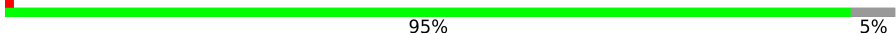


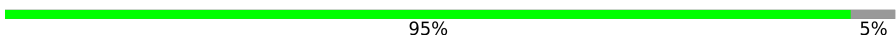

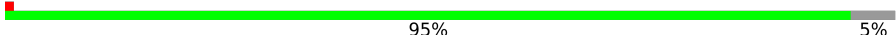

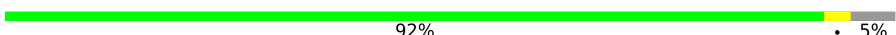
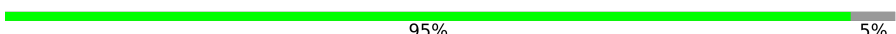
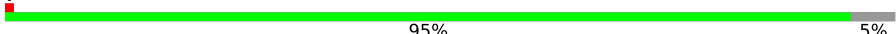
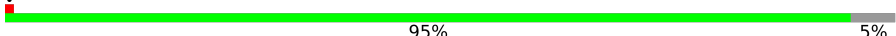

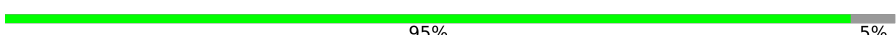
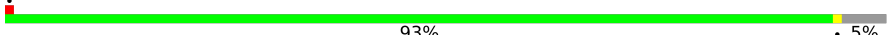
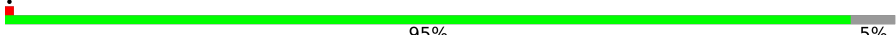

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	ID	74	 93% 5%
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%

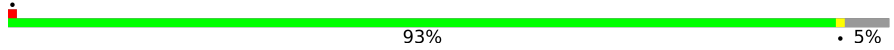
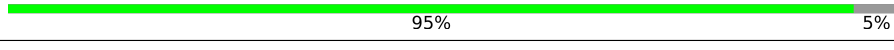
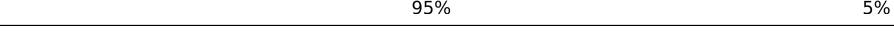
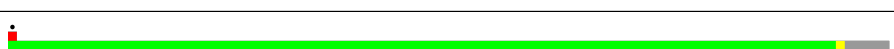

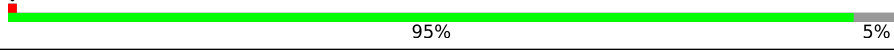
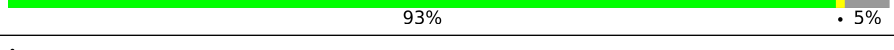
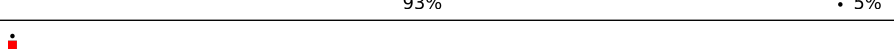
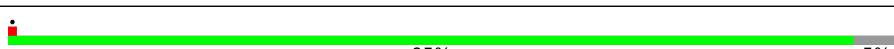
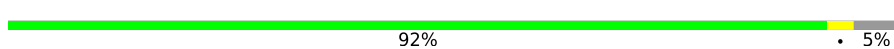
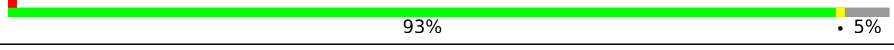
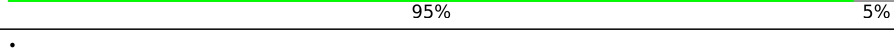
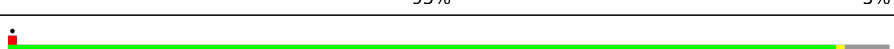
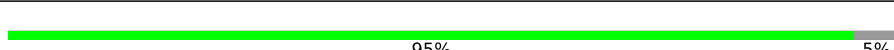
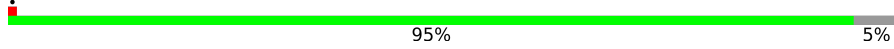
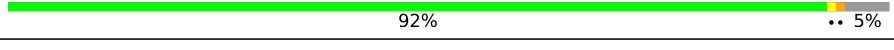
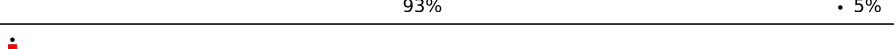

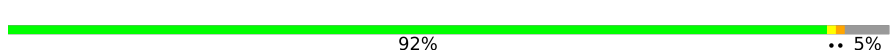
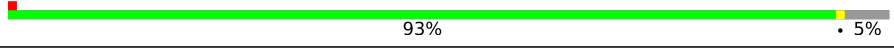
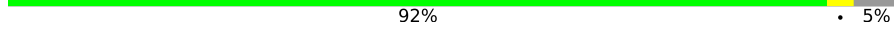



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	ND	74	 92% • 5%
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%

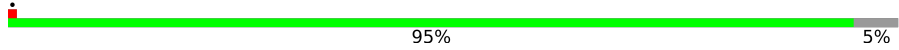
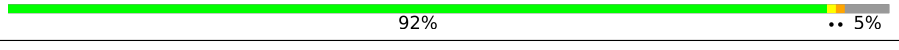
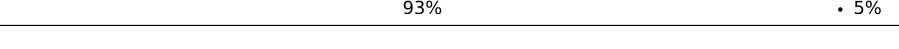
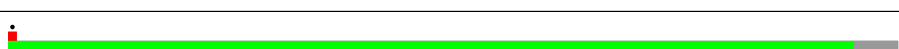

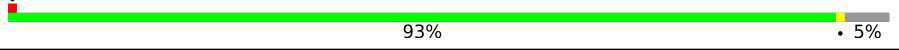
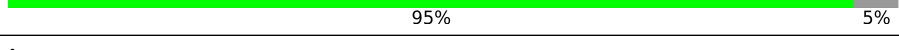
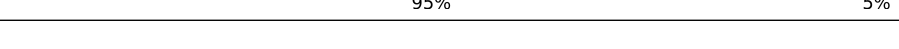

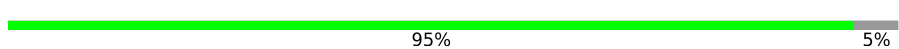
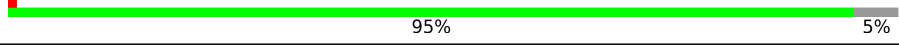
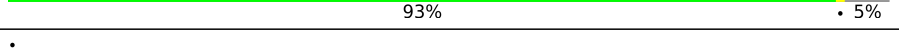
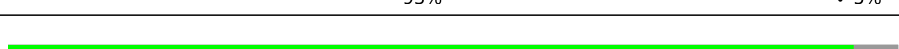
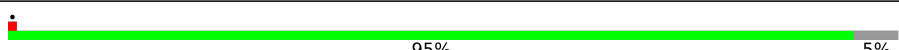
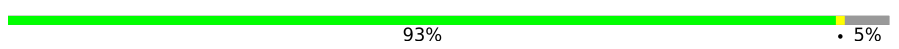
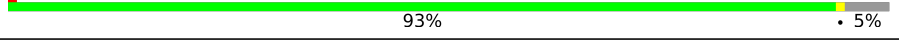
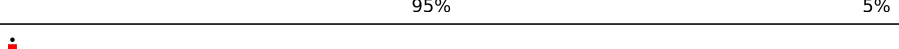

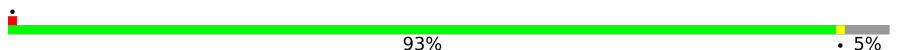
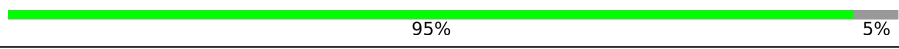
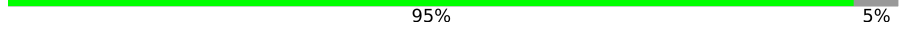



Continued on next page...

Continued from previous page...

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

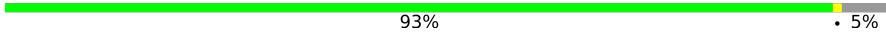
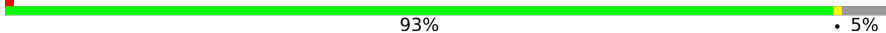
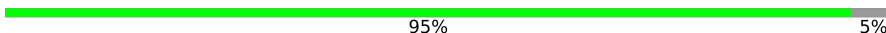
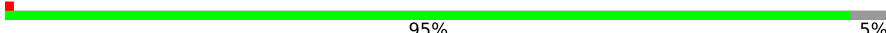

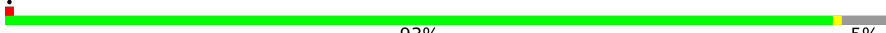
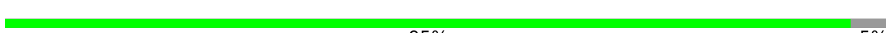








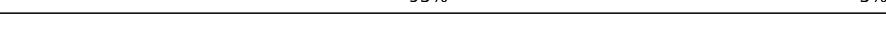
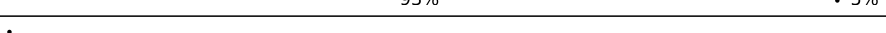
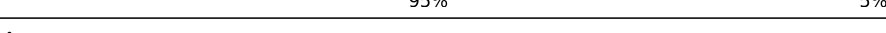
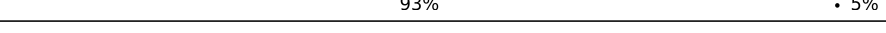
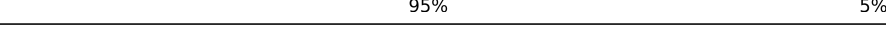
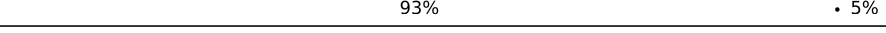
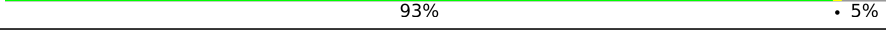
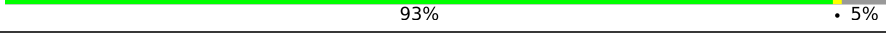
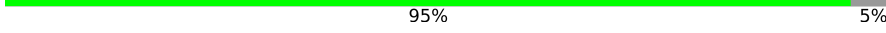
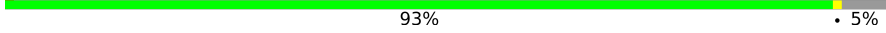
Continued on next page...

Continued from previous page...

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

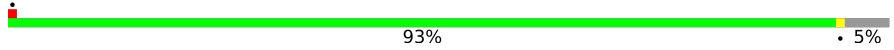
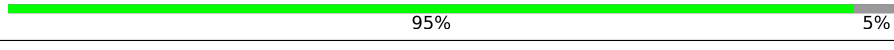
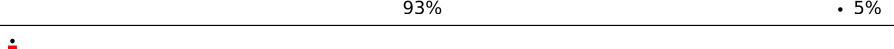
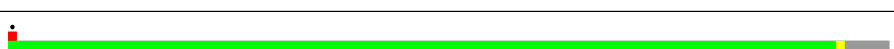
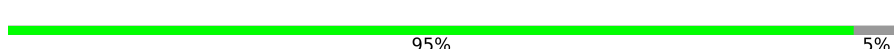
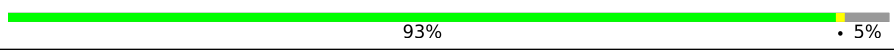
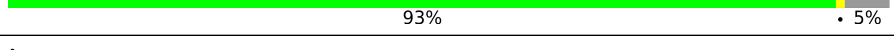
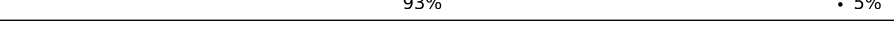
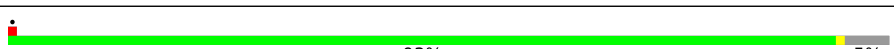
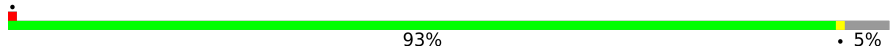
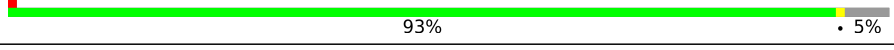
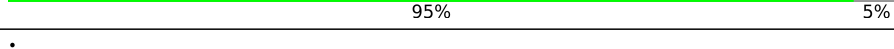
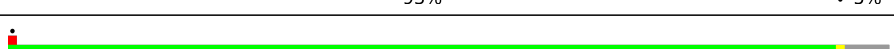
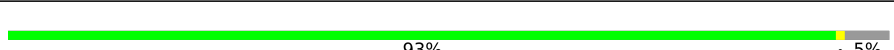
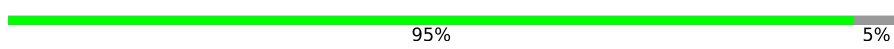
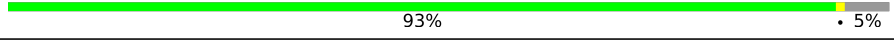
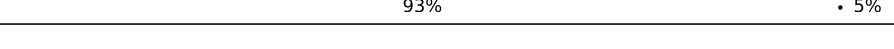

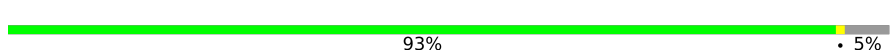
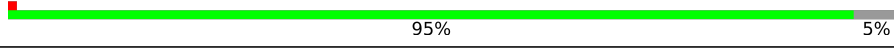
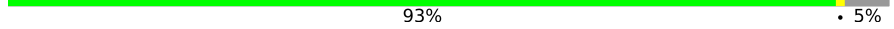



Continued on next page...

Continued from previous page...

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

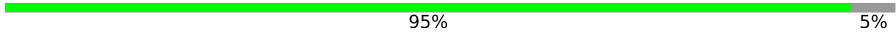
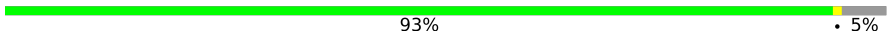
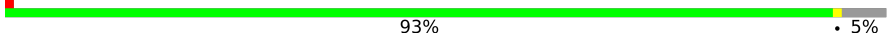
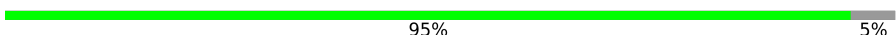
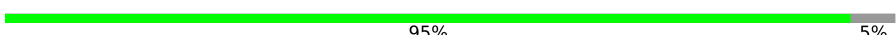
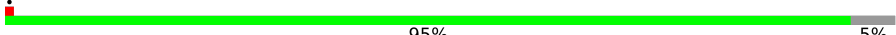





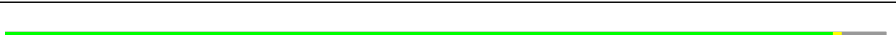

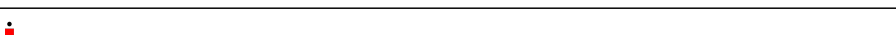
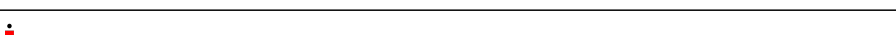
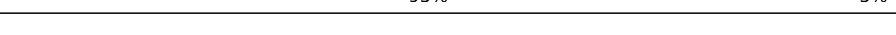
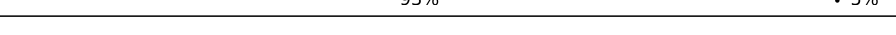
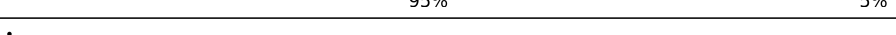
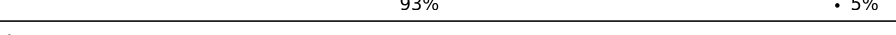
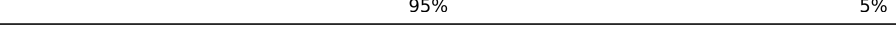
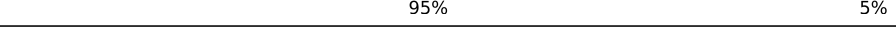
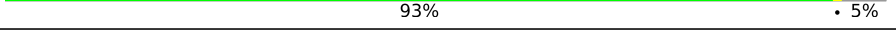
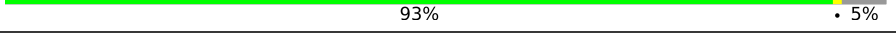
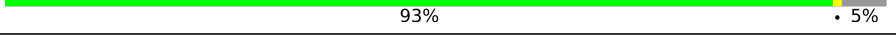
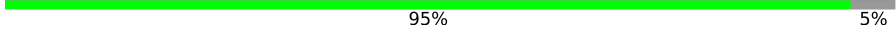
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	yC	74	<div><div></div><div>93%</div><div>• 5%</div></div>
1	z	74	<div><div></div><div>95%</div><div>5%</div></div>
1	zA	74	<div><div></div><div>93%</div><div>• 5%</div></div>
1	zB	74	<div><div></div><div>93%</div><div>• 5%</div></div>
1	zC	74	<div><div></div><div>93%</div><div>• 5%</div></div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
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	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	D	70	Total 547	C 341	N 102	O 104	0	0
1	TA	70	Total 547	C 341	N 102	O 104	0	0
1	UA	70	Total 547	C 341	N 102	O 104	0	0
1	VA	70	Total 547	C 341	N 102	O 104	0	0
1	WA	70	Total 547	C 341	N 102	O 104	0	0
1	XA	70	Total 547	C 341	N 102	O 104	0	0
1	YA	70	Total 547	C 341	N 102	O 104	0	0
1	ZA	70	Total 547	C 341	N 102	O 104	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
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	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	I	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
1	RC	70	Total 547	C 341	N 102	O 104	0	0
1	SC	70	Total 547	C 341	N 102	O 104	0	0
1	TC	70	Total 547	C 341	N 102	O 104	0	0
1	UC	70	Total 547	C 341	N 102	O 104	0	0
1	VC	70	Total 547	C 341	N 102	O 104	0	0
1	WC	70	Total 547	C 341	N 102	O 104	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
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	XB	1	Total 1	Co 1	0
2	YB	1	Total 1	Co 1	0
2	ZB	1	Total 1	Co 1	0
2	G	1	Total 1	Co 1	0
2	aB	1	Total 1	Co 1	0
2	bB	1	Total 1	Co 1	0
2	cB	1	Total 1	Co 1	0
2	dB	1	Total 1	Co 1	0
2	eB	1	Total 1	Co 1	0
2	fB	1	Total 1	Co 1	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
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	aC	1	Total 1	Co 1	0
2	bC	1	Total 1	Co 1	0
2	cC	1	Total 1	Co 1	0
2	dC	1	Total 1	Co 1	0
2	eC	1	Total 1	Co 1	0
2	fC	1	Total 1	Co 1	0
2	gC	1	Total 1	Co 1	0
2	J	1	Total 1	Co 1	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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%



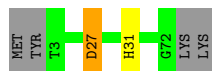
- Molecule 1: Transcription attenuation protein MtrB

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%



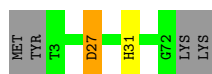
- Molecule 1: Transcription attenuation protein MtrB

Chain e:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain f:  92% •• 5%



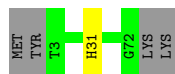
- Molecule 1: Transcription attenuation protein MtrB

Chain g:  93% • 5%



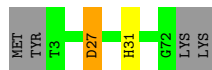
- Molecule 1: Transcription attenuation protein MtrB

Chain h:  93% • 5%



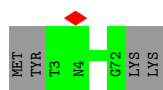
- Molecule 1: Transcription attenuation protein MtrB

Chain i:  92% •• 5%



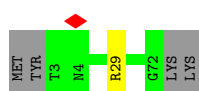
- Molecule 1: Transcription attenuation protein MtrB

Chain B:  95% 5%



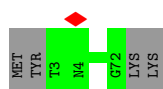
- Molecule 1: Transcription attenuation protein MtrB

Chain j:  93% • 5%




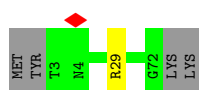
- Molecule 1: Transcription attenuation protein MtrB

Chain k:  95% 5%



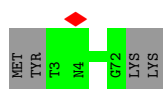
- Molecule 1: Transcription attenuation protein MtrB

Chain l:  93% 5%



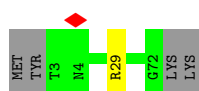
- Molecule 1: Transcription attenuation protein MtrB

Chain m:  95% 5%



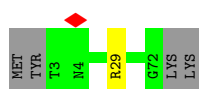
- Molecule 1: Transcription attenuation protein MtrB

Chain n:  93% 5%



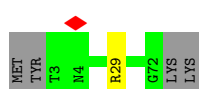
- Molecule 1: Transcription attenuation protein MtrB

Chain o:  93% 5%



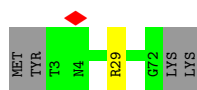
- Molecule 1: Transcription attenuation protein MtrB

Chain p:  93% 5%

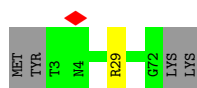


- Molecule 1: Transcription attenuation protein MtrB

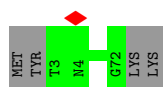
Chain q:  93% 5%



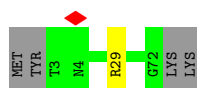
- Molecule 1: Transcription attenuation protein MtrB



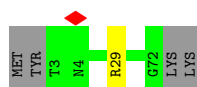
- Molecule 1: Transcription attenuation protein MtrB



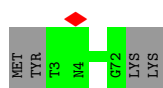
- Molecule 1: Transcription attenuation protein MtrB



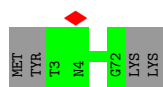
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

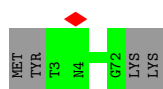


- Molecule 1: Transcription attenuation protein MtrB



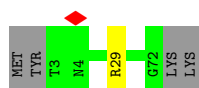
- Molecule 1: Transcription attenuation protein MtrB

Chain x:  95% 5%



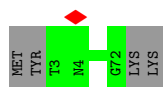
- Molecule 1: Transcription attenuation protein MtrB

Chain y:  93% 5%



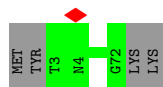
- Molecule 1: Transcription attenuation protein MtrB

Chain z:  95% 5%



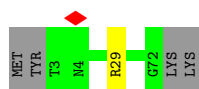
- Molecule 1: Transcription attenuation protein MtrB

Chain 0:  95% 5%



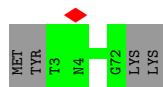
- Molecule 1: Transcription attenuation protein MtrB

Chain 1:  93% 5%



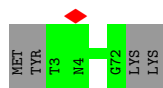
- Molecule 1: Transcription attenuation protein MtrB

Chain 2:  95% 5%



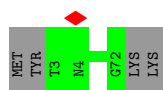
- Molecule 1: Transcription attenuation protein MtrB

Chain 3:  95% 5%



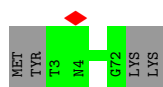
- Molecule 1: Transcription attenuation protein MtrB

Chain 4:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 5:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain C:  95% 5%



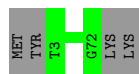
- Molecule 1: Transcription attenuation protein MtrB

Chain 6:  95% 5%



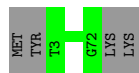
- Molecule 1: Transcription attenuation protein MtrB

Chain 7:  95% 5%



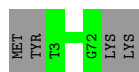
- Molecule 1: Transcription attenuation protein MtrB

Chain 8:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 9:  95% 5%



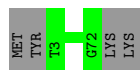
- Molecule 1: Transcription attenuation protein MtrB

Chain AA:  95% 5%



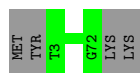
- Molecule 1: Transcription attenuation protein MtrB

Chain BA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain CA:  95% 5%



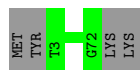
- Molecule 1: Transcription attenuation protein MtrB

Chain DA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain EA:  95% 5%



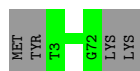
- Molecule 1: Transcription attenuation protein MtrB

Chain FA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain GA:  95% 5%



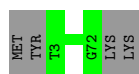
- Molecule 1: Transcription attenuation protein MtrB

Chain HA:  95% 5%



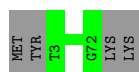
- Molecule 1: Transcription attenuation protein MtrB

Chain IA:  95% 5%



- 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%



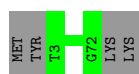
- Molecule 1: Transcription attenuation protein MtrB

Chain MA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain NA:  95% 5%



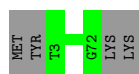
- Molecule 1: Transcription attenuation protein MtrB

Chain OA:  95% 5%



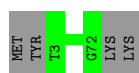
- Molecule 1: Transcription attenuation protein MtrB

Chain PA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain QA:  95% 5%



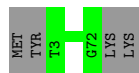
- Molecule 1: Transcription attenuation protein MtrB

Chain RA:  95% 5%



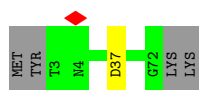
- Molecule 1: Transcription attenuation protein MtrB

Chain SA:  95% 5%



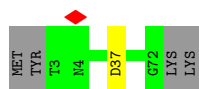
- Molecule 1: Transcription attenuation protein MtrB

Chain D:  93% 5%



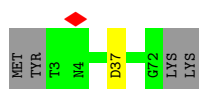
- Molecule 1: Transcription attenuation protein MtrB

Chain TA:  93% 5%



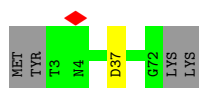
- Molecule 1: Transcription attenuation protein MtrB

Chain UA:  93% • 5%



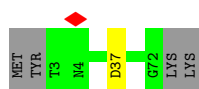
- Molecule 1: Transcription attenuation protein MtrB

Chain VA:  93% • 5%



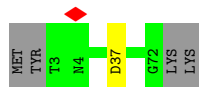
- Molecule 1: Transcription attenuation protein MtrB

Chain WA:  93% • 5%



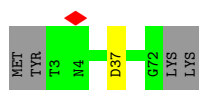
- Molecule 1: Transcription attenuation protein MtrB

Chain XA:  93% • 5%



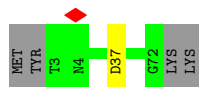
- Molecule 1: Transcription attenuation protein MtrB

Chain YA:  93% • 5%



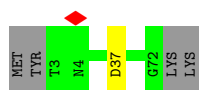
- Molecule 1: Transcription attenuation protein MtrB

Chain ZA:  93% • 5%



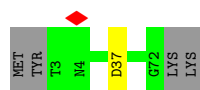
- Molecule 1: Transcription attenuation protein MtrB

Chain aA:  93% • 5%



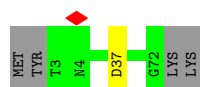
- Molecule 1: Transcription attenuation protein MtrB

Chain bA:  93% 5%



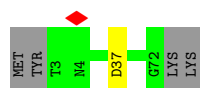
- Molecule 1: Transcription attenuation protein MtrB

Chain cA:  93% 5%



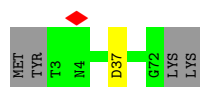
- Molecule 1: Transcription attenuation protein MtrB

Chain dA:  93% 5%



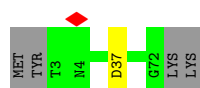
- Molecule 1: Transcription attenuation protein MtrB

Chain eA:  93% 5%



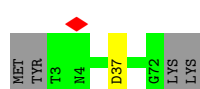
- Molecule 1: Transcription attenuation protein MtrB

Chain fA:  93% 5%



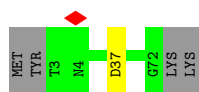
- Molecule 1: Transcription attenuation protein MtrB

Chain gA:  93% 5%



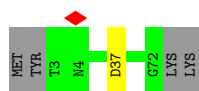
- Molecule 1: Transcription attenuation protein MtrB

Chain hA:  93% 5%



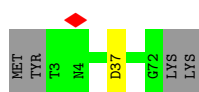
- Molecule 1: Transcription attenuation protein MtrB

Chain iA: 93% • 5%



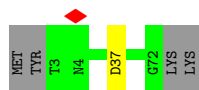
- Molecule 1: Transcription attenuation protein MtrB

Chain jA: 93% • 5%



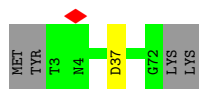
- Molecule 1: Transcription attenuation protein MtrB

Chain kA: 93% • 5%



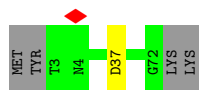
- Molecule 1: Transcription attenuation protein MtrB

Chain lA: 93% • 5%



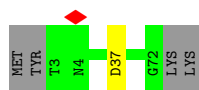
- Molecule 1: Transcription attenuation protein MtrB

Chain mA: 93% • 5%



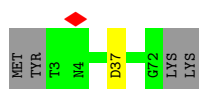
- Molecule 1: Transcription attenuation protein MtrB

Chain nA: 93% • 5%



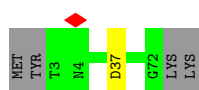
- Molecule 1: Transcription attenuation protein MtrB

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

Chain qA:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain rA:  93% 5%



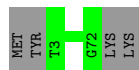
- Molecule 1: Transcription attenuation protein MtrB

Chain sA:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain tA:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain uA:  93% • 5%



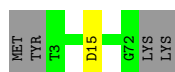
- Molecule 1: Transcription attenuation protein MtrB

Chain vA:  93% • 5%



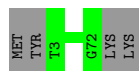
- Molecule 1: Transcription attenuation protein MtrB

Chain wA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain xA:  95% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain yA:  95% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain zA:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 0A:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 1A:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 2A:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 3A:  93% • 5%



- 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%



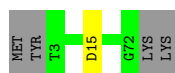
- Molecule 1: Transcription attenuation protein MtrB

Chain 7A:  93% • 5%



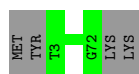
- Molecule 1: Transcription attenuation protein MtrB

Chain 8A:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain 9A:  95% 5%



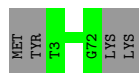
- Molecule 1: Transcription attenuation protein MtrB

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%



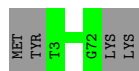
- Molecule 1: Transcription attenuation protein MtrB

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%



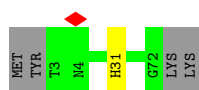
- Molecule 1: Transcription attenuation protein MtrB

Chain LB:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain MB:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain NB:  93% • 5%



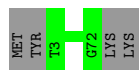
- Molecule 1: Transcription attenuation protein MtrB

Chain OB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain PB:  95% 5%



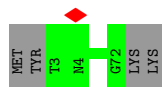
- Molecule 1: Transcription attenuation protein MtrB

Chain QB:  93% • 5%



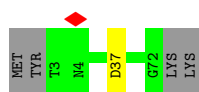
- Molecule 1: Transcription attenuation protein MtrB

Chain RB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain SB:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain TB:  95% 5%



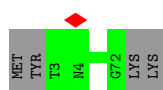
- Molecule 1: Transcription attenuation protein MtrB

Chain UB:  93% 5%



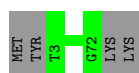
- Molecule 1: Transcription attenuation protein MtrB

Chain VB:  95% 5%



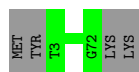
- Molecule 1: Transcription attenuation protein MtrB

Chain WB:  95% 5%



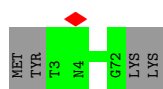
- Molecule 1: Transcription attenuation protein MtrB

Chain XB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain YB:  95% 5%



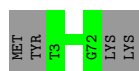
- Molecule 1: Transcription attenuation protein MtrB

Chain ZB:  92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain G:  95% 5%



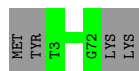
- Molecule 1: Transcription attenuation protein MtrB

Chain aB:  95% 5%



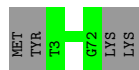
- Molecule 1: Transcription attenuation protein MtrB

Chain bB:  95% 5%



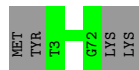
- Molecule 1: Transcription attenuation protein MtrB

Chain cB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain dB:  95% 5%



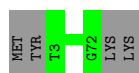
- Molecule 1: Transcription attenuation protein MtrB

Chain eB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain fB:  95% 5%



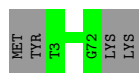
- Molecule 1: Transcription attenuation protein MtrB

Chain gB:  95% 5%



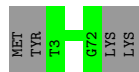
- Molecule 1: Transcription attenuation protein MtrB

Chain hB:  95% 5%



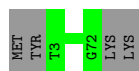
- Molecule 1: Transcription attenuation protein MtrB

Chain iB:  95% 5%



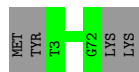
- Molecule 1: Transcription attenuation protein MtrB

Chain jB:  95% 5%



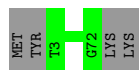
- Molecule 1: Transcription attenuation protein MtrB

Chain kB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain lB:  95% 5%



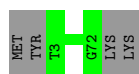
- Molecule 1: Transcription attenuation protein MtrB

Chain mB:  95% 5%



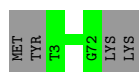
- Molecule 1: Transcription attenuation protein MtrB

Chain nB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain oB:  95% 5%



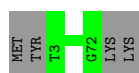
- Molecule 1: Transcription attenuation protein MtrB

Chain pB:  95% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain qB:  95% 5%



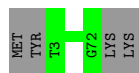
- Molecule 1: Transcription attenuation protein MtrB

Chain rB:  95% 5%



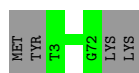
- Molecule 1: Transcription attenuation protein MtrB

Chain sB:  95% 5%



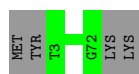
- Molecule 1: Transcription attenuation protein MtrB

Chain tB:  95% 5%



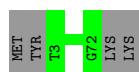
- Molecule 1: Transcription attenuation protein MtrB

Chain uB:  95% 5%



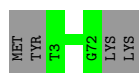
- Molecule 1: Transcription attenuation protein MtrB

Chain vB:  95% 5%



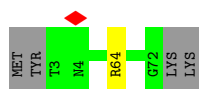
- Molecule 1: Transcription attenuation protein MtrB

Chain wB:  95% 5%



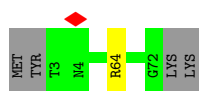
- Molecule 1: Transcription attenuation protein MtrB

Chain H:  93% 5%



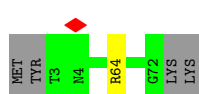
- Molecule 1: Transcription attenuation protein MtrB

Chain xB:  93% 5%



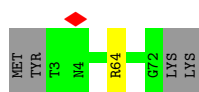
- Molecule 1: Transcription attenuation protein MtrB

Chain yB:  93% 5%



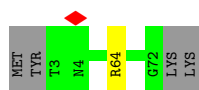
- Molecule 1: Transcription attenuation protein MtrB

Chain zB:  93% • 5%



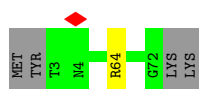
- Molecule 1: Transcription attenuation protein MtrB

Chain 0B:  93% • 5%



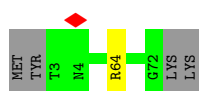
- Molecule 1: Transcription attenuation protein MtrB

Chain 1B:  93% • 5%



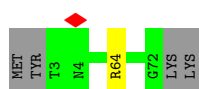
- Molecule 1: Transcription attenuation protein MtrB

Chain 2B:  93% • 5%



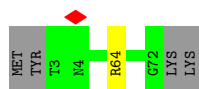
- Molecule 1: Transcription attenuation protein MtrB

Chain 3B:  93% • 5%



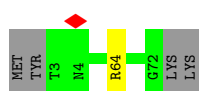
- Molecule 1: Transcription attenuation protein MtrB

Chain 4B:  93% • 5%



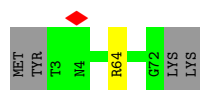
- Molecule 1: Transcription attenuation protein MtrB

Chain 5B:  93% • 5%



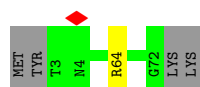
- Molecule 1: Transcription attenuation protein MtrB

Chain 6B:  93% • 5%



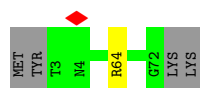
- Molecule 1: Transcription attenuation protein MtrB

Chain 7B:  93% • 5%



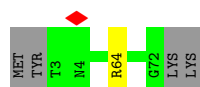
- Molecule 1: Transcription attenuation protein MtrB

Chain 8B:  93% • 5%



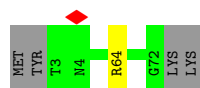
- Molecule 1: Transcription attenuation protein MtrB

Chain 9B:  93% • 5%



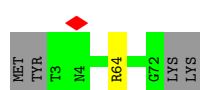
- Molecule 1: Transcription attenuation protein MtrB

Chain AC:  93% • 5%



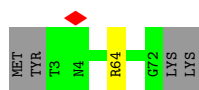
- Molecule 1: Transcription attenuation protein MtrB

Chain BC:  93% • 5%

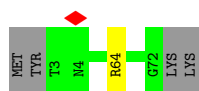


- Molecule 1: Transcription attenuation protein MtrB

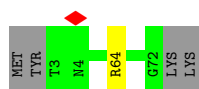
Chain CC:  93% • 5%



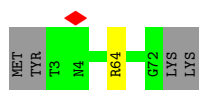
- Molecule 1: Transcription attenuation protein MtrB



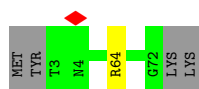
- Molecule 1: Transcription attenuation protein MtrB



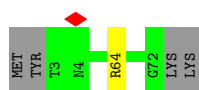
- Molecule 1: Transcription attenuation protein MtrB



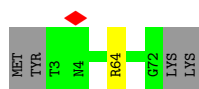
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

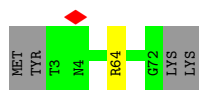


- Molecule 1: Transcription attenuation protein MtrB



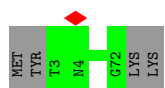
- Molecule 1: Transcription attenuation protein MtrB

Chain JC:  93% 5%



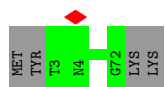
- Molecule 1: Transcription attenuation protein MtrB

Chain I:  95% 5%



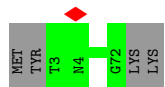
- Molecule 1: Transcription attenuation protein MtrB

Chain KC:  95% 5%



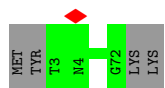
- Molecule 1: Transcription attenuation protein MtrB

Chain LC:  95% 5%



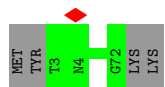
- Molecule 1: Transcription attenuation protein MtrB

Chain MC:  95% 5%



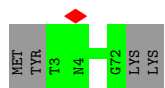
- Molecule 1: Transcription attenuation protein MtrB

Chain NC:  95% 5%



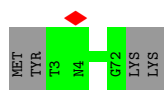
- Molecule 1: Transcription attenuation protein MtrB

Chain OC:  95% 5%



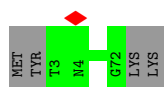
- Molecule 1: Transcription attenuation protein MtrB

Chain PC:  95% 5%



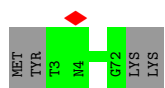
- Molecule 1: Transcription attenuation protein MtrB

Chain QC:  95% 5%



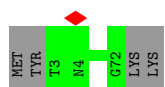
- Molecule 1: Transcription attenuation protein MtrB

Chain RC:  95% 5%



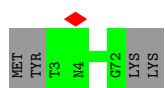
- Molecule 1: Transcription attenuation protein MtrB

Chain SC:  95% 5%



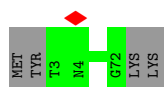
- Molecule 1: Transcription attenuation protein MtrB

Chain TC:  95% 5%



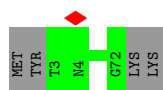
- Molecule 1: Transcription attenuation protein MtrB

Chain UC:  95% 5%

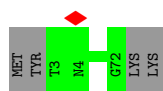


- Molecule 1: Transcription attenuation protein MtrB

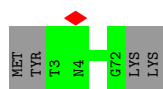
Chain VC:  95% 5%



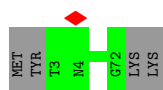
- Molecule 1: Transcription attenuation protein MtrB



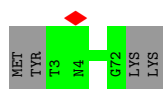
- Molecule 1: Transcription attenuation protein MtrB



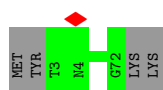
- Molecule 1: Transcription attenuation protein MtrB



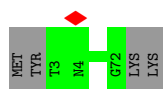
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

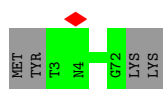


- Molecule 1: Transcription attenuation protein MtrB



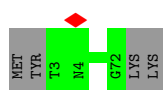
- Molecule 1: Transcription attenuation protein MtrB

Chain cC:  95% 5%



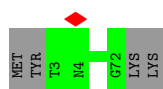
- Molecule 1: Transcription attenuation protein MtrB

Chain dC:  95% 5%



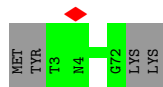
- Molecule 1: Transcription attenuation protein MtrB

Chain eC:  95% 5%



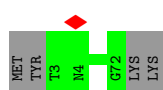
- Molecule 1: Transcription attenuation protein MtrB

Chain fC:  95% 5%



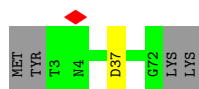
- Molecule 1: Transcription attenuation protein MtrB

Chain gC:  95% 5%



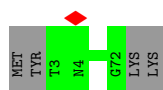
- Molecule 1: Transcription attenuation protein MtrB

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%



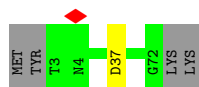
- Molecule 1: Transcription attenuation protein MtrB

Chain kC:  93% 5%



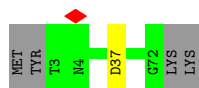
- Molecule 1: Transcription attenuation protein MtrB

Chain lC:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain mC:  93% 5%



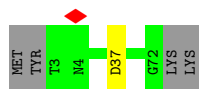
- Molecule 1: Transcription attenuation protein MtrB

Chain nC:  93% 5%



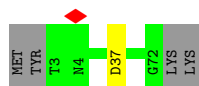
- Molecule 1: Transcription attenuation protein MtrB

Chain oC:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain pC:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain qC:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain rC:  93% 5%



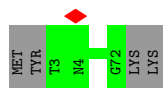
- Molecule 1: Transcription attenuation protein MtrB

Chain sC:  93% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain tC:  95% 5%



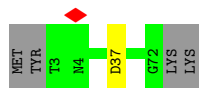
- Molecule 1: Transcription attenuation protein MtrB

Chain uC:  93% 5%



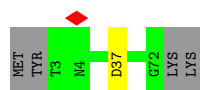
- Molecule 1: Transcription attenuation protein MtrB

Chain vC:  93% 5%



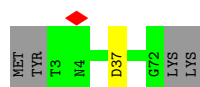
- Molecule 1: Transcription attenuation protein MtrB

Chain wC:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain xC:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain yC:  93% • 5%



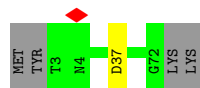
- Molecule 1: Transcription attenuation protein MtrB

Chain zC:  93% • 5%



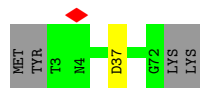
- Molecule 1: Transcription attenuation protein MtrB

Chain 0C:  93% • 5%



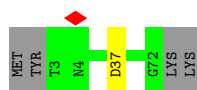
- Molecule 1: Transcription attenuation protein MtrB

Chain 1C:  93% • 5%

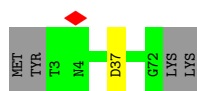


- Molecule 1: Transcription attenuation protein MtrB

Chain 2C:  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 9C: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain AD: 93% • 5%



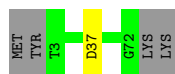
- Molecule 1: Transcription attenuation protein MtrB

Chain BD: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain CD: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain DD: 92% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ED: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain FD: 93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain GD:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain HD:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain ID:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain JD:  93% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain KD:  93% • 5%



- 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
Maximum map value	5.123	Depositor
Minimum map value	-2.557	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.278	Depositor
Recommended contour level	0.493	Depositor
Map size (Å)	387.0, 387.0, 387.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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(°)	Ideal(°)
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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	l	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

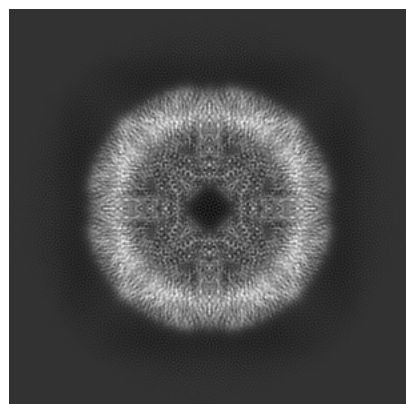
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18904. These allow visual inspection of the internal detail of the map and identification of artifacts.

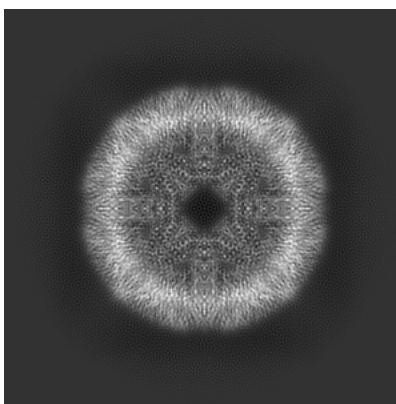
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

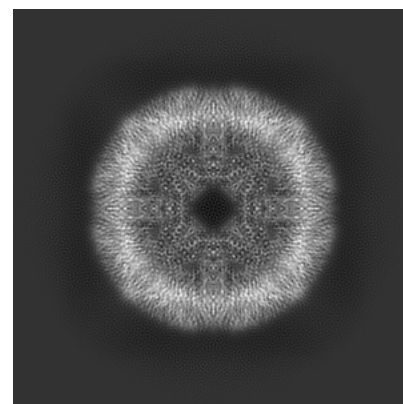
6.1.1 Primary map



X

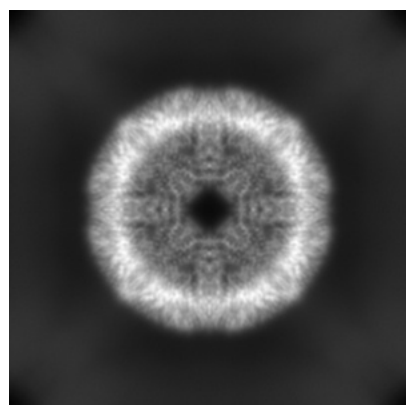


Y

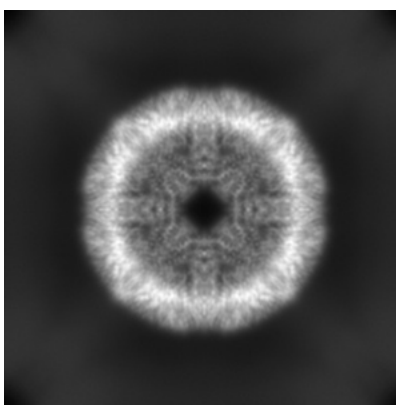


Z

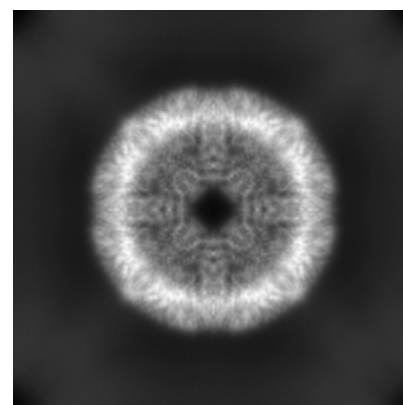
6.1.2 Raw map



X



Y

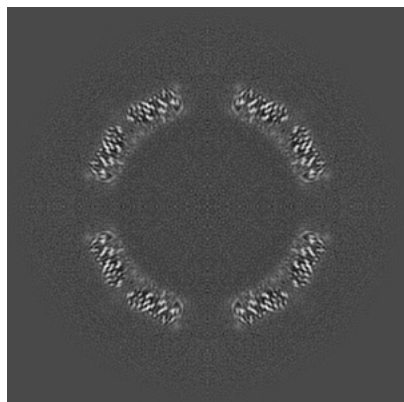


Z

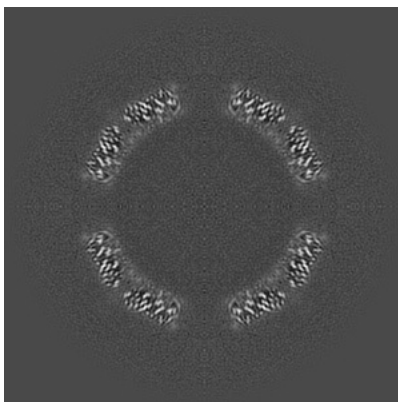
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

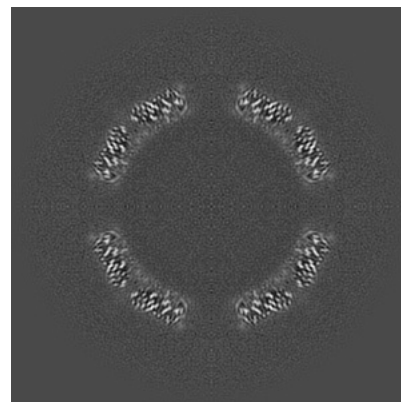
6.2.1 Primary map



X Index: 225

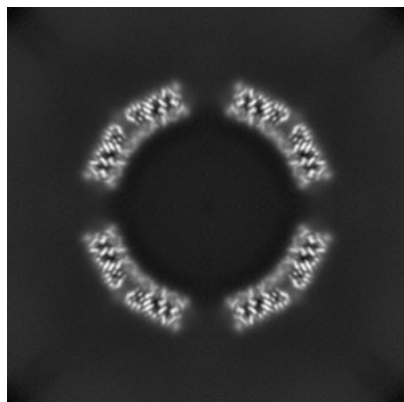


Y Index: 225

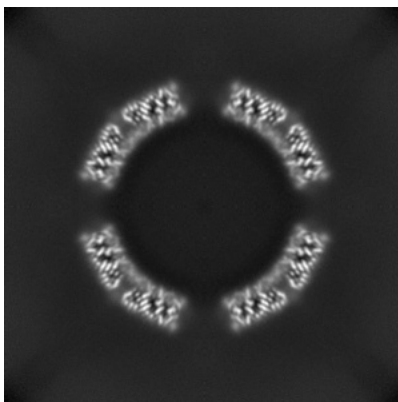


Z Index: 225

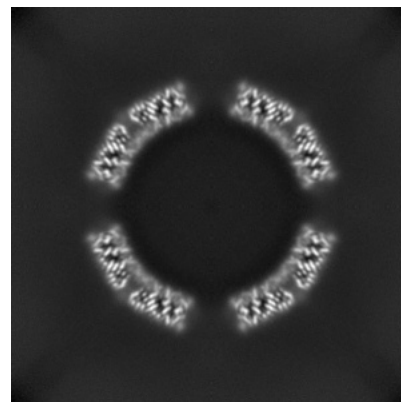
6.2.2 Raw map



X Index: 225



Y Index: 225

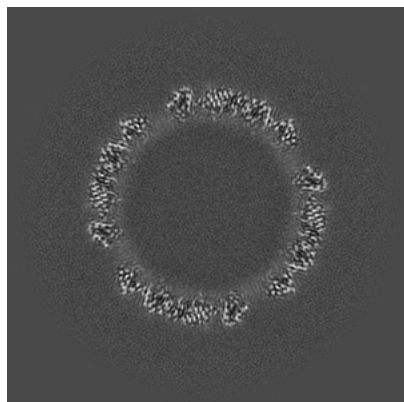


Z Index: 225

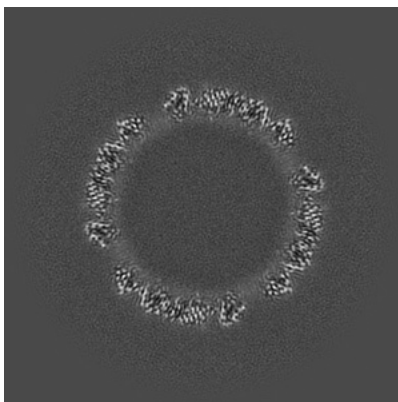
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

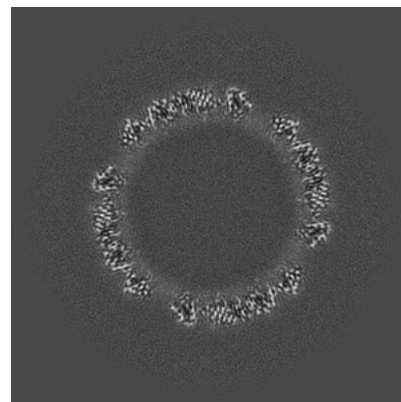
6.3.1 Primary map



X Index: 262

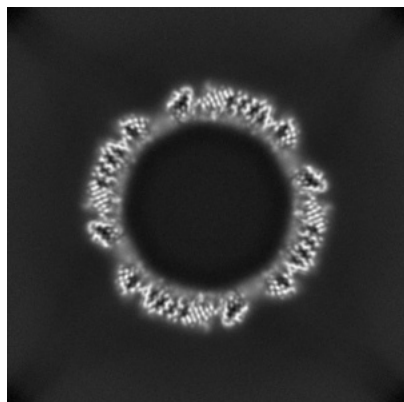


Y Index: 262

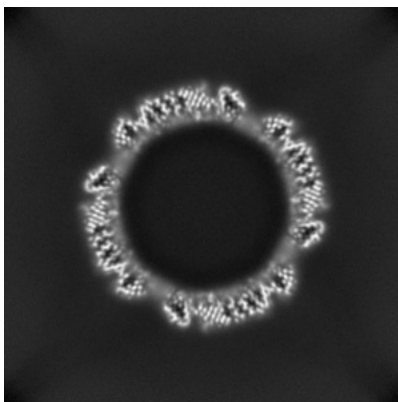


Z Index: 188

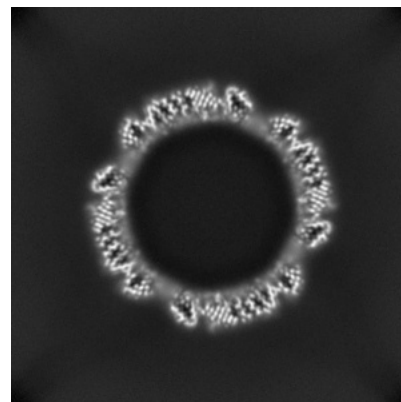
6.3.2 Raw map



X Index: 262



Y Index: 188

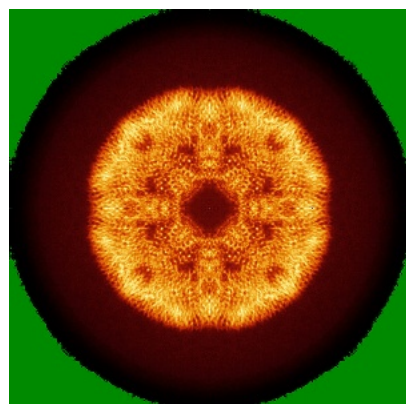


Z Index: 188

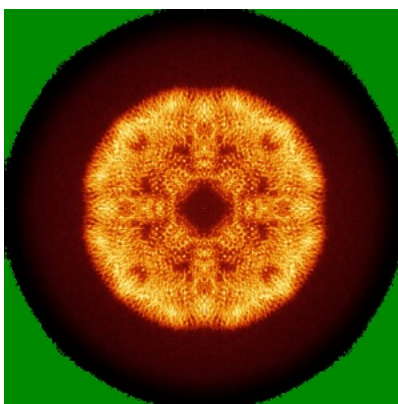
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

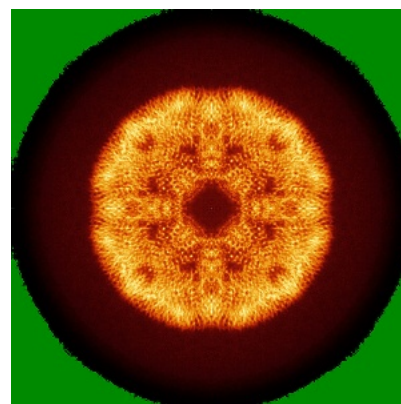
6.4.1 Primary map



X

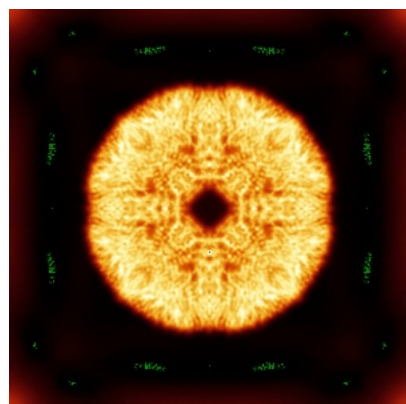


Y

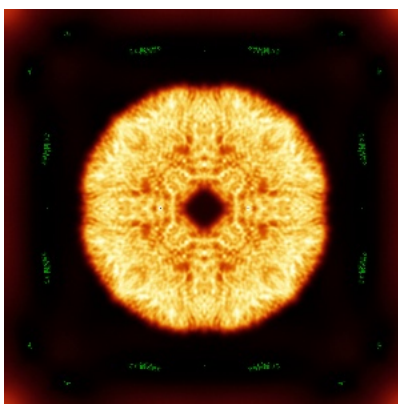


Z

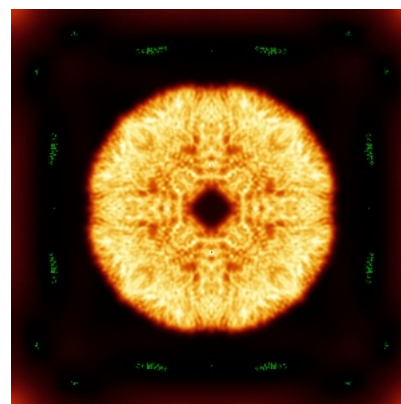
6.4.2 Raw map



X



Y

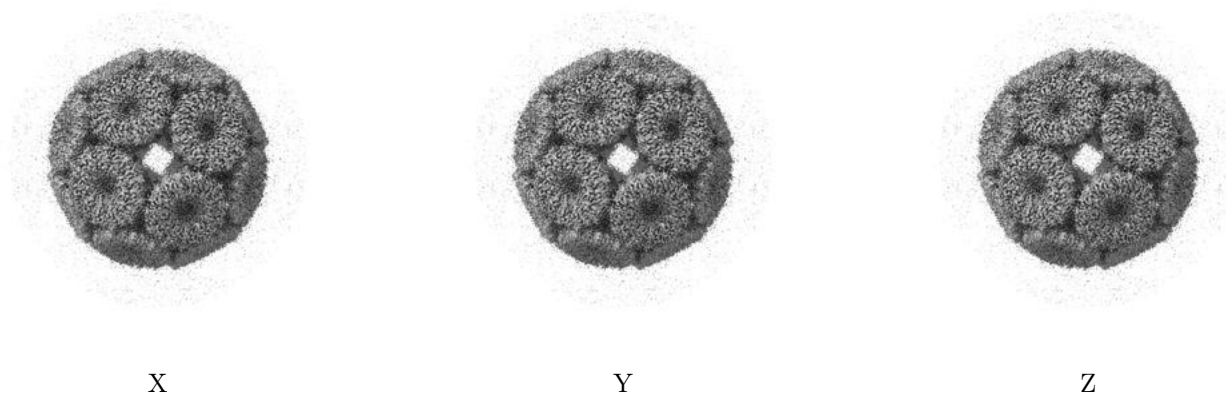


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

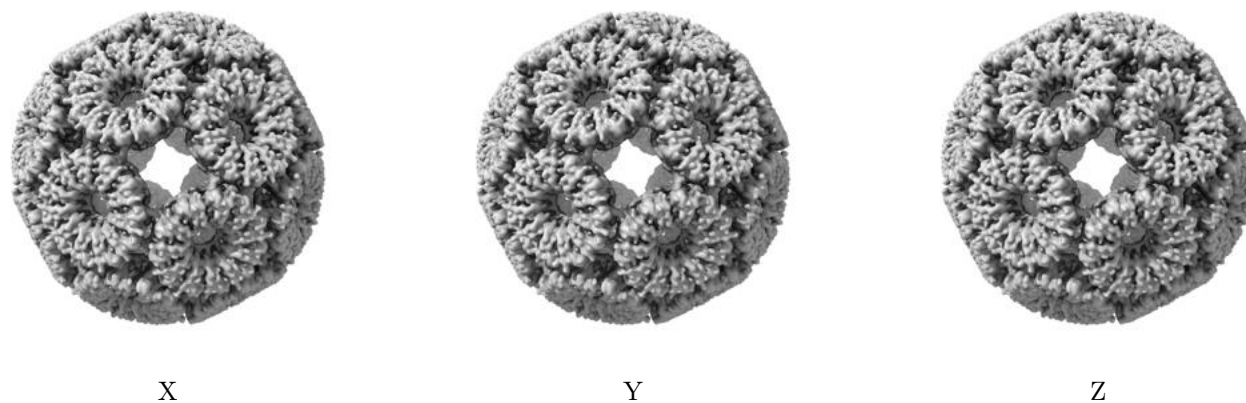
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.493. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

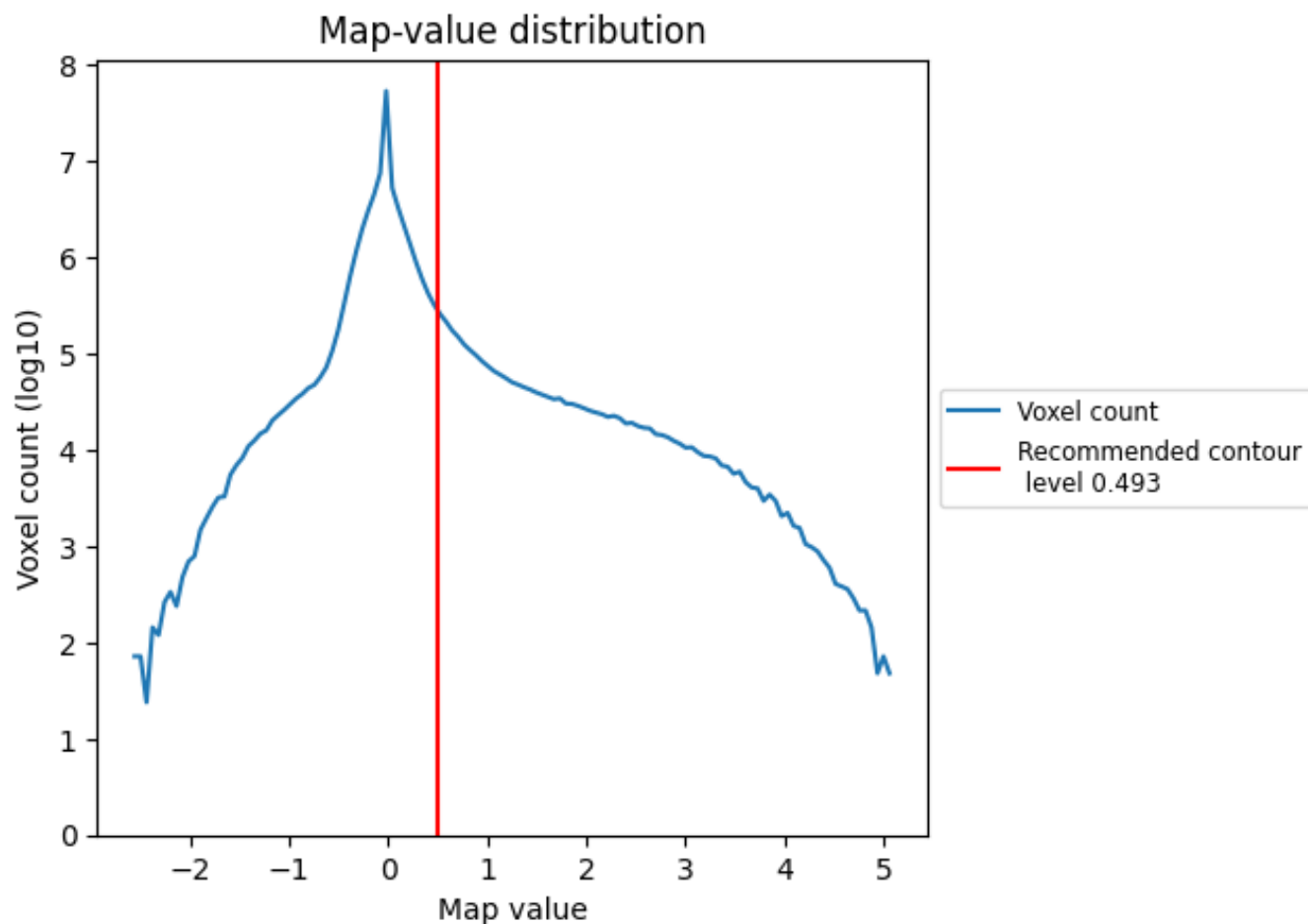
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

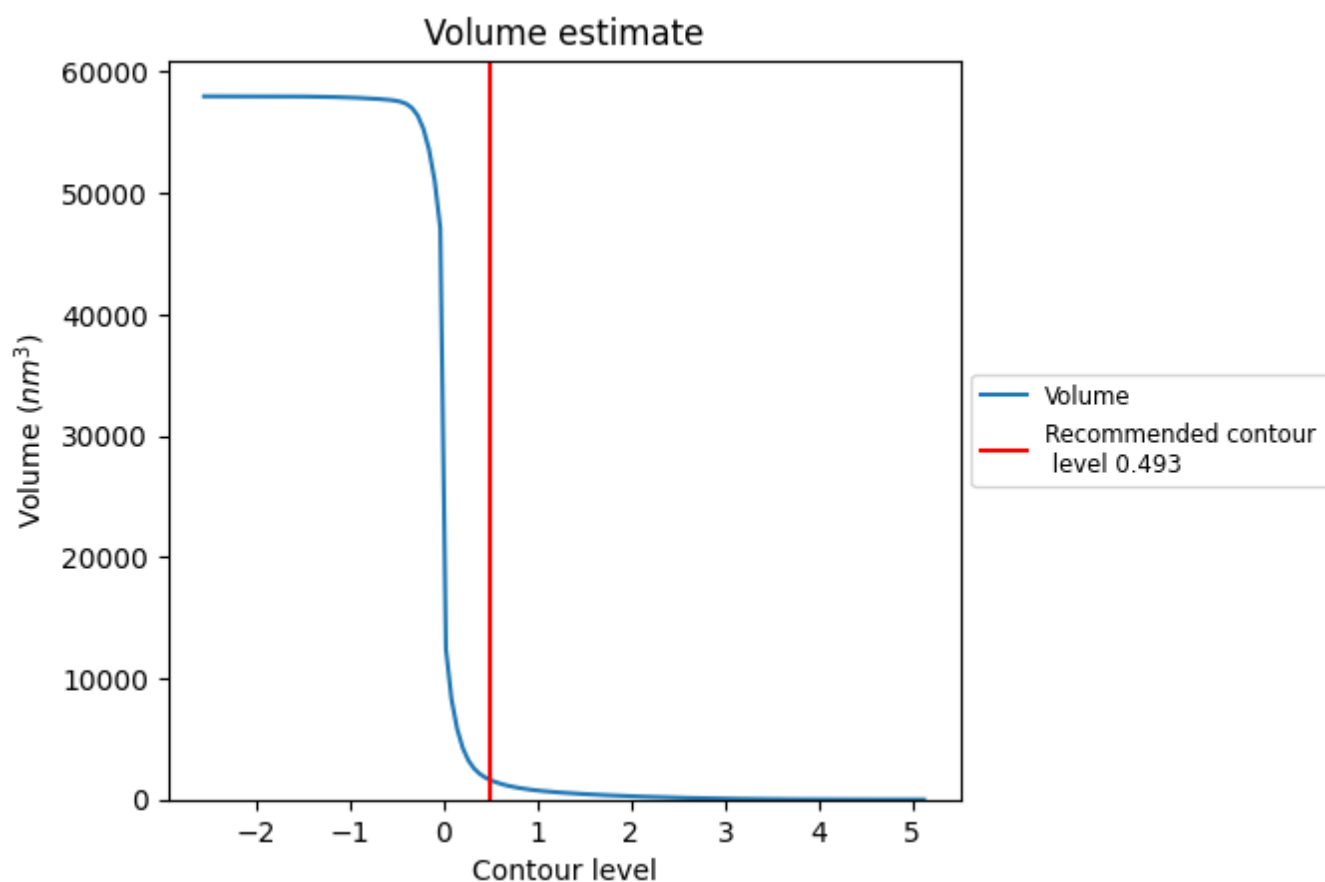
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

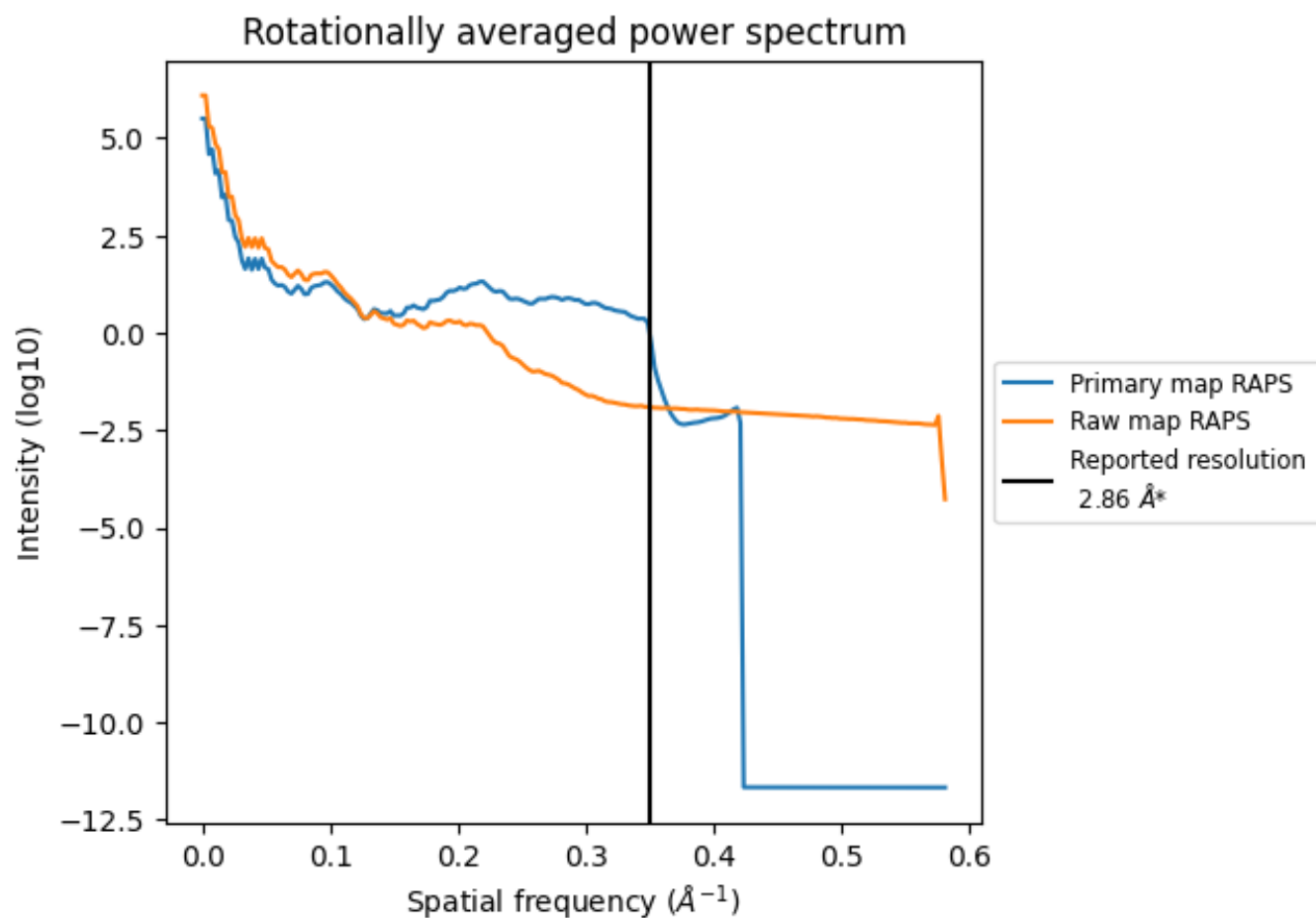
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1626 nm³; this corresponds to an approximate mass of 1469 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

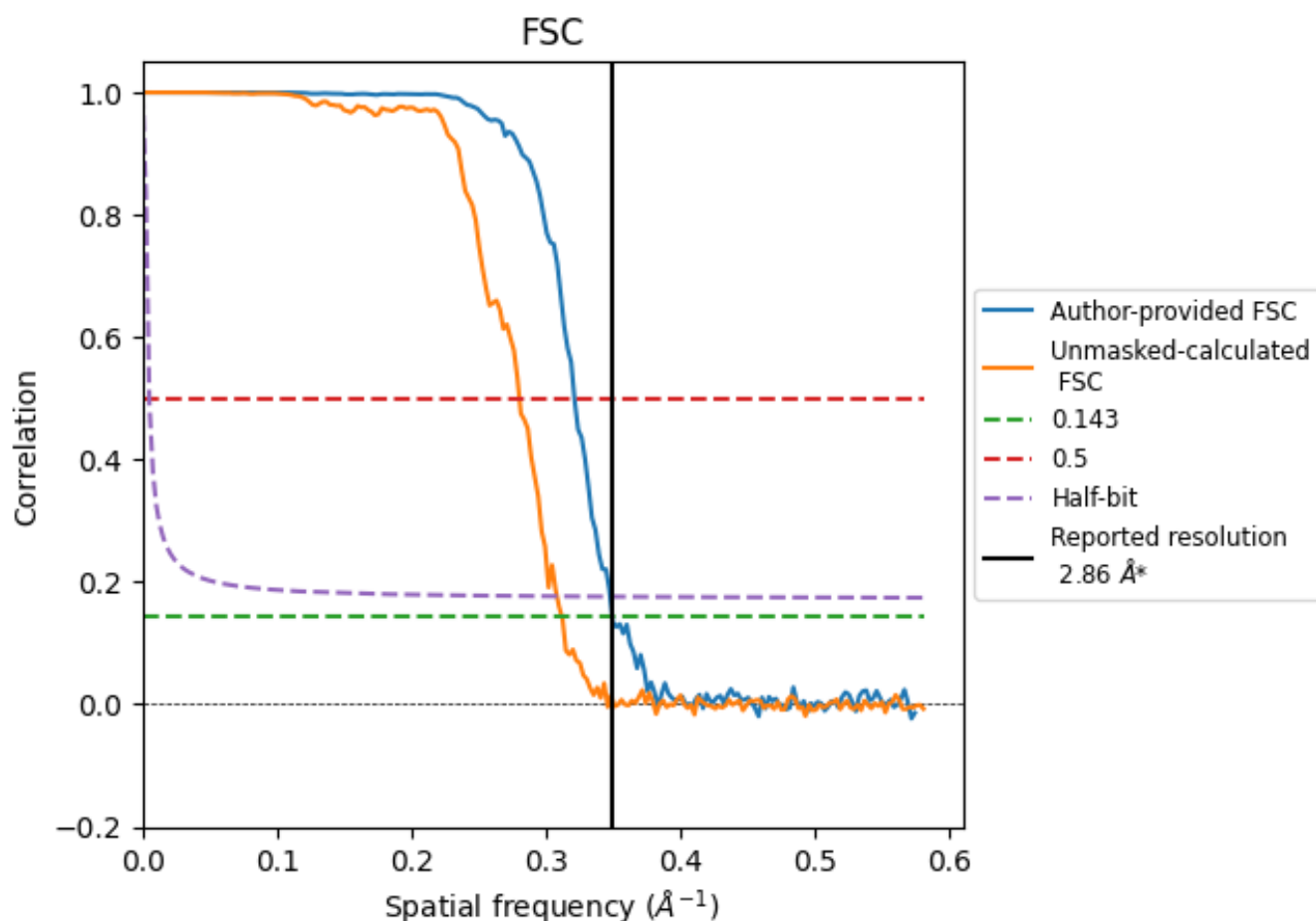


*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

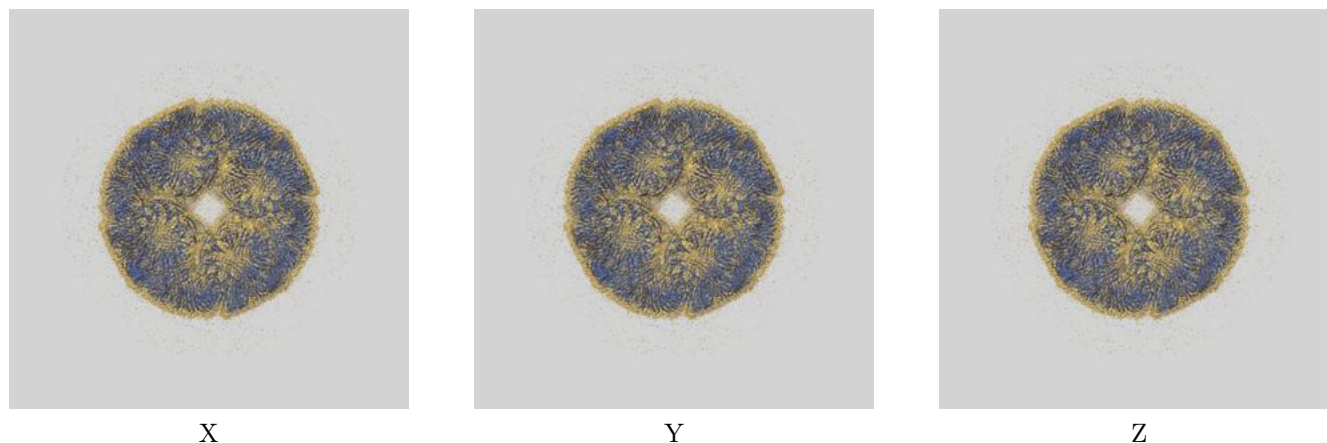
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.11	2.87
Unmasked-calculated*	3.20	3.56	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

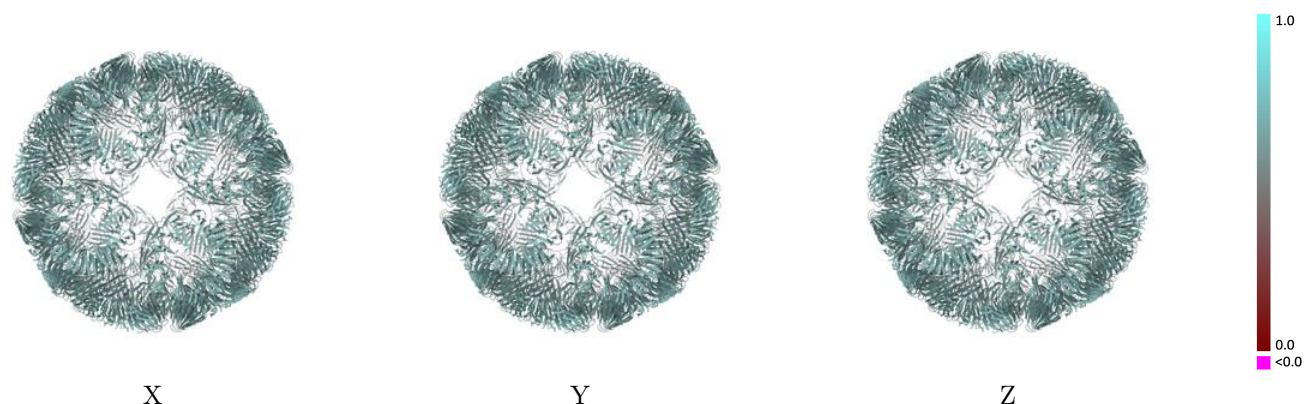
This section contains information regarding the fit between EMDB map EMD-18904 and PDB model 8R59. Per-residue inclusion information can be found in section [3](#) on page [46](#).

9.1 Map-model overlay [i](#)



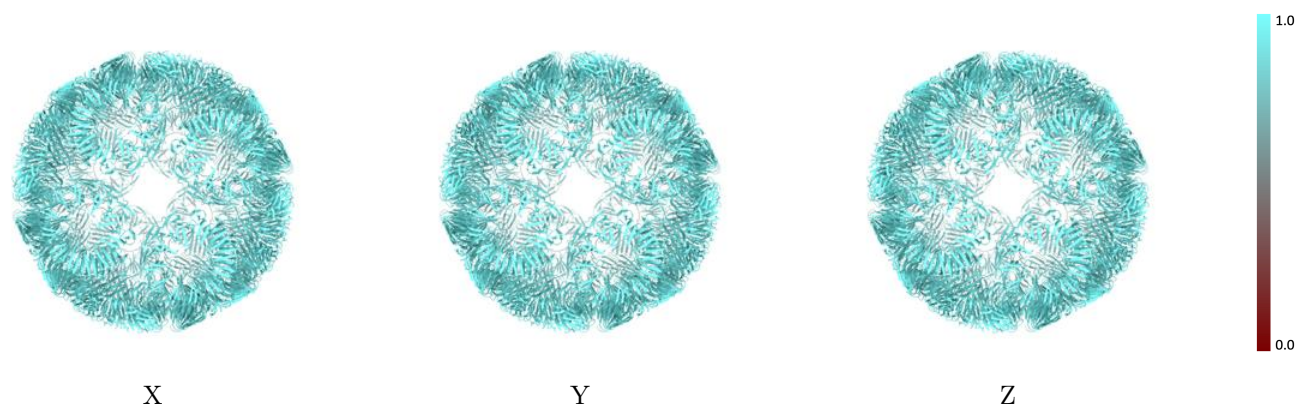
The images above show the 3D surface view of the map at the recommended contour level 0.493 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



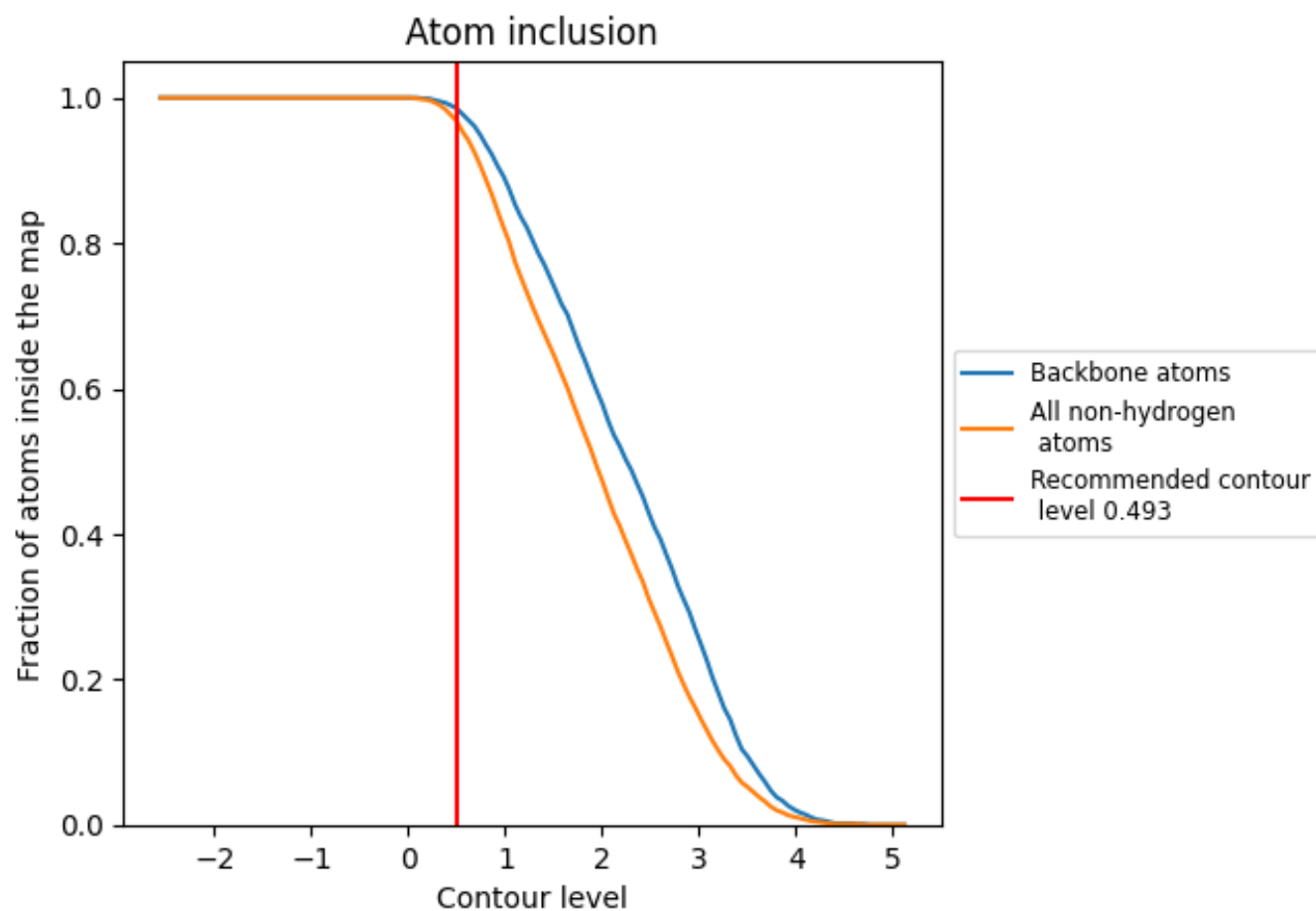
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.493).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.493) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.6060
0	 0.9720	 0.6090
0A	 0.9760	 0.6100
0B	 0.9700	 0.6030
0C	 0.9560	 0.5910
1	 0.9720	 0.6120
1A	 0.9740	 0.6090
1B	 0.9700	 0.6010
1C	 0.9590	 0.5930
2	 0.9720	 0.6120
2A	 0.9720	 0.6050
2B	 0.9670	 0.6000
2C	 0.9560	 0.5930
3	 0.9720	 0.6090
3A	 0.9720	 0.6090
3B	 0.9700	 0.6000
3C	 0.9570	 0.5910
4	 0.9720	 0.6100
4A	 0.9760	 0.6060
4B	 0.9700	 0.6010
4C	 0.9720	 0.6100
5	 0.9740	 0.6100
5A	 0.9740	 0.6080
5B	 0.9680	 0.5990
5C	 0.9720	 0.6080
6	 0.9720	 0.6110
6A	 0.9740	 0.6110
6B	 0.9700	 0.6010
6C	 0.9690	 0.6070
7	 0.9700	 0.6140
7A	 0.9760	 0.6070
7B	 0.9680	 0.6040
7C	 0.9720	 0.6130
8	 0.9720	 0.6100
8A	 0.9740	 0.6090























































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
8B	 0.9700	 0.6000
8C	 0.9720	 0.6170
9	 0.9700	 0.6150
9A	 0.9740	 0.6060
9B	 0.9700	 0.5960
9C	 0.9720	 0.6130
A	 0.9800	 0.6110
AA	 0.9700	 0.6170
AB	 0.9740	 0.6070
AC	 0.9700	 0.6020
AD	 0.9740	 0.6150
B	 0.9720	 0.6050
BA	 0.9700	 0.6160
BB	 0.9720	 0.6040
BC	 0.9700	 0.6010
BD	 0.9720	 0.6170
C	 0.9700	 0.6130
CA	 0.9700	 0.6170
CB	 0.9760	 0.6110
CC	 0.9680	 0.6030
CD	 0.9690	 0.6120
D	 0.9630	 0.6030
DA	 0.9700	 0.6160
DB	 0.9650	 0.5990
DC	 0.9700	 0.6020
DD	 0.9720	 0.6170
E	 0.9740	 0.6070
EA	 0.9700	 0.6160
EB	 0.9630	 0.5930
EC	 0.9680	 0.6050
ED	 0.9690	 0.6120
F	 0.9630	 0.6010
FA	 0.9720	 0.6160
FB	 0.9630	 0.5900
FC	 0.9680	 0.6050
FD	 0.9720	 0.6100
G	 0.9690	 0.6080
GA	 0.9720	 0.6150
GB	 0.9610	 0.5950
GC	 0.9680	 0.6030
GD	 0.9720	 0.6080
H	 0.9720	 0.6040





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HA	 0.9700	 0.6130
HB	 0.9630	 0.5950
HC	 0.9680	 0.6000
HD	 0.9720	 0.6080
I	 0.9720	 0.6090
IA	 0.9700	 0.6120
IB	 0.9610	 0.5950
IC	 0.9670	 0.6030
ID	 0.9720	 0.6080
J	 0.9570	 0.5960
JA	 0.9700	 0.6130
JB	 0.9610	 0.5970
JC	 0.9680	 0.6000
JD	 0.9720	 0.6160
K	 0.9690	 0.6100
KA	 0.9700	 0.6110
KB	 0.9650	 0.6010
KC	 0.9690	 0.6070
KD	 0.9720	 0.6150
L	 0.9800	 0.6090
LA	 0.9700	 0.6160
LB	 0.9630	 0.6030
LC	 0.9690	 0.6060
LD	 0.9720	 0.6110
M	 0.9800	 0.6080
MA	 0.9700	 0.6130
MB	 0.9630	 0.6010
MC	 0.9700	 0.6060
MD	 0.9690	 0.6160
N	 0.9800	 0.6080
NA	 0.9700	 0.6150
NB	 0.9610	 0.5970
NC	 0.9690	 0.6080
ND	 0.9720	 0.6150
O	 0.9800	 0.6180
OA	 0.9700	 0.6170
OB	 0.9630	 0.5930
OC	 0.9690	 0.6090
OD	 0.9720	 0.6110
P	 0.9800	 0.6140
PA	 0.9700	 0.6150
PB	 0.9630	 0.5920





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PC	 0.9690	 0.6070
PD	 0.9720	 0.6150
Q	 0.9800	 0.6150
QA	 0.9700	 0.6150
QB	 0.9610	 0.5930
QC	 0.9690	 0.6100
QD	 0.9740	 0.6150
R	 0.9800	 0.6160
RA	 0.9720	 0.6150
RB	 0.9610	 0.5900
RC	 0.9700	 0.6100
S	 0.9800	 0.6150
SA	 0.9720	 0.6140
SB	 0.9590	 0.5960
SC	 0.9700	 0.6060
T	 0.9800	 0.6160
TA	 0.9590	 0.5960
TB	 0.9630	 0.5960
TC	 0.9690	 0.6090
U	 0.9800	 0.6140
UA	 0.9630	 0.6030
UB	 0.9610	 0.5930
UC	 0.9700	 0.6060
V	 0.9800	 0.6140
VA	 0.9610	 0.5980
VB	 0.9610	 0.5950
VC	 0.9700	 0.6090
W	 0.9800	 0.6110
WA	 0.9630	 0.6030
WB	 0.9630	 0.5940
WC	 0.9690	 0.6050
XA	 0.9670	 0.6090
XB	 0.9630	 0.5930
XC	 0.9700	 0.6080
Y	 0.9800	 0.6080
YA	 0.9610	 0.6020
YB	 0.9610	 0.5930
YC	 0.9700	 0.6070
Z	 0.9800	 0.6100
ZA	 0.9570	 0.6010
ZB	 0.9630	 0.6060
ZC	 0.9720	 0.6080





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9800	 0.6090
aA	 0.9590	 0.6030
aB	 0.9700	 0.6080
aC	 0.9690	 0.6090
b	 0.9800	 0.6160
bA	 0.9590	 0.5990
bB	 0.9670	 0.6080
bC	 0.9690	 0.6100
c	 0.9800	 0.6150
cA	 0.9630	 0.6030
cB	 0.9700	 0.6050
cC	 0.9700	 0.6100
d	 0.9800	 0.6130
dA	 0.9630	 0.6030
dB	 0.9720	 0.6100
dC	 0.9700	 0.6090
e	 0.9800	 0.6160
eA	 0.9590	 0.5980
eB	 0.9690	 0.6100
eC	 0.9690	 0.6050
f	 0.9800	 0.6160
fA	 0.9670	 0.6010
fB	 0.9690	 0.6050
fC	 0.9700	 0.6090
g	 0.9800	 0.6140
gA	 0.9630	 0.6020
gB	 0.9720	 0.6110
gC	 0.9700	 0.6060
h	 0.9800	 0.6140
hA	 0.9650	 0.6030
hB	 0.9690	 0.6100
hC	 0.9560	 0.5910
i	 0.9800	 0.6150
iA	 0.9630	 0.6040
iB	 0.9690	 0.6070
iC	 0.9670	 0.5940
j	 0.9720	 0.6050
jA	 0.9650	 0.6060
jB	 0.9700	 0.6070
jC	 0.9590	 0.5930
k	 0.9720	 0.6050
kA	 0.9630	 0.6040









































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
kB	 0.9670	 0.6100
kC	 0.9650	 0.5970
l	 0.9720	 0.6030
lA	 0.9630	 0.6070
lB	 0.9700	 0.6090
lC	 0.9590	 0.5960
m	 0.9720	 0.6110
mA	 0.9630	 0.6020
mB	 0.9700	 0.6040
mC	 0.9590	 0.5940
n	 0.9720	 0.6120
nA	 0.9630	 0.6040
nB	 0.9700	 0.6060
nC	 0.9610	 0.5970
o	 0.9720	 0.6100
oA	 0.9610	 0.6010
oB	 0.9700	 0.6060
oC	 0.9590	 0.5950
p	 0.9720	 0.6110
pA	 0.9650	 0.6040
pB	 0.9720	 0.6100
pC	 0.9570	 0.5910
q	 0.9720	 0.6080
qA	 0.9720	 0.6070
qB	 0.9690	 0.6080
qC	 0.9630	 0.5970
r	 0.9720	 0.6090
rA	 0.9740	 0.6080
rB	 0.9700	 0.6080
rC	 0.9610	 0.5940
s	 0.9720	 0.6110
sA	 0.9740	 0.6060
sB	 0.9690	 0.6110
sC	 0.9610	 0.5970
t	 0.9720	 0.6080
tA	 0.9740	 0.6090
tB	 0.9700	 0.6090
tC	 0.9560	 0.5920
u	 0.9720	 0.6060
uA	 0.9720	 0.6080
uB	 0.9720	 0.6070
uC	 0.9630	 0.5970

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
v	 0.9720	 0.6060
vA	 0.9740	 0.6100
vB	 0.9700	 0.6080
vC	 0.9570	 0.5880
w	 0.9720	 0.6070
wA	 0.9720	 0.6100
wB	 0.9690	 0.6080
wC	 0.9560	 0.5960
x	 0.9720	 0.6050
xA	 0.9740	 0.6050
xB	 0.9700	 0.6010
xC	 0.9610	 0.5930
y	 0.9720	 0.6110
yA	 0.9740	 0.6090
yB	 0.9700	 0.6000
yC	 0.9590	 0.5950
z	 0.9720	 0.6120
zA	 0.9760	 0.6040
zB	 0.9680	 0.5970
zC	 0.9650	 0.5970