



## wwPDB EM Validation Summary Report ⓘ

Mar 24, 2025 – 02:50 pm GMT

PDB ID : 8R5A  
EMDB ID : EMD-18905  
Title : Structure of the Co(II) triggered TRAP (S33HK35H) protein cage (dextro form)  
Authors : Biela, A.P.; Heddle, J.G.  
Deposited on : 2023-11-16  
Resolution : 2.84 Å(reported)  
Based on initial model : 4v4f

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

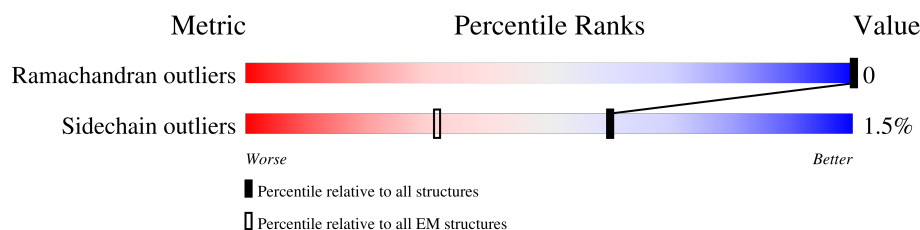
EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 2.84 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  $\geq 3$ , 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	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	0A	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	0B	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	0C	74	<div> <div>11%</div> <div>93%</div> <div>5%</div> </div>
1	1	74	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	1A	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	1B	74	<div> <div>9%</div> <div>95%</div> <div>5%</div> </div>
1	1C	74	<div> <div>11%</div> <div>93%</div> <div>5%</div> </div>
1	2	74	<div> <div>8%</div> <div>91%</div> <div>5%</div> </div>

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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	

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Mol	Chain	Length	Quality of chain
1	8B	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	8C	74	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	9	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	9A	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	9B	74	<div> <div>9%</div> <div>95%</div> <div>5%</div> </div>
1	9C	74	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	A	74	<div> <div>7%</div> <div>92%</div> <div>5%</div> </div>
1	AA	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	AB	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	AC	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	AD	74	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	B	74	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	BA	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	BB	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	BC	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	BD	74	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	C	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	CA	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	CB	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	CC	74	<div> <div>11%</div> <div>95%</div> <div>5%</div> </div>
1	CD	74	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	D	74	<div> <div>11%</div> <div>95%</div> <div>5%</div> </div>
1	DA	74	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
1	DB	74	<div> <div>11%</div> <div>92%</div> <div>5%</div> </div>
1	DC	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>

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

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

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

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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	

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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	

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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	

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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	

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Mol	Chain	Length	Quality of chain
1	sB	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	sC	74	<div> <div>11%</div> <div>92%</div> <div>5%</div> </div>
1	t	74	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	tA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	tB	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	tC	74	<div> <div>11%</div> <div>92%</div> <div>5%</div> </div>
1	u	74	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>
1	uA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	uB	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	uC	74	<div> <div>11%</div> <div>92%</div> <div>5%</div> </div>
1	v	74	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	vA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	vB	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	vC	74	<div> <div>9%</div> <div>93%</div> <div>5%</div> </div>
1	w	74	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>
1	wA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	wB	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
1	wC	74	<div> <div>9%</div> <div>92%</div> <div>5%</div> </div>
1	x	74	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	xA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	xB	74	<div> <div>9%</div> <div>95%</div> <div>5%</div> </div>
1	xC	74	<div> <div>11%</div> <div>93%</div> <div>5%</div> </div>
1	y	74	<div> <div>8%</div> <div>92%</div> <div>5%</div> </div>
1	yA	74	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	yB	74	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	yC	74	 11% 93% 5%
1	z	74	 5% 95% 5%
1	zA	74	 8% 93% 5%
1	zB	74	 8% 95% 5%
1	zC	74	 11% 93% 5%

## 2 Entry composition [i](#)

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	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
1	W	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	a	70	Total 547	C 341	N 102	O 104	0	0
1	b	70	Total 547	C 341	N 102	O 104	0	0

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
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

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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

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
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

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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

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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

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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

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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

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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

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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

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

There are 528 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total Co 1 1	0
2	6	1	Total Co 1 1	0
2	7	1	Total Co 1 1	0
2	8	1	Total Co 1 1	0
2	9	1	Total Co 1 1	0
2	AA	1	Total Co 1 1	0
2	BA	1	Total Co 1 1	0
2	CA	1	Total Co 1 1	0
2	DA	1	Total Co 1 1	0
2	EA	1	Total Co 1 1	0
2	FA	1	Total Co 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	GA	1	Total 1	Co 1	0
2	HA	1	Total 1	Co 1	0
2	IA	1	Total 1	Co 1	0
2	JA	1	Total 1	Co 1	0
2	KA	1	Total 1	Co 1	0
2	LA	1	Total 1	Co 1	0
2	MA	1	Total 1	Co 1	0
2	NA	1	Total 1	Co 1	0
2	OA	1	Total 1	Co 1	0
2	PA	1	Total 1	Co 1	0
2	QA	1	Total 1	Co 1	0
2	RA	1	Total 1	Co 1	0
2	SA	1	Total 1	Co 1	0
2	E	1	Total 1	Co 1	0
2	qA	1	Total 1	Co 1	0
2	rA	1	Total 1	Co 1	0
2	sA	1	Total 1	Co 1	0
2	tA	1	Total 1	Co 1	0
2	uA	1	Total 1	Co 1	0
2	vA	1	Total 1	Co 1	0
2	wA	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	xA	1	Total 1	Co 1	0
2	yA	1	Total 1	Co 1	0
2	zA	1	Total 1	Co 1	0
2	0A	1	Total 1	Co 1	0
2	1A	1	Total 1	Co 1	0
2	2A	1	Total 1	Co 1	0
2	3A	1	Total 1	Co 1	0
2	4A	1	Total 1	Co 1	0
2	5A	1	Total 1	Co 1	0
2	6A	1	Total 1	Co 1	0
2	7A	1	Total 1	Co 1	0
2	8A	1	Total 1	Co 1	0
2	9A	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	F	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
2	GB	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
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	XB	1	Total 1	Co 1	0
2	YB	1	Total 1	Co 1	0
2	ZB	1	Total 1	Co 1	0
2	eB	1	Total 1	Co 1	0
2	iB	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	jB	1	Total 1	Co 1	0
2	H	1	Total 1	Co 1	0
2	0B	1	Total 1	Co 1	0
2	1B	1	Total 1	Co 1	0
2	2B	1	Total 1	Co 1	0
2	3B	1	Total 1	Co 1	0
2	4B	1	Total 1	Co 1	0
2	5B	1	Total 1	Co 1	0
2	6B	1	Total 1	Co 1	0
2	7B	1	Total 1	Co 1	0
2	8B	1	Total 1	Co 1	0
2	9B	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	HC	1	Total 1	Co 1	0
2	IC	1	Total 1	Co 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	JC	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
2	MD	1	Total 1	Co 1	0

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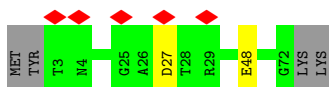
Mol	Chain	Residues	Atoms		AltConf
2	ND	1	Total 1	Co 1	0
2	OD	1	Total 1	Co 1	0
2	PD	1	Total 1	Co 1	0
2	QD	1	Total 1	Co 1	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: 



- Molecule 1: Transcription attenuation protein MtrB

Chain L: 



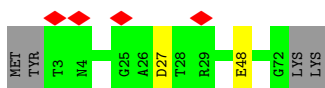
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Chain M: 



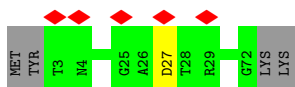
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Chain N: 

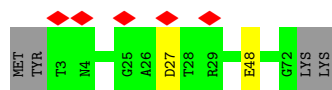
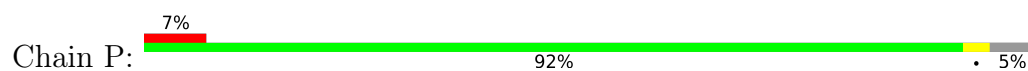


- Molecule 1: Transcription attenuation protein MtrB

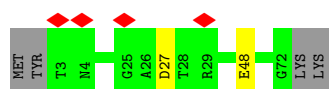
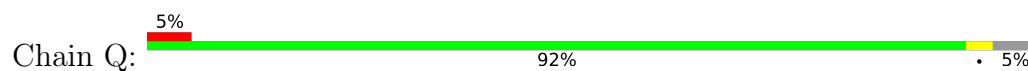
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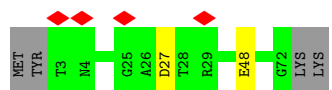
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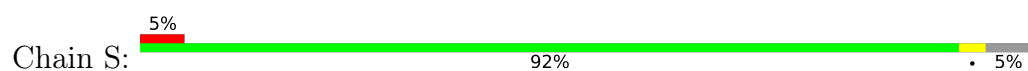
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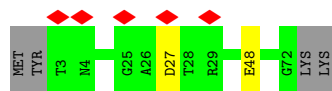
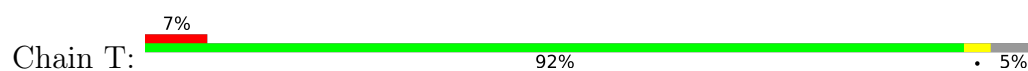
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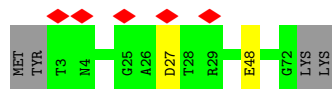
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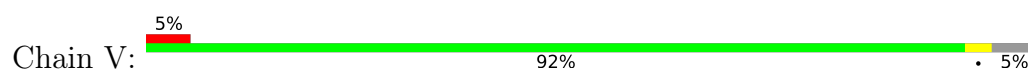
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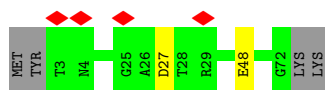


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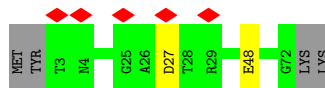
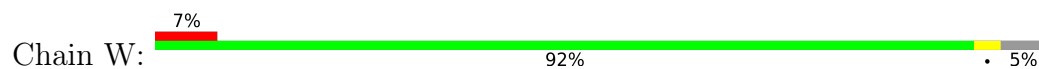


- Molecule 1: Transcription attenuation protein MtrB





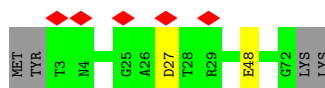
- Molecule 1: Transcription attenuation protein MtrB



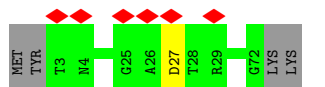
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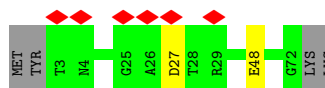
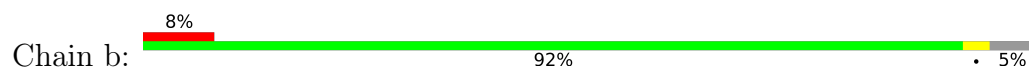
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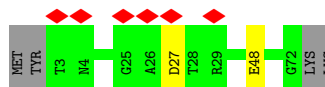
- Molecule 1: Transcription attenuation protein MtrB



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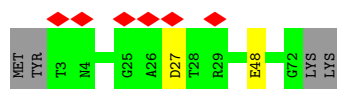
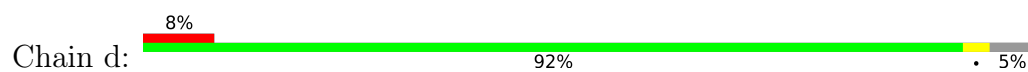


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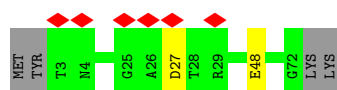
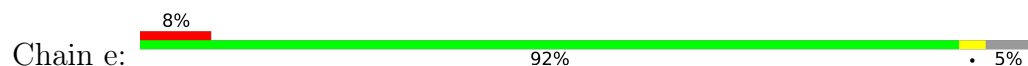


- Molecule 1: Transcription attenuation protein MtrB





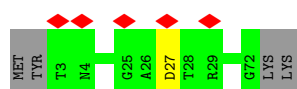
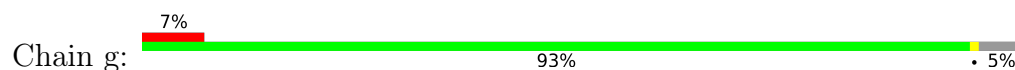
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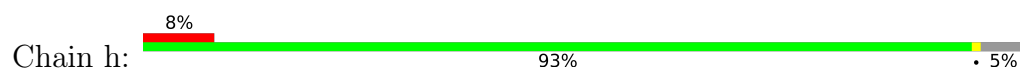
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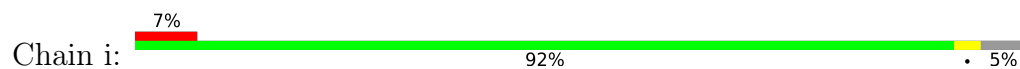
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- Molecule 1: Transcription attenuation protein MtrB

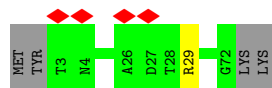


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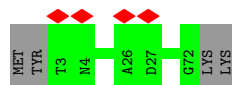
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Chain j: 



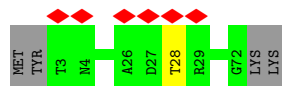
- Molecule 1: Transcription attenuation protein MtrB

Chain k: 



- Molecule 1: Transcription attenuation protein MtrB

Chain l: 

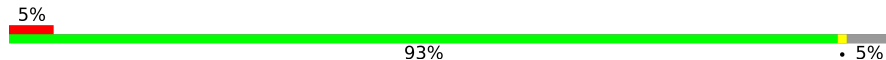


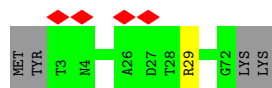
- Molecule 1: Transcription attenuation protein MtrB

Chain m: 

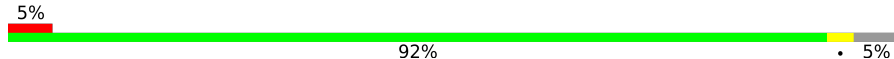


- Molecule 1: Transcription attenuation protein MtrB

Chain n: 

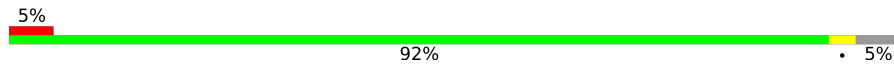


- Molecule 1: Transcription attenuation protein MtrB

Chain o: 

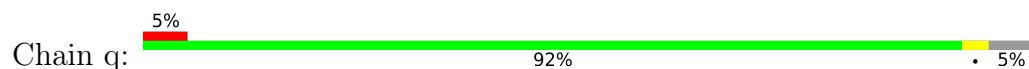


- Molecule 1: Transcription attenuation protein MtrB

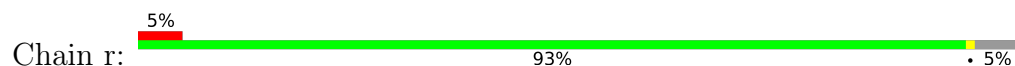
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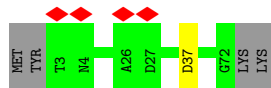
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- Molecule 1: Transcription attenuation protein MtrB



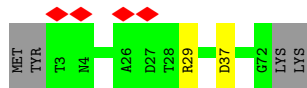
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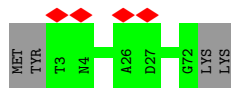
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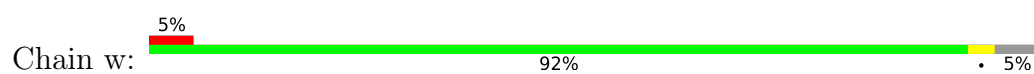
- Molecule 1: Transcription attenuation protein MtrB



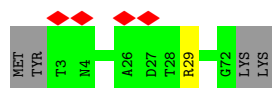
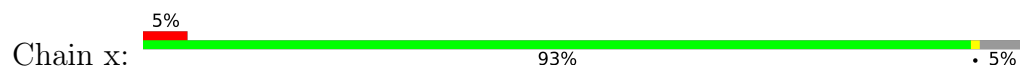
- Molecule 1: Transcription attenuation protein MtrB



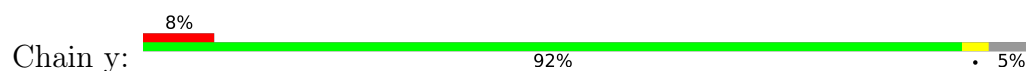
- Molecule 1: Transcription attenuation protein MtrB



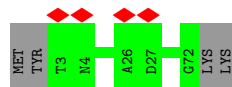
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



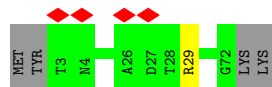
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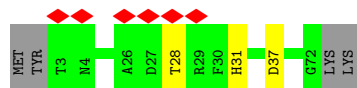
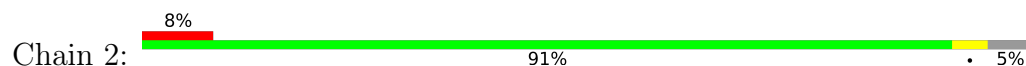
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- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



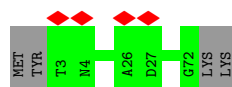
- Molecule 1: Transcription attenuation protein MtrB

Chain 3:  5% 93% 5%

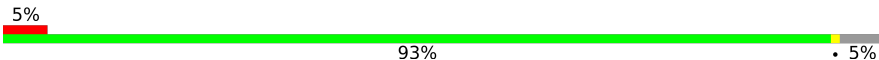


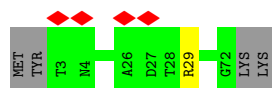
- Molecule 1: Transcription attenuation protein MtrB

Chain 4:  5% 95% 5%



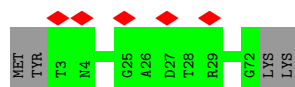
- Molecule 1: Transcription attenuation protein MtrB

Chain 5:  5% 93% 5%



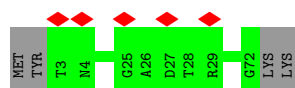
- Molecule 1: Transcription attenuation protein MtrB

Chain C:  7% 95% 5%



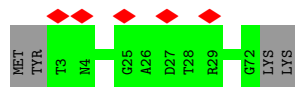
- Molecule 1: Transcription attenuation protein MtrB

Chain 6:  7% 95% 5%

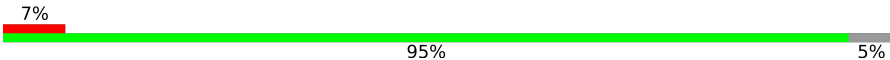


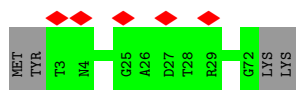
- Molecule 1: Transcription attenuation protein MtrB

Chain 7:  7% 95% 5%

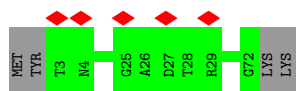


- Molecule 1: Transcription attenuation protein MtrB

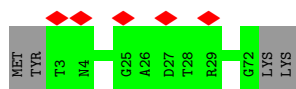
Chain 8:  7% 95% 5%



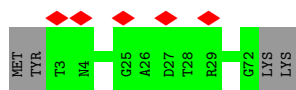
- Molecule 1: Transcription attenuation protein MtrB



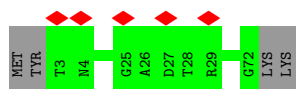
- Molecule 1: Transcription attenuation protein MtrB



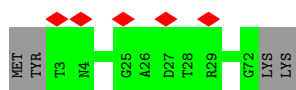
- Molecule 1: Transcription attenuation protein MtrB



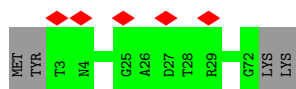
- Molecule 1: Transcription attenuation protein MtrB



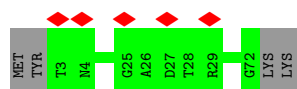
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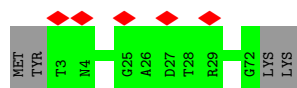
- Molecule 1: Transcription attenuation protein MtrB



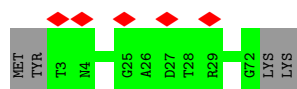
- Molecule 1: Transcription attenuation protein MtrB



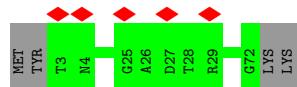
- Molecule 1: Transcription attenuation protein MtrB



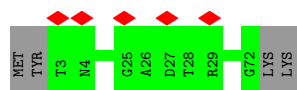
- Molecule 1: Transcription attenuation protein MtrB



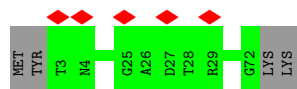
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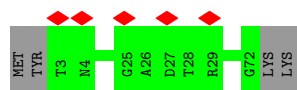
- Molecule 1: Transcription attenuation protein MtrB



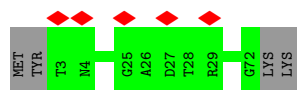
- Molecule 1: Transcription attenuation protein MtrB



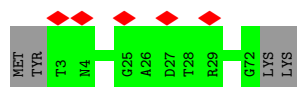
- Molecule 1: Transcription attenuation protein MtrB



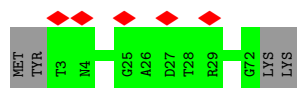
- Molecule 1: Transcription attenuation protein MtrB



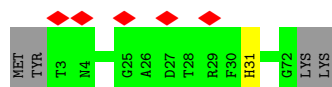
- Molecule 1: Transcription attenuation protein MtrB



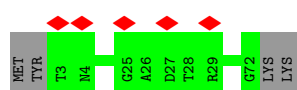
- Molecule 1: Transcription attenuation protein MtrB



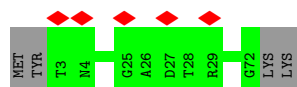
- Molecule 1: Transcription attenuation protein MtrB



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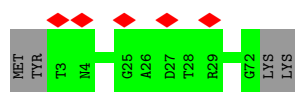
- Molecule 1: Transcription attenuation protein MtrB



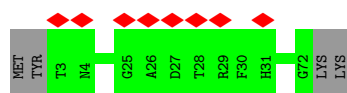
- Molecule 1: Transcription attenuation protein MtrB







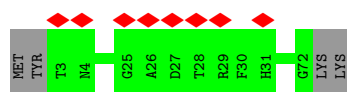
- Molecule 1: Transcription attenuation protein MtrB



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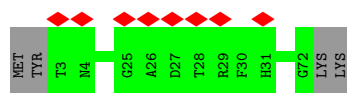
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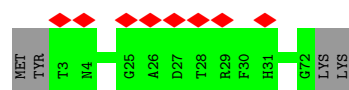
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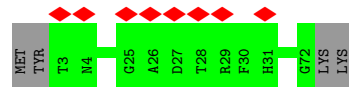
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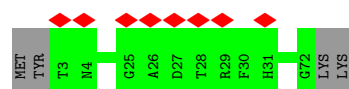
- Molecule 1: Transcription attenuation protein MtrB



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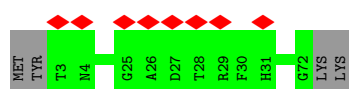
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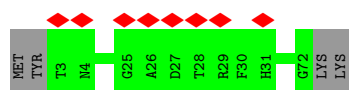
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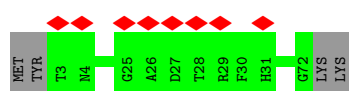
- Molecule 1: Transcription attenuation protein MtrB



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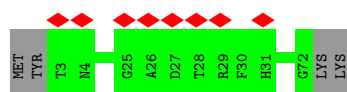


- Molecule 1: Transcription attenuation protein MtrB



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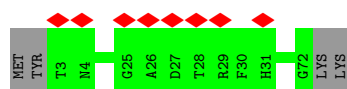
- Molecule 1: Transcription attenuation protein MtrB



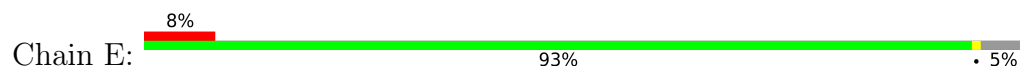
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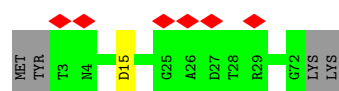
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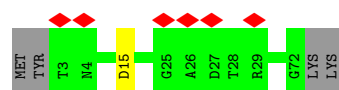
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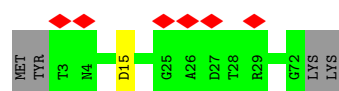
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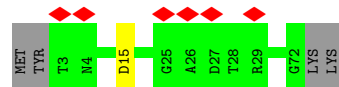
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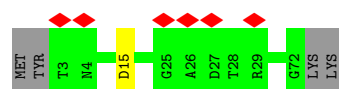
- Molecule 1: Transcription attenuation protein MtrB



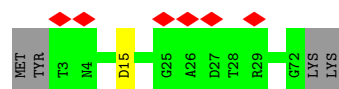
- Molecule 1: Transcription attenuation protein MtrB



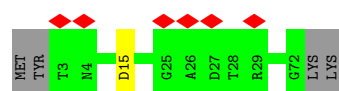
- Molecule 1: Transcription attenuation protein MtrB



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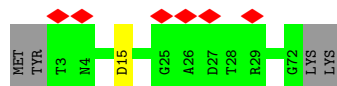


- Molecule 1: Transcription attenuation protein MtrB



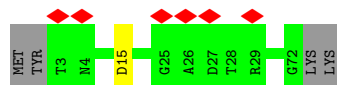
- Molecule 1: Transcription attenuation protein MtrB

Chain yA: 



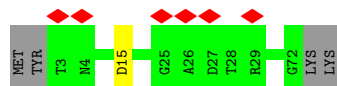
- Molecule 1: Transcription attenuation protein MtrB

Chain zA: 



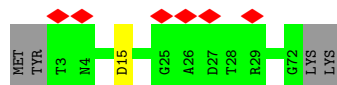
- Molecule 1: Transcription attenuation protein MtrB

Chain 0A: 



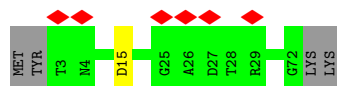
- Molecule 1: Transcription attenuation protein MtrB

Chain 1A: 



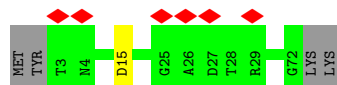
- Molecule 1: Transcription attenuation protein MtrB

Chain 2A: 



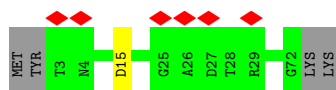
- Molecule 1: Transcription attenuation protein MtrB

Chain 3A: 

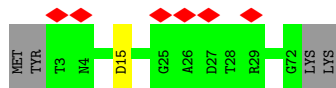


- Molecule 1: Transcription attenuation protein MtrB

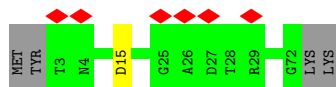
Chain 4A: 



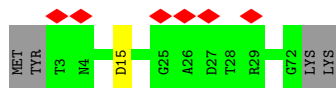
- Molecule 1: Transcription attenuation protein MtrB



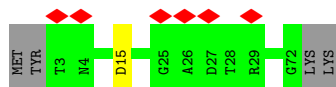
- Molecule 1: Transcription attenuation protein MtrB



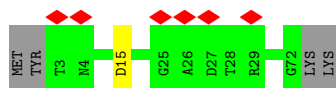
- Molecule 1: Transcription attenuation protein MtrB



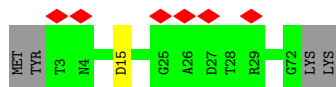
- Molecule 1: Transcription attenuation protein MtrB



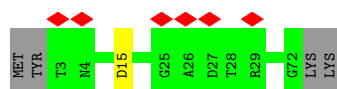
- Molecule 1: Transcription attenuation protein MtrB



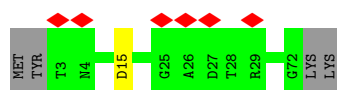
- Molecule 1: Transcription attenuation protein MtrB



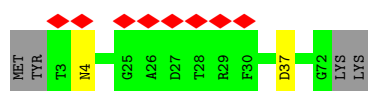
- Molecule 1: Transcription attenuation protein MtrB



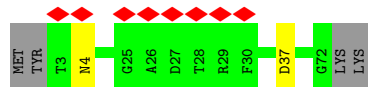
- Molecule 1: Transcription attenuation protein MtrB



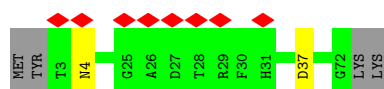
- Molecule 1: Transcription attenuation protein MtrB



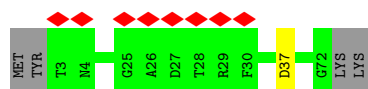
- Molecule 1: Transcription attenuation protein MtrB



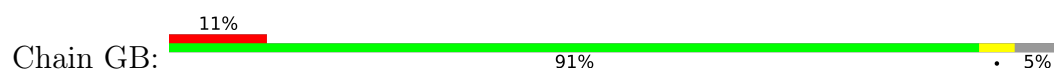
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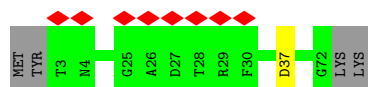
- Molecule 1: Transcription attenuation protein MtrB

Chain HB:  11% 91% 5%



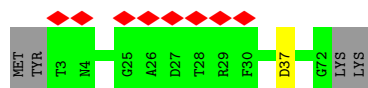
- Molecule 1: Transcription attenuation protein MtrB

Chain IB:  11% 93% 5%




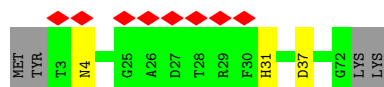
- Molecule 1: Transcription attenuation protein MtrB

Chain JB:  11% 93% 5%



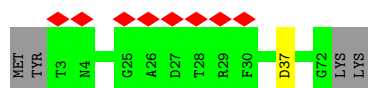
- Molecule 1: Transcription attenuation protein MtrB

Chain KB:  11% 91% 5%



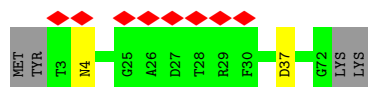
- Molecule 1: Transcription attenuation protein MtrB

Chain LB:  11% 93% 5%



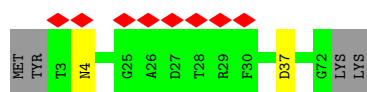
- Molecule 1: Transcription attenuation protein MtrB

Chain MB:  11% 92% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain NB:  11% 92% 5%



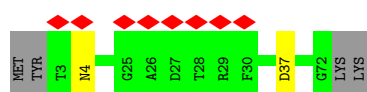
- Molecule 1: Transcription attenuation protein MtrB



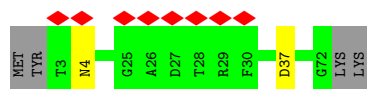
- Molecule 1: Transcription attenuation protein MtrB



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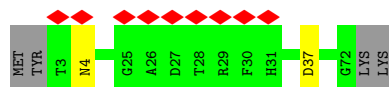
- Molecule 1: Transcription attenuation protein MtrB



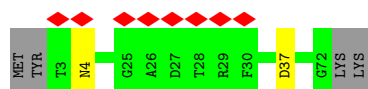
- Molecule 1: Transcription attenuation protein MtrB



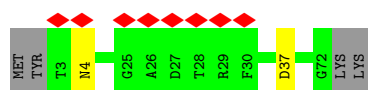
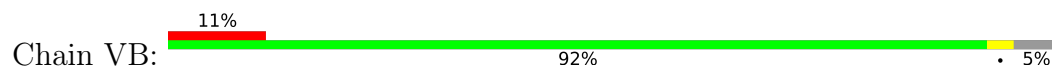
- Molecule 1: Transcription attenuation protein MtrB



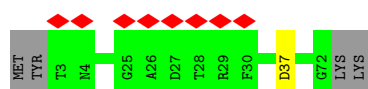
- Molecule 1: Transcription attenuation protein MtrB



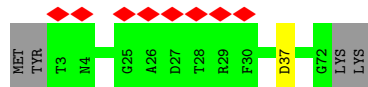
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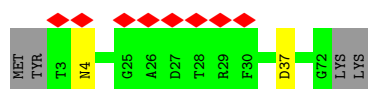
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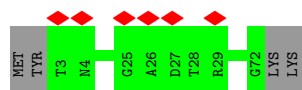
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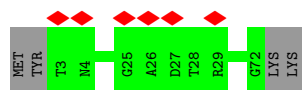
- Molecule 1: Transcription attenuation protein MtrB



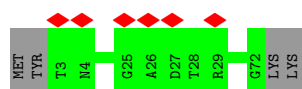
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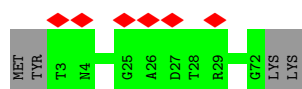
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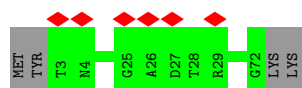
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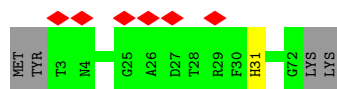
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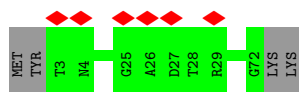


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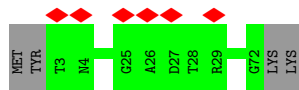


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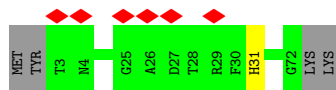
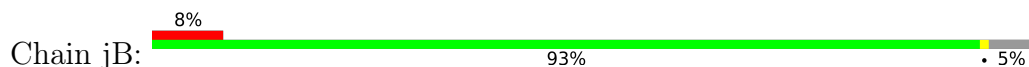
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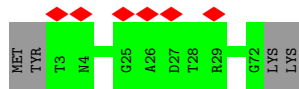
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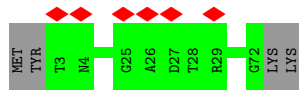
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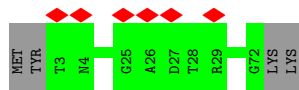
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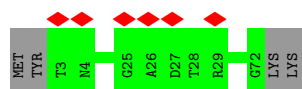
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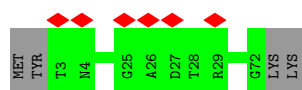
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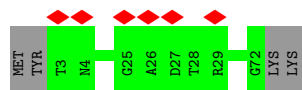
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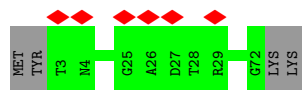
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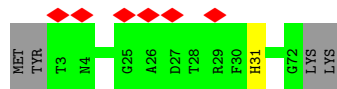
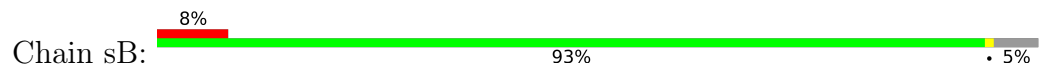
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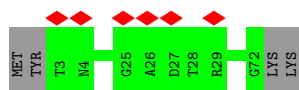


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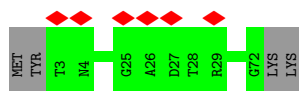


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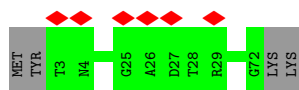
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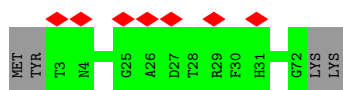
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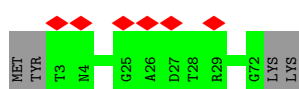
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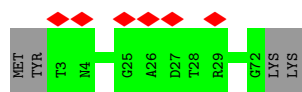
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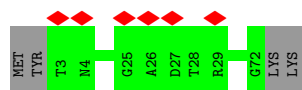
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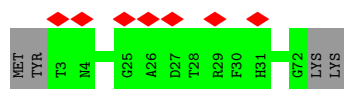
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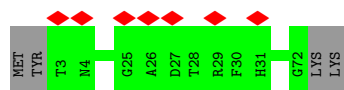
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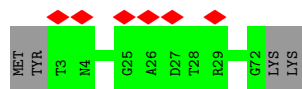
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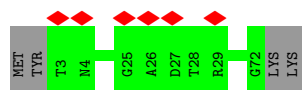
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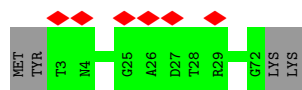


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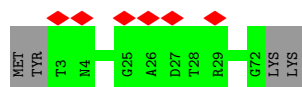




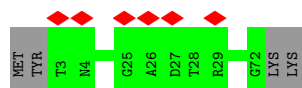
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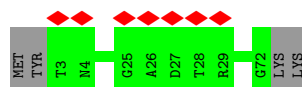
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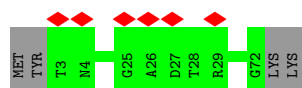
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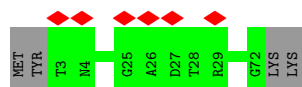
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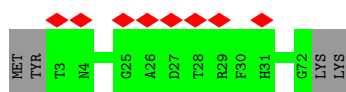


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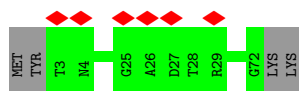


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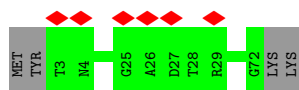
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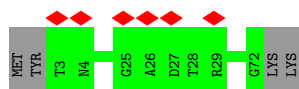
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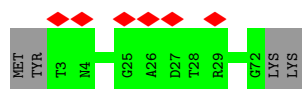
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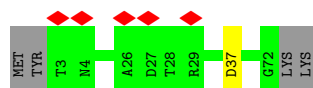
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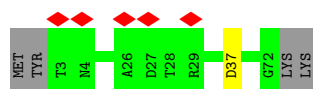
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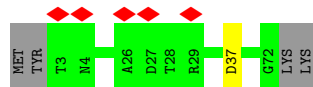
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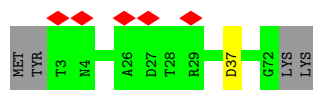
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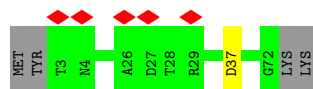
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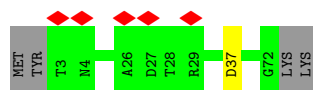
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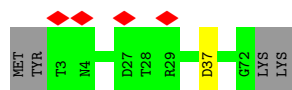
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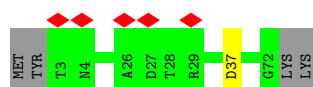
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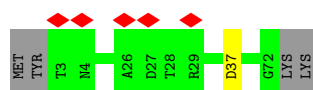
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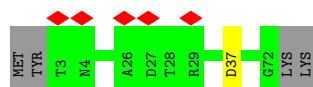
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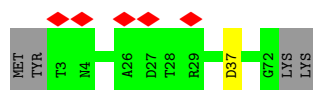
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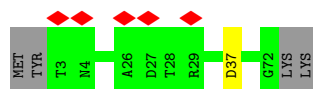
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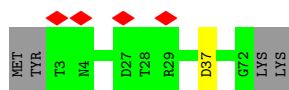


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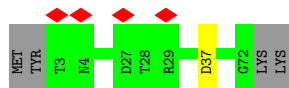


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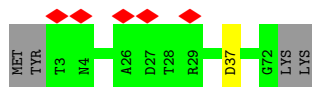




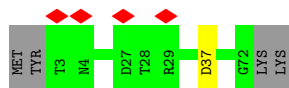
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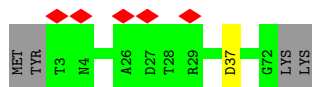
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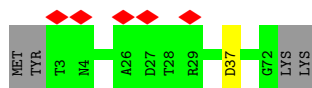
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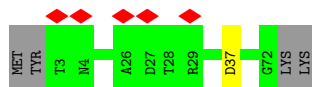
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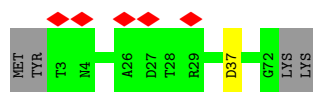
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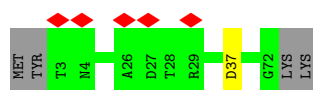
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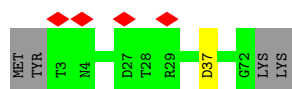
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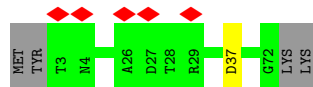
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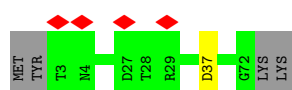
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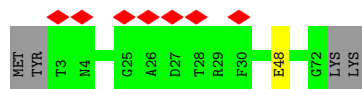
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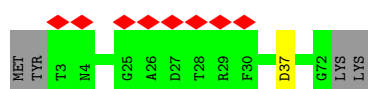
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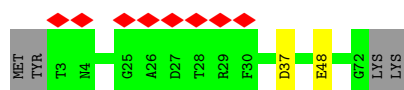
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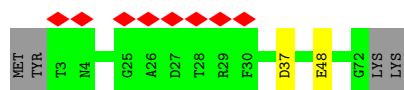
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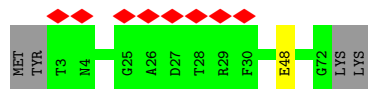
- Molecule 1: Transcription attenuation protein MtrB

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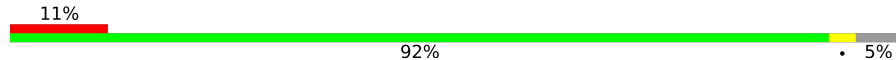


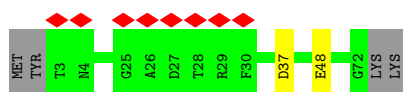
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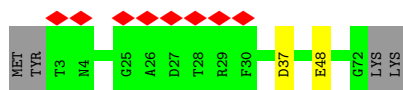
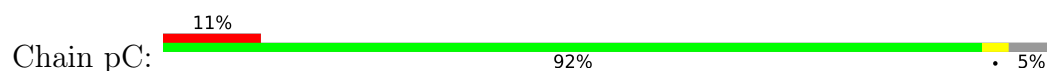


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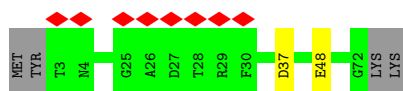
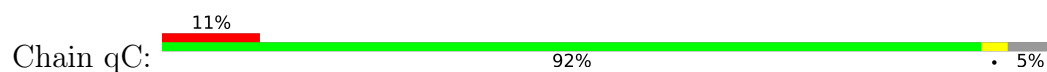
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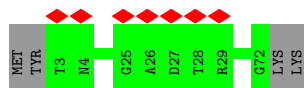
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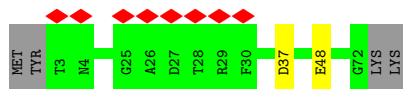
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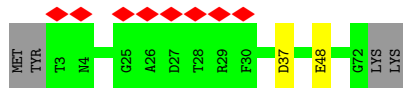
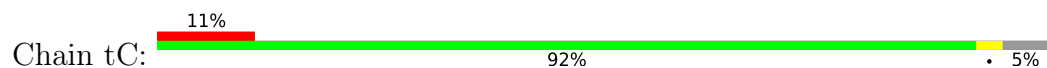
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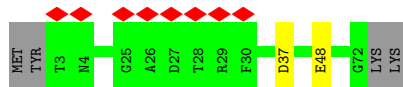
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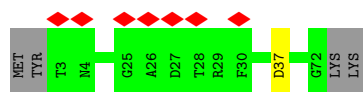


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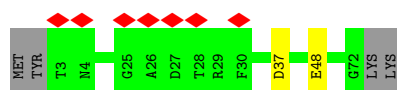


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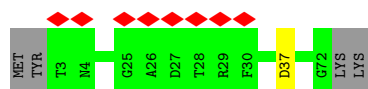




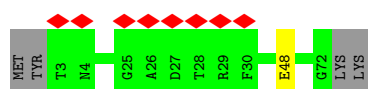
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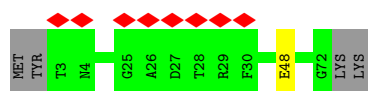
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



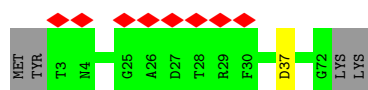
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



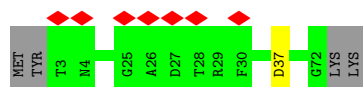
- Molecule 1: Transcription attenuation protein MtrB



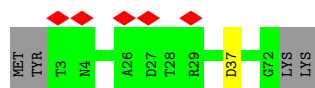
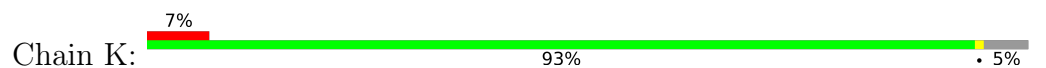
- Molecule 1: Transcription attenuation protein MtrB



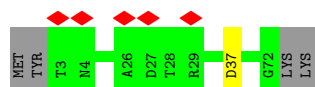
- Molecule 1: Transcription attenuation protein MtrB



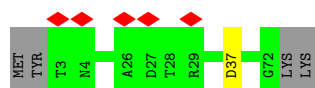
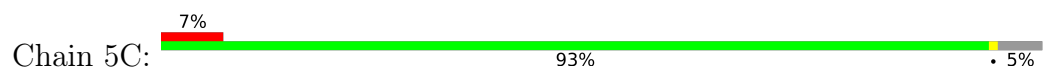
- Molecule 1: Transcription attenuation protein MtrB



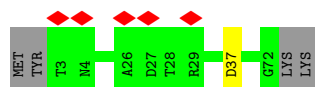
- Molecule 1: Transcription attenuation protein MtrB



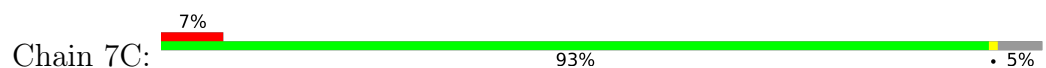
- Molecule 1: Transcription attenuation protein MtrB

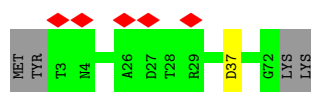


- Molecule 1: Transcription attenuation protein MtrB

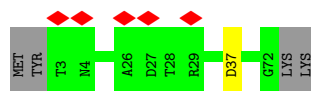


- Molecule 1: Transcription attenuation protein MtrB

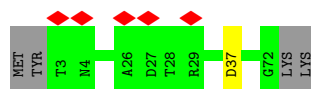




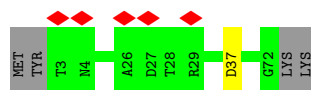
- Molecule 1: Transcription attenuation protein MtrB



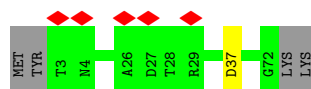
- Molecule 1: Transcription attenuation protein MtrB



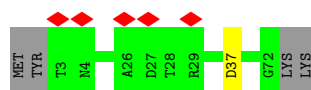
- Molecule 1: Transcription attenuation protein MtrB



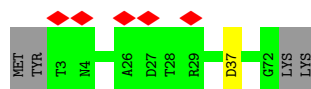
- Molecule 1: Transcription attenuation protein MtrB



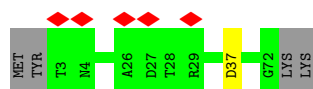
- Molecule 1: Transcription attenuation protein MtrB



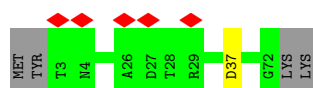
- Molecule 1: Transcription attenuation protein MtrB



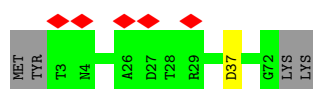
- Molecule 1: Transcription attenuation protein MtrB



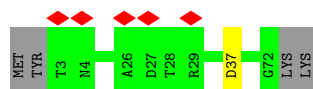
- Molecule 1: Transcription attenuation protein MtrB



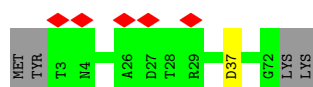
- Molecule 1: Transcription attenuation protein MtrB



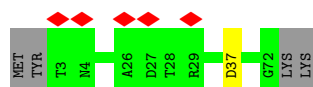
- Molecule 1: Transcription attenuation protein MtrB



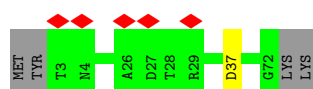
- Molecule 1: Transcription attenuation protein MtrB



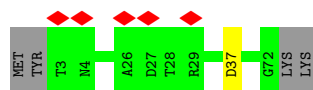
- Molecule 1: Transcription attenuation protein MtrB



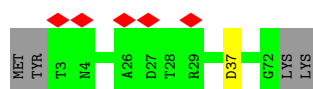
- Molecule 1: Transcription attenuation protein MtrB



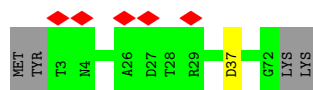
- Molecule 1: Transcription attenuation protein MtrB



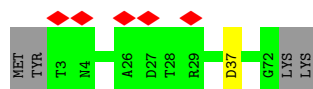
- Molecule 1: Transcription attenuation protein MtrB



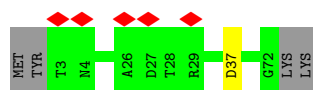
- Molecule 1: Transcription attenuation protein MtrB



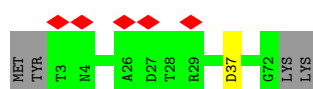
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	161631	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	5.224	Depositor
Minimum map value	-2.655	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.278	Depositor
Recommended contour level	0.976	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	0.27	0/556	0.53	0/749
1	0A	0.27	0/556	0.52	0/749
1	0B	0.28	0/556	0.53	0/749
1	0C	0.27	0/556	0.53	0/749
1	1	0.28	0/556	0.55	0/749
1	1A	0.28	0/556	0.53	0/749
1	1B	0.28	0/556	0.53	0/749
1	1C	0.27	0/556	0.53	0/749
1	2	0.27	0/556	0.53	0/749
1	2A	0.28	0/556	0.53	0/749
1	2B	0.27	0/556	0.52	0/749
1	2C	0.28	0/556	0.53	0/749
1	3	0.27	0/556	0.53	0/749
1	3A	0.28	0/556	0.53	0/749
1	3B	0.28	0/556	0.53	0/749
1	3C	0.27	0/556	0.53	0/749
1	4	0.27	0/556	0.53	0/749
1	4A	0.27	0/556	0.53	0/749
1	4B	0.28	0/556	0.53	0/749
1	4C	0.27	0/556	0.53	0/749
1	5	0.27	0/556	0.53	0/749
1	5A	0.27	0/556	0.52	0/749
1	5B	0.28	0/556	0.53	0/749
1	5C	0.27	0/556	0.53	0/749
1	6	0.27	0/556	0.54	0/749
1	6A	0.27	0/556	0.53	0/749
1	6B	0.28	0/556	0.53	0/749
1	6C	0.27	0/556	0.53	0/749
1	7	0.27	0/556	0.55	0/749
1	7A	0.28	0/556	0.53	0/749
1	7B	0.28	0/556	0.53	0/749
1	7C	0.27	0/556	0.53	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	8	0.27	0/556	0.54	0/749
1	8A	0.28	0/556	0.53	0/749
1	8B	0.28	0/556	0.52	0/749
1	8C	0.27	0/556	0.53	0/749
1	9	0.27	0/556	0.54	0/749
1	9A	0.27	0/556	0.53	0/749
1	9B	0.27	0/556	0.52	0/749
1	9C	0.27	0/556	0.53	0/749
1	A	0.27	0/556	0.53	0/749
1	AA	0.27	0/556	0.54	0/749
1	AB	0.27	0/556	0.53	0/749
1	AC	0.28	0/556	0.53	0/749
1	AD	0.27	0/556	0.53	0/749
1	B	0.27	0/556	0.53	0/749
1	BA	0.27	0/556	0.55	0/749
1	BB	0.28	0/556	0.53	0/749
1	BC	0.28	0/556	0.53	0/749
1	BD	0.27	0/556	0.53	0/749
1	C	0.27	0/556	0.55	0/749
1	CA	0.27	0/556	0.55	0/749
1	CB	0.27	0/556	0.53	0/749
1	CC	0.27	0/556	0.53	0/749
1	CD	0.27	0/556	0.53	0/749
1	D	0.27	0/556	0.54	0/749
1	DA	0.27	0/556	0.55	0/749
1	DB	0.27	0/556	0.53	0/749
1	DC	0.28	0/556	0.53	0/749
1	DD	0.27	0/556	0.53	0/749
1	E	0.27	0/556	0.52	0/749
1	EA	0.27	0/556	0.54	0/749
1	EB	0.27	0/556	0.53	0/749
1	EC	0.27	0/556	0.53	0/749
1	ED	0.27	0/556	0.53	0/749
1	F	0.27	0/556	0.53	0/749
1	FA	0.27	0/556	0.55	0/749
1	FB	0.27	0/556	0.53	0/749
1	FC	0.28	0/556	0.53	0/749
1	FD	0.27	0/556	0.53	0/749
1	G	0.27	0/556	0.54	0/749
1	GA	0.27	0/556	0.54	0/749
1	GB	0.27	0/556	0.53	0/749
1	GC	0.28	0/556	0.53	0/749
1	GD	0.27	0/556	0.54	0/749



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.27	0/556	0.53	0/749
1	HA	0.27	0/556	0.55	0/749
1	HB	0.27	0/556	0.54	0/749
1	HC	0.28	0/556	0.53	0/749
1	HD	0.27	0/556	0.53	0/749
1	I	0.26	0/556	0.53	0/749
1	IA	0.27	0/556	0.55	0/749
1	IB	0.27	0/556	0.53	0/749
1	IC	0.27	0/556	0.52	0/749
1	ID	0.27	0/556	0.54	0/749
1	J	0.27	0/556	0.53	0/749
1	JA	0.27	0/556	0.55	0/749
1	JB	0.27	0/556	0.53	0/749
1	JC	0.28	0/556	0.53	0/749
1	JD	0.27	0/556	0.53	0/749
1	K	0.27	0/556	0.53	0/749
1	KA	0.27	0/556	0.55	0/749
1	KB	0.28	0/556	0.54	0/749
1	KC	0.26	0/556	0.52	0/749
1	KD	0.27	0/556	0.53	0/749
1	L	0.26	0/556	0.54	0/749
1	LA	0.27	0/556	0.55	0/749
1	LB	0.27	0/556	0.53	0/749
1	LC	0.27	0/556	0.52	0/749
1	LD	0.27	0/556	0.53	0/749
1	M	0.27	0/556	0.53	0/749
1	MA	0.27	0/556	0.55	0/749
1	MB	0.27	0/556	0.53	0/749
1	MC	0.27	0/556	0.52	0/749
1	MD	0.27	0/556	0.53	0/749
1	N	0.27	0/556	0.55	0/749
1	NA	0.27	0/556	0.55	0/749
1	NB	0.27	0/556	0.53	0/749
1	NC	0.27	0/556	0.52	0/749
1	ND	0.27	0/556	0.53	0/749
1	O	0.27	0/556	0.54	0/749
1	OA	0.27	0/556	0.54	0/749
1	OB	0.27	0/556	0.54	0/749
1	OC	0.27	0/556	0.53	0/749
1	OD	0.27	0/556	0.53	0/749
1	P	0.27	0/556	0.53	0/749
1	PA	0.27	0/556	0.55	0/749
1	PB	0.27	0/556	0.55	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	PC	0.26	0/556	0.52	0/749
1	PD	0.27	0/556	0.53	0/749
1	Q	0.27	0/556	0.54	0/749
1	QA	0.27	0/556	0.55	0/749
1	QB	0.27	0/556	0.53	0/749
1	QC	0.26	0/556	0.52	0/749
1	QD	0.27	0/556	0.53	0/749
1	R	0.27	0/556	0.54	0/749
1	RA	0.27	0/556	0.55	0/749
1	RB	0.27	0/556	0.53	0/749
1	RC	0.26	0/556	0.53	0/749
1	S	0.27	0/556	0.53	0/749
1	SA	0.27	0/556	0.55	0/749
1	SB	0.27	0/556	0.53	0/749
1	SC	0.27	0/556	0.53	0/749
1	T	0.27	0/556	0.55	0/749
1	TA	0.27	0/556	0.54	0/749
1	TB	0.27	0/556	0.53	0/749
1	TC	0.26	0/556	0.52	0/749
1	U	0.27	0/556	0.53	0/749
1	UA	0.27	0/556	0.54	0/749
1	UB	0.27	0/556	0.53	0/749
1	UC	0.26	0/556	0.52	0/749
1	V	0.27	0/556	0.54	0/749
1	VA	0.27	0/556	0.54	0/749
1	VB	0.27	0/556	0.53	0/749
1	VC	0.26	0/556	0.52	0/749
1	W	0.27	0/556	0.53	0/749
1	WA	0.27	0/556	0.54	0/749
1	WB	0.27	0/556	0.53	0/749
1	WC	0.26	0/556	0.52	0/749
1	XA	0.27	0/556	0.54	0/749
1	XB	0.27	0/556	0.53	0/749
1	XC	0.26	0/556	0.52	0/749
1	Y	0.27	0/556	0.54	0/749
1	YA	0.27	0/556	0.54	0/749
1	YB	0.27	0/556	0.53	0/749
1	YC	0.26	0/556	0.53	0/749
1	Z	0.27	0/556	0.53	0/749
1	ZA	0.27	0/556	0.54	0/749
1	ZB	0.27	0/556	0.53	0/749
1	ZC	0.27	0/556	0.53	0/749
1	a	0.27	0/556	0.54	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	aA	0.27	0/556	0.54	0/749
1	aB	0.27	0/556	0.55	0/749
1	aC	0.27	0/556	0.53	0/749
1	b	0.27	0/556	0.53	0/749
1	bA	0.27	0/556	0.54	0/749
1	bB	0.27	0/556	0.54	0/749
1	bC	0.27	0/556	0.53	0/749
1	c	0.27	0/556	0.53	0/749
1	cA	0.27	0/556	0.55	0/749
1	cB	0.27	0/556	0.55	0/749
1	cC	0.26	0/556	0.52	0/749
1	d	0.27	0/556	0.55	0/749
1	dA	0.27	0/556	0.54	0/749
1	dB	0.27	0/556	0.55	0/749
1	dC	0.27	0/556	0.53	0/749
1	e	0.27	0/556	0.55	0/749
1	eA	0.27	0/556	0.54	0/749
1	eB	0.27	0/556	0.54	0/749
1	eC	0.26	0/556	0.52	0/749
1	f	0.27	0/556	0.53	0/749
1	fA	0.27	0/556	0.54	0/749
1	fB	0.27	0/556	0.55	0/749
1	fC	0.26	0/556	0.52	0/749
1	g	0.27	0/556	0.53	0/749
1	gA	0.27	0/556	0.54	0/749
1	gB	0.27	0/556	0.55	0/749
1	gC	0.26	0/556	0.52	0/749
1	h	0.27	0/556	0.54	0/749
1	hA	0.27	0/556	0.54	0/749
1	hB	0.27	0/556	0.55	0/749
1	hC	0.27	0/556	0.53	0/749
1	i	0.27	0/556	0.53	0/749
1	iA	0.27	0/556	0.55	0/749
1	iB	0.27	0/556	0.54	0/749
1	iC	0.27	0/556	0.53	0/749
1	j	0.28	0/556	0.53	0/749
1	jA	0.27	0/556	0.54	0/749
1	jB	0.27	0/556	0.56	0/749
1	jC	0.27	0/556	0.53	0/749
1	k	0.27	0/556	0.53	0/749
1	kA	0.27	0/556	0.54	0/749
1	kB	0.27	0/556	0.55	0/749
1	kC	0.27	0/556	0.53	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	l	0.27	0/556	0.53	0/749
1	lA	0.27	0/556	0.55	0/749
1	lB	0.27	0/556	0.54	0/749
1	lC	0.27	0/556	0.54	0/749
1	m	0.28	0/556	0.53	0/749
1	mA	0.27	0/556	0.54	0/749
1	mB	0.27	0/556	0.54	0/749
1	mC	0.27	0/556	0.53	0/749
1	n	0.27	0/556	0.53	0/749
1	nA	0.27	0/556	0.54	0/749
1	nB	0.27	0/556	0.55	0/749
1	nC	0.27	0/556	0.54	0/749
1	o	0.27	0/556	0.52	0/749
1	oA	0.27	0/556	0.55	0/749
1	oB	0.27	0/556	0.54	0/749
1	oC	0.27	0/556	0.53	0/749
1	p	0.27	0/556	0.53	0/749
1	pA	0.27	0/556	0.54	0/749
1	pB	0.27	0/556	0.54	0/749
1	pC	0.27	0/556	0.53	0/749
1	q	0.27	0/556	0.53	0/749
1	qA	0.28	0/556	0.53	0/749
1	qB	0.27	0/556	0.55	0/749
1	qC	0.27	0/556	0.52	0/749
1	r	0.28	0/556	0.53	0/749
1	rA	0.28	0/556	0.53	0/749
1	rB	0.27	0/556	0.54	0/749
1	rC	0.27	0/556	0.53	0/749
1	s	0.27	0/556	0.53	0/749
1	sA	0.27	0/556	0.53	0/749
1	sB	0.27	0/556	0.55	0/749
1	sC	0.27	0/556	0.52	0/749
1	t	0.27	0/556	0.53	0/749
1	tA	0.28	0/556	0.53	0/749
1	tB	0.27	0/556	0.55	0/749
1	tC	0.27	0/556	0.53	0/749
1	u	0.27	0/556	0.53	0/749
1	uA	0.27	0/556	0.52	0/749
1	uB	0.27	0/556	0.54	0/749
1	uC	0.27	0/556	0.53	0/749
1	v	0.27	0/556	0.53	0/749
1	vA	0.28	0/556	0.53	0/749
1	vB	0.27	0/556	0.54	0/749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	vC	0.27	0/556	0.53	0/749
1	w	0.27	0/556	0.53	0/749
1	wA	0.27	0/556	0.52	0/749
1	wB	0.27	0/556	0.55	0/749
1	wC	0.27	0/556	0.53	0/749
1	x	0.27	0/556	0.53	0/749
1	xA	0.27	0/556	0.53	0/749
1	xB	0.28	0/556	0.54	0/749
1	xC	0.27	0/556	0.53	0/749
1	y	0.27	0/556	0.53	0/749
1	yA	0.27	0/556	0.52	0/749
1	yB	0.28	0/556	0.53	0/749
1	yC	0.27	0/556	0.53	0/749
1	z	0.27	0/556	0.53	0/749
1	zA	0.28	0/556	0.53	0/749
1	zB	0.28	0/556	0.53	0/749
1	zC	0.27	0/556	0.53	0/749
All	All	0.27	0/146784	0.53	0/197736

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	0A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	0B	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	1B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	1C	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	2	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	2A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	2B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	2C	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	3	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	3A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	3B	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	4B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	4C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	5	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	5A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	5B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	5C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	6	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	6A	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	6B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	6C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	7	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	7A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	7B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	7C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	67 (98%)	1 (2%)	0	100	100
1	8C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	9	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	9A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	9B	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	9C	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	A	68/74 (92%)	66 (97%)	2 (3%)	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%)	67 (98%)	1 (2%)	0	100	100
1	AD	68/74 (92%)	65 (96%)	3 (4%)	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%)	66 (97%)	2 (3%)	0	100	100
1	BC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	BD	68/74 (92%)	65 (96%)	3 (4%)	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
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	CD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	D	68/74 (92%)	66 (97%)	2 (3%)	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%)	67 (98%)	1 (2%)	0	100	100
1	DD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	E	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	EA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	EB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	ED	68/74 (92%)	65 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
1	FC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	FD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	G	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	GA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	GB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	GC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	GD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	H	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	HA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	HB	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	HC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	HD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	I	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	IA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	IB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	IC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	ID	68/74 (92%)	65 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
1	JC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	JD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	K	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	KA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	KB	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	KC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	L	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LA	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
1	LB	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	LC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	LD	68/74 (92%)	65 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
1	MC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	MD	68/74 (92%)	65 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
1	NC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	ND	68/74 (92%)	65 (96%)	3 (4%)	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%)	65 (96%)	3 (4%)	0	100	100
1	OC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	OD	68/74 (92%)	65 (96%)	3 (4%)	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%)	65 (96%)	3 (4%)	0	100	100
1	PC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	PD	68/74 (92%)	65 (96%)	3 (4%)	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%)	67 (98%)	1 (2%)	0	100	100
1	QC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	QD	68/74 (92%)	65 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	67 (98%)	1 (2%)	0	100	100
1	RC	68/74 (92%)	67 (98%)	1 (2%)	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%)	67 (98%)	1 (2%)	0	100	100
1	SC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	T	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	TA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	TB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	UB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	VB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	VC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	W	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	WA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	WB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	WC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	XA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	XB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	YB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	YC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ZA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	ZB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	ZC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	a	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	aA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	aB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	aC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	b	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	bA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	bB	68/74 (92%)	68 (100%)	0	0	100	100
1	bC	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
1	cB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	dB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	dC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	e	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	eA	68/74 (92%)	66 (97%)	2 (3%)	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%)	66 (97%)	2 (3%)	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%)	66 (97%)	2 (3%)	0	100	100
1	gB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	66 (97%)	2 (3%)	0	100	100
1	hB	68/74 (92%)	68 (100%)	0	0	100	100
1	hC	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%)	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%)	66 (97%)	2 (3%)	0	100	100
1	jB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	jC	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%)	67 (98%)	1 (2%)	0	100	100
1	kC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	l	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	lA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	lB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	lC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	m	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	mA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	mB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	nB	68/74 (92%)	68 (100%)	0	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%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	oB	68/74 (92%)	68 (100%)	0	0	100	100
1	oC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	p	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	pA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	pB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	pC	68/74 (92%)	67 (98%)	1 (2%)	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%)	67 (98%)	1 (2%)	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%)	67 (98%)	1 (2%)	0	100	100
1	rC	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	s	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	sA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	sB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	sC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	t	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	tA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	tB	68/74 (92%)	67 (98%)	1 (2%)	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%)	68 (100%)	0	0	100	100
1	uC	68/74 (92%)	67 (98%)	1 (2%)	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%)	68 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	wA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	wB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	xB	68/74 (92%)	67 (98%)	1 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
1	yB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	yC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	z	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	zA	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
1	zB	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	zC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
All	All	17952/19536 (92%)	17515 (98%)	437 (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%)	57 (98%)	1 (2%)	56	78
1	0A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	0B	58/62 (94%)	58 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1B	58/62 (94%)	58 (100%)	0	100	100
1	1C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	2	58/62 (94%)	55 (95%)	3 (5%)	19	39
1	2A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	2B	58/62 (94%)	58 (100%)	0	100	100
1	2C	58/62 (94%)	58 (100%)	0	100	100
1	3	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	3A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	3B	58/62 (94%)	58 (100%)	0	100	100
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%)	58 (100%)	0	100	100
1	4C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	5	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	5A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	5B	58/62 (94%)	58 (100%)	0	100	100
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
1	6B	58/62 (94%)	58 (100%)	0	100	100
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%)	58 (100%)	0	100	100
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%)	58 (100%)	0	100	100
1	8C	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	9	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9A	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	9B	58/62 (94%)	58 (100%)	0	100	100
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%)	58 (100%)	0	100	100
1	AD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	B	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	BA	58/62 (94%)	58 (100%)	0	100	100
1	BB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	BC	58/62 (94%)	58 (100%)	0	100	100
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%)	58 (100%)	0	100	100
1	CD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	D	58/62 (94%)	58 (100%)	0	100	100
1	DA	58/62 (94%)	58 (100%)	0	100	100
1	DB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	DC	58/62 (94%)	58 (100%)	0	100	100
1	DD	58/62 (94%)	57 (98%)	1 (2%)	56	78
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%)	56 (97%)	2 (3%)	32	57
1	EC	58/62 (94%)	58 (100%)	0	100	100
1	ED	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	F	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	FA	58/62 (94%)	58 (100%)	0	100	100
1	FB	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FC	58/62 (94%)	58 (100%)	0	100	100
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%)	55 (95%)	3 (5%)	19	39
1	GC	58/62 (94%)	58 (100%)	0	100	100
1	GD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	H	58/62 (94%)	58 (100%)	0	100	100
1	HA	58/62 (94%)	58 (100%)	0	100	100
1	HB	58/62 (94%)	55 (95%)	3 (5%)	19	39
1	HC	58/62 (94%)	58 (100%)	0	100	100
1	HD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	I	58/62 (94%)	57 (98%)	1 (2%)	56	78
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%)	58 (100%)	0	100	100
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
1	JC	58/62 (94%)	58 (100%)	0	100	100
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%)	55 (95%)	3 (5%)	19	39
1	KC	58/62 (94%)	57 (98%)	1 (2%)	56	78
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%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	M	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	MA	58/62 (94%)	58 (100%)	0	100	100
1	MB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	MC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	MD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	N	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	NA	58/62 (94%)	58 (100%)	0	100	100
1	NB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	NC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	ND	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%)	58 (100%)	0	100	100
1	OB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	OC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	OD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	P	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	PA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	PB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	PC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	PD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	Q	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	QA	58/62 (94%)	58 (100%)	0	100	100
1	QB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	QC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	QD	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	R	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	RA	58/62 (94%)	58 (100%)	0	100	100
1	RB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	RC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	S	58/62 (94%)	56 (97%)	2 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SA	58/62 (94%)	58 (100%)	0	100	100
1	SB	58/62 (94%)	55 (95%)	3 (5%)	19	39
1	SC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	T	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	TA	58/62 (94%)	58 (100%)	0	100	100
1	TB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	TC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	U	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	UA	58/62 (94%)	58 (100%)	0	100	100
1	UB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	UC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	V	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	VA	58/62 (94%)	58 (100%)	0	100	100
1	VB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	VC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	W	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	WA	58/62 (94%)	58 (100%)	0	100	100
1	WB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	WC	58/62 (94%)	57 (98%)	1 (2%)	56	78
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%)	56 (97%)	2 (3%)	32	57
1	YA	58/62 (94%)	58 (100%)	0	100	100
1	YB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	YC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	Z	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	ZA	58/62 (94%)	58 (100%)	0	100	100
1	ZB	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	ZC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	a	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	58/62 (94%)	58 (100%)	0	100	100
1	aB	58/62 (94%)	58 (100%)	0	100	100
1	aC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	b	58/62 (94%)	56 (97%)	2 (3%)	32	57
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	c	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	cA	58/62 (94%)	58 (100%)	0	100	100
1	cB	58/62 (94%)	58 (100%)	0	100	100
1	cC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	d	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	dA	58/62 (94%)	58 (100%)	0	100	100
1	dB	58/62 (94%)	58 (100%)	0	100	100
1	dC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	e	58/62 (94%)	56 (97%)	2 (3%)	32	57
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	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%)	57 (98%)	1 (2%)	56	78
1	fC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	g	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	gA	58/62 (94%)	58 (100%)	0	100	100
1	gB	58/62 (94%)	58 (100%)	0	100	100
1	gC	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%)	56 (97%)	2 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	iA	58/62 (94%)	58 (100%)	0	100	100
1	iB	58/62 (94%)	58 (100%)	0	100	100
1	iC	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
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%)	58 (100%)	0	100	100
1	kB	58/62 (94%)	58 (100%)	0	100	100
1	kC	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	58 (100%)	0	100	100
1	lC	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%)	58 (100%)	0	100	100
1	mC	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	58 (100%)	0	100	100
1	nC	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	o	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	56 (97%)	2 (3%)	32	57
1	p	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	pA	58/62 (94%)	58 (100%)	0	100	100
1	pB	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	pC	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	q	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	56 (97%)	2 (3%)	32	57
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%)	58 (100%)	0	100	100
1	s	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	sA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	sB	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	sC	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	56 (97%)	2 (3%)	32	57
1	u	58/62 (94%)	56 (97%)	2 (3%)	32	57
1	uA	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	uB	58/62 (94%)	58 (100%)	0	100	100
1	uC	58/62 (94%)	56 (97%)	2 (3%)	32	57
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%)	56 (97%)	2 (3%)	32	57
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%)	56 (97%)	2 (3%)	32	57
1	x	58/62 (94%)	57 (98%)	1 (2%)	56	78
1	xA	58/62 (94%)	57 (98%)	1 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	xB	58/62 (94%)	58 (100%)	0	100	100
1	xC	58/62 (94%)	57 (98%)	1 (2%)	56	78
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%)	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%)	58 (100%)	0	100	100
1	zC	58/62 (94%)	57 (98%)	1 (2%)	56	78
All	All	15312/16368 (94%)	15089 (98%)	223 (2%)	60	81

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	MB	37	ASP
1	PD	37	ASP
1	I	37	ASP
1	ND	37	ASP
1	K	37	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	OC	31	HIS
1	eC	31	HIS
1	TC	31	HIS
1	dC	32	HIS
1	bC	31	HIS

### 5.3.3 RNA ⓘ

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.



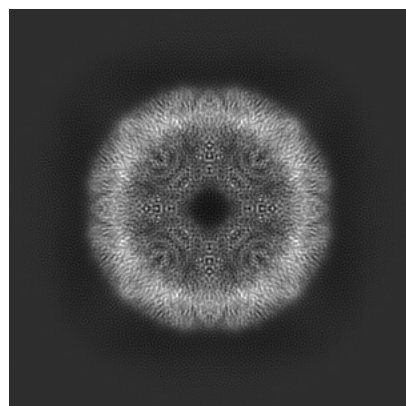
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18905. These allow visual inspection of the internal detail of the map and identification of artifacts.

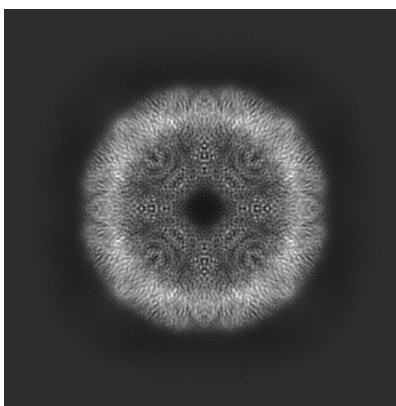
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

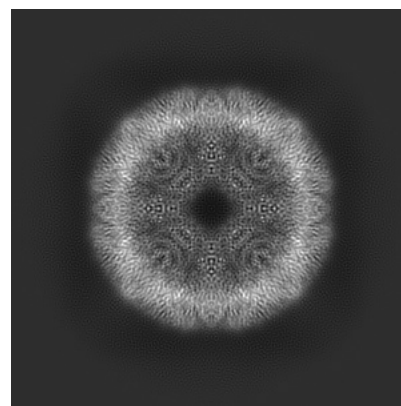
#### 6.1.1 Primary map



X

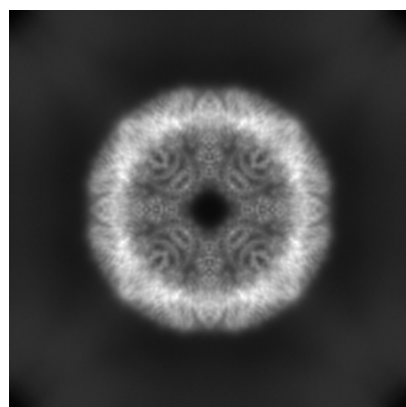


Y

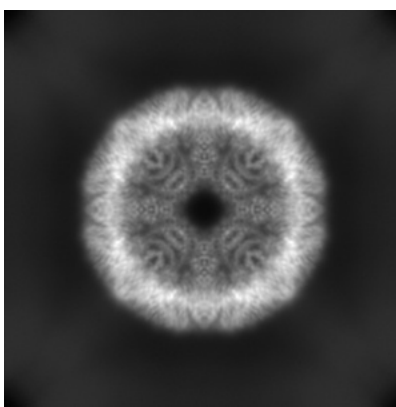


Z

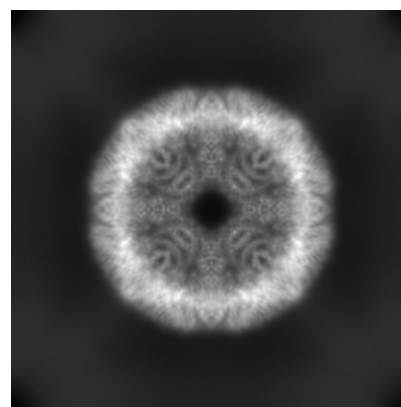
#### 6.1.2 Raw map



X



Y

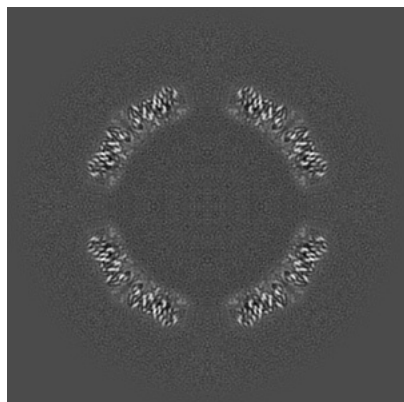


Z

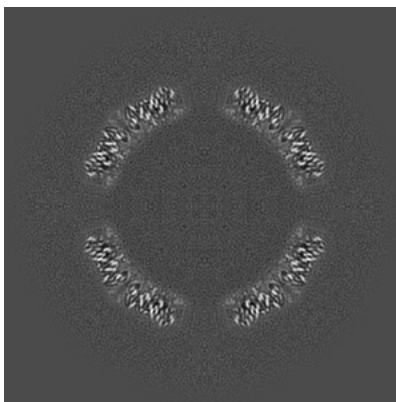
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

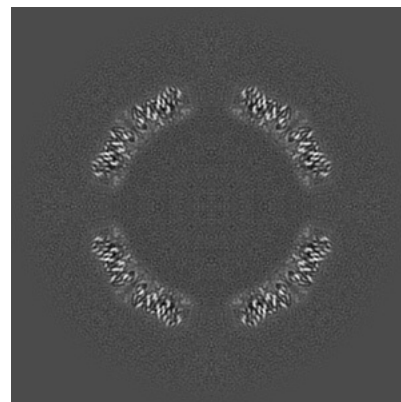
### 6.2.1 Primary map



X Index: 225

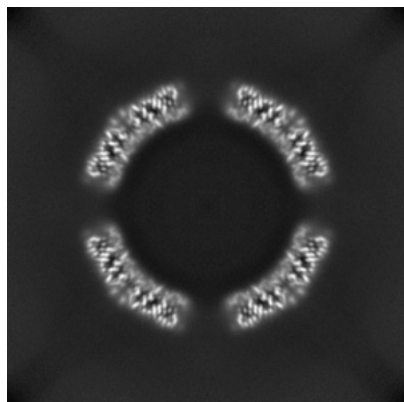


Y Index: 225

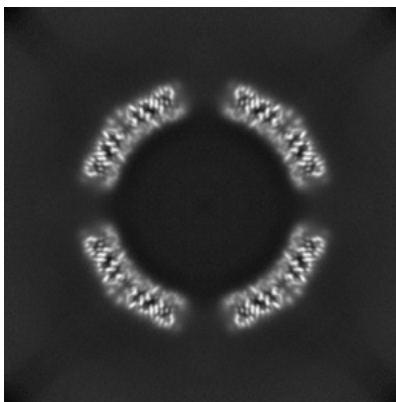


Z Index: 225

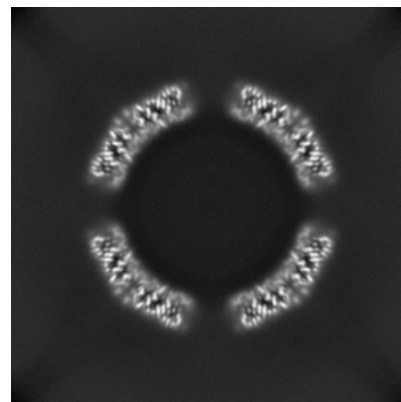
### 6.2.2 Raw map



X Index: 225



Y Index: 225

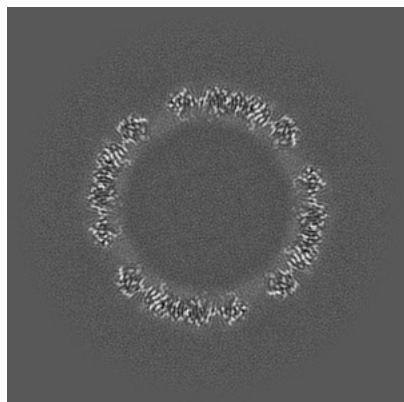


Z Index: 225

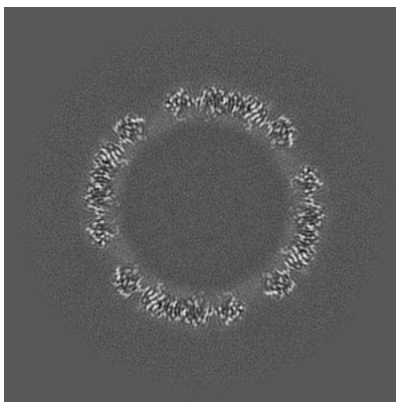
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

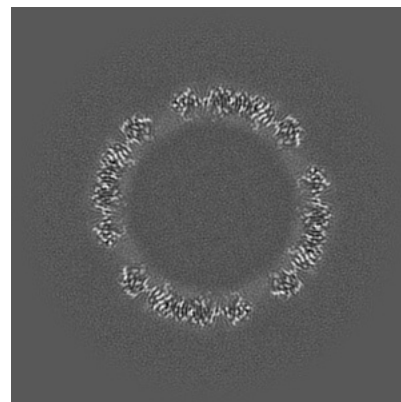
### 6.3.1 Primary map



X Index: 189

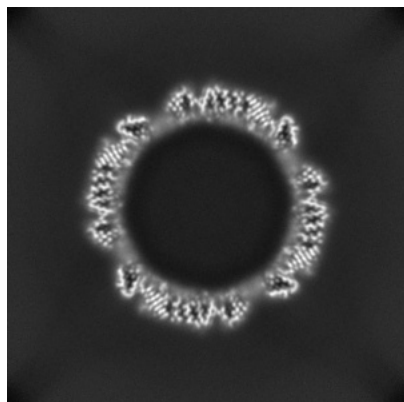


Y Index: 189

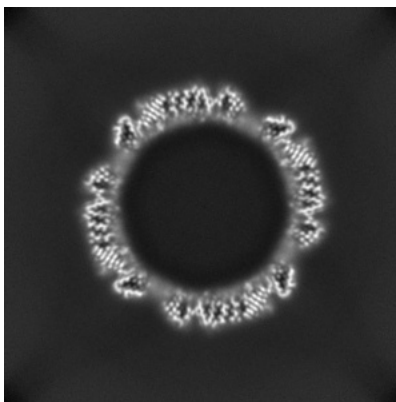


Z Index: 189

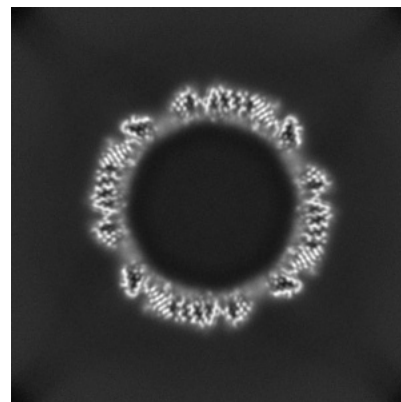
### 6.3.2 Raw map



X Index: 188



Y Index: 262

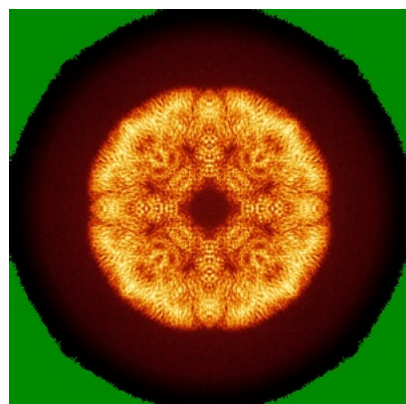


Z Index: 188

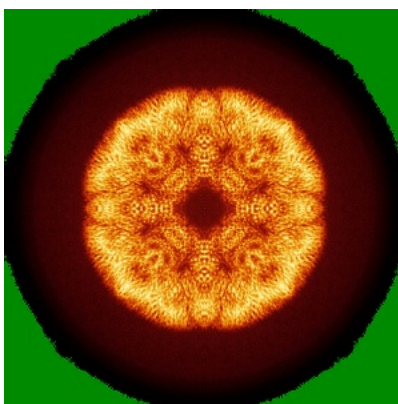
The images above show the largest variance slices of the map in three orthogonal directions.

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

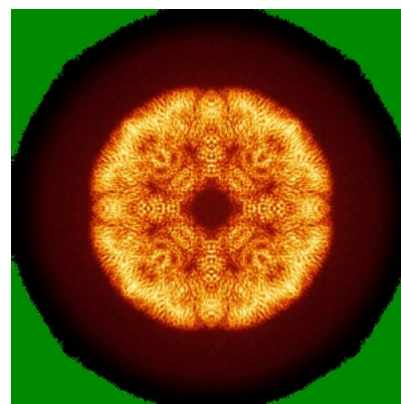
### 6.4.1 Primary map



X

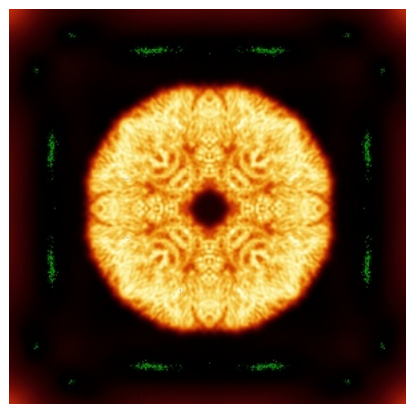


Y

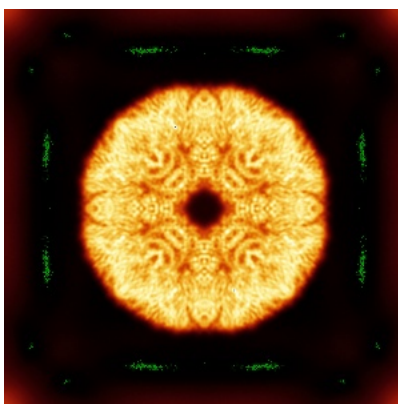


Z

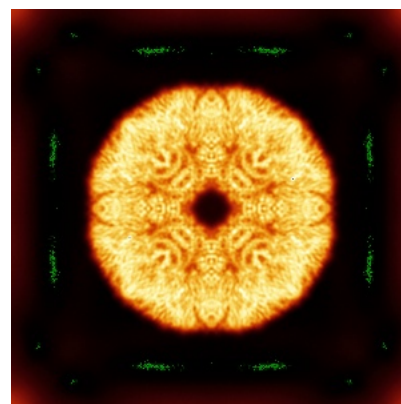
### 6.4.2 Raw map



X



Y

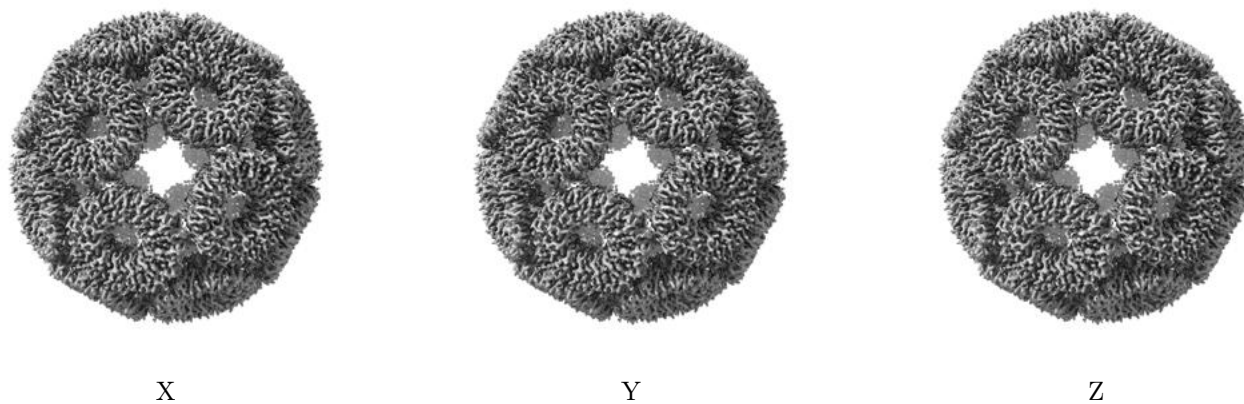


Z

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.

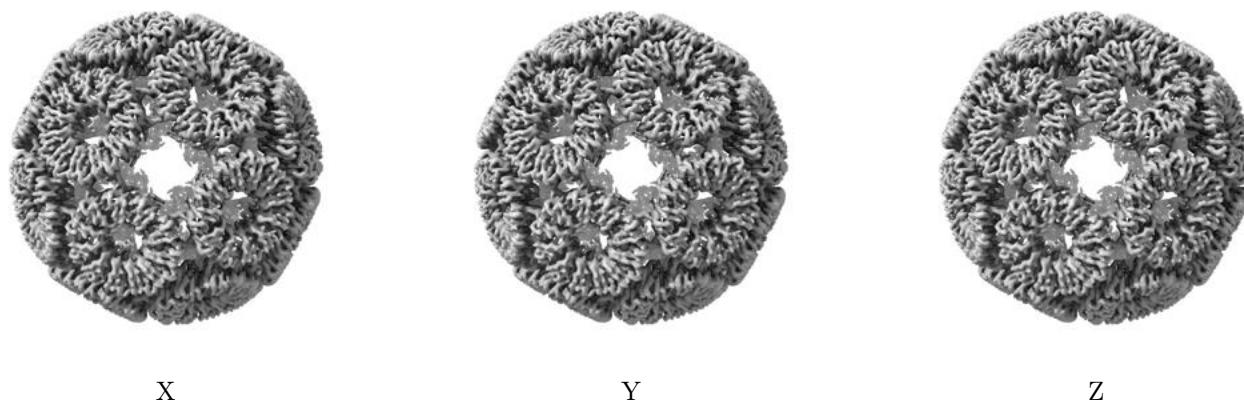
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.976. 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.

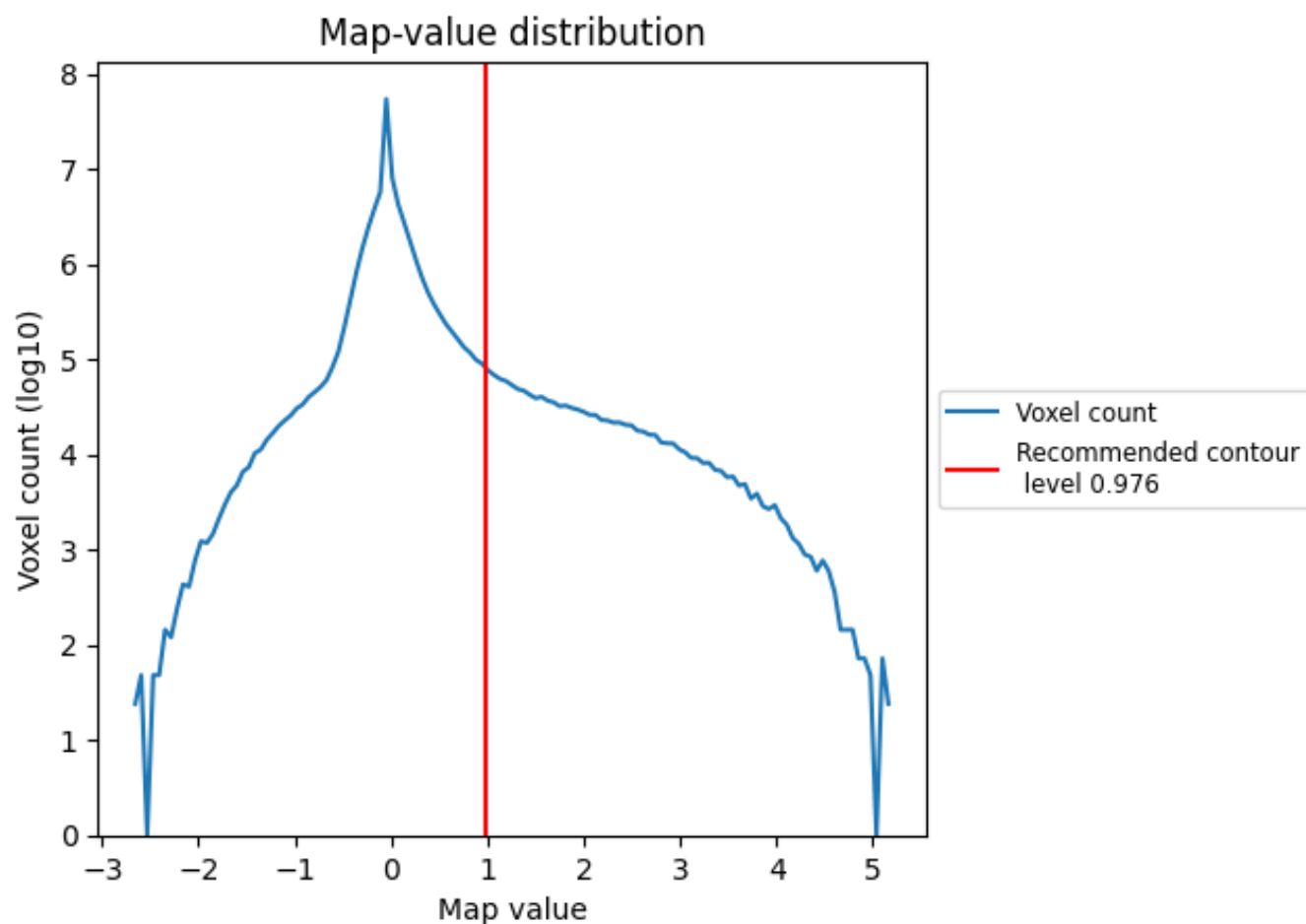
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

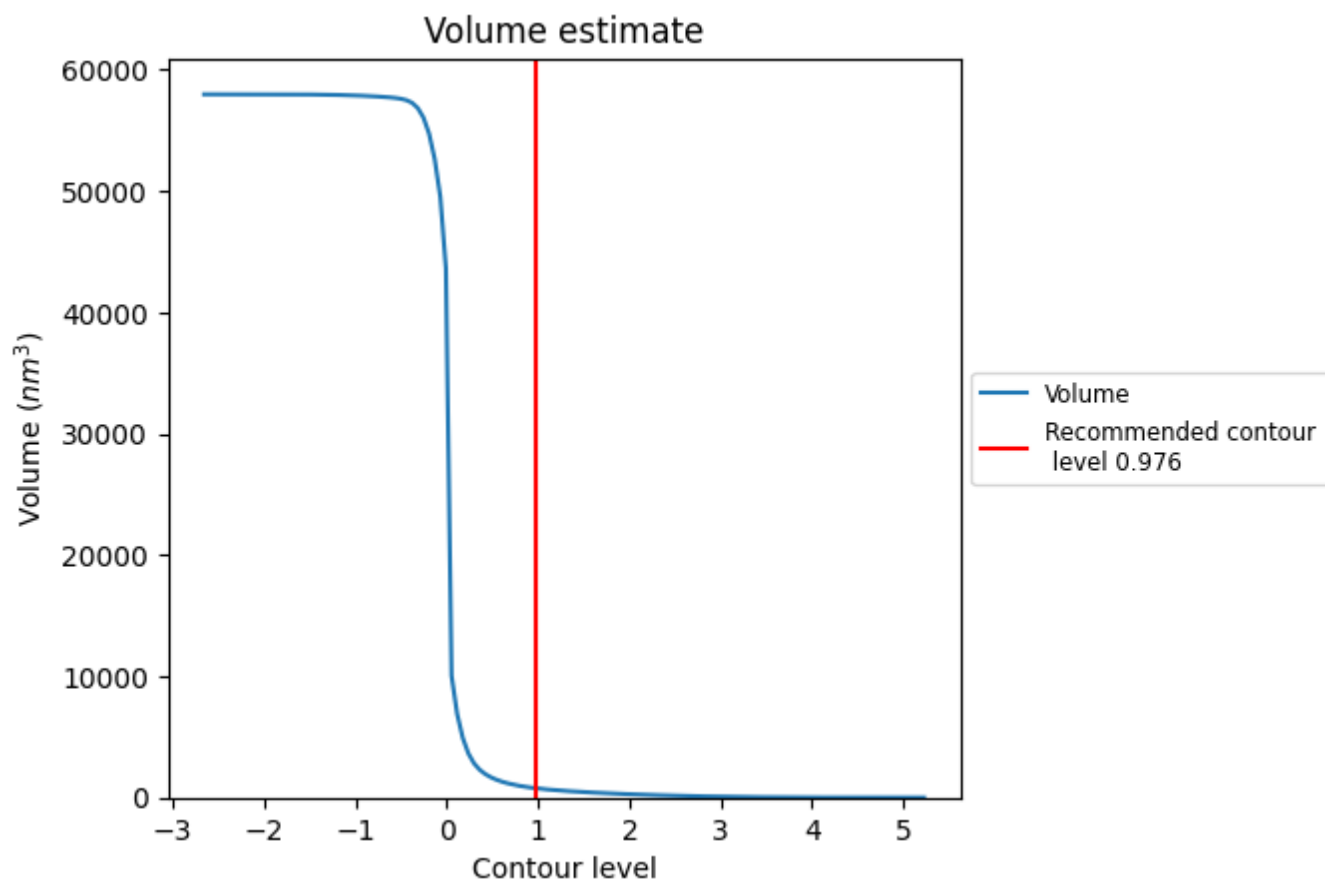
This section contains the results of statistical analysis of the map.

### 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](#)

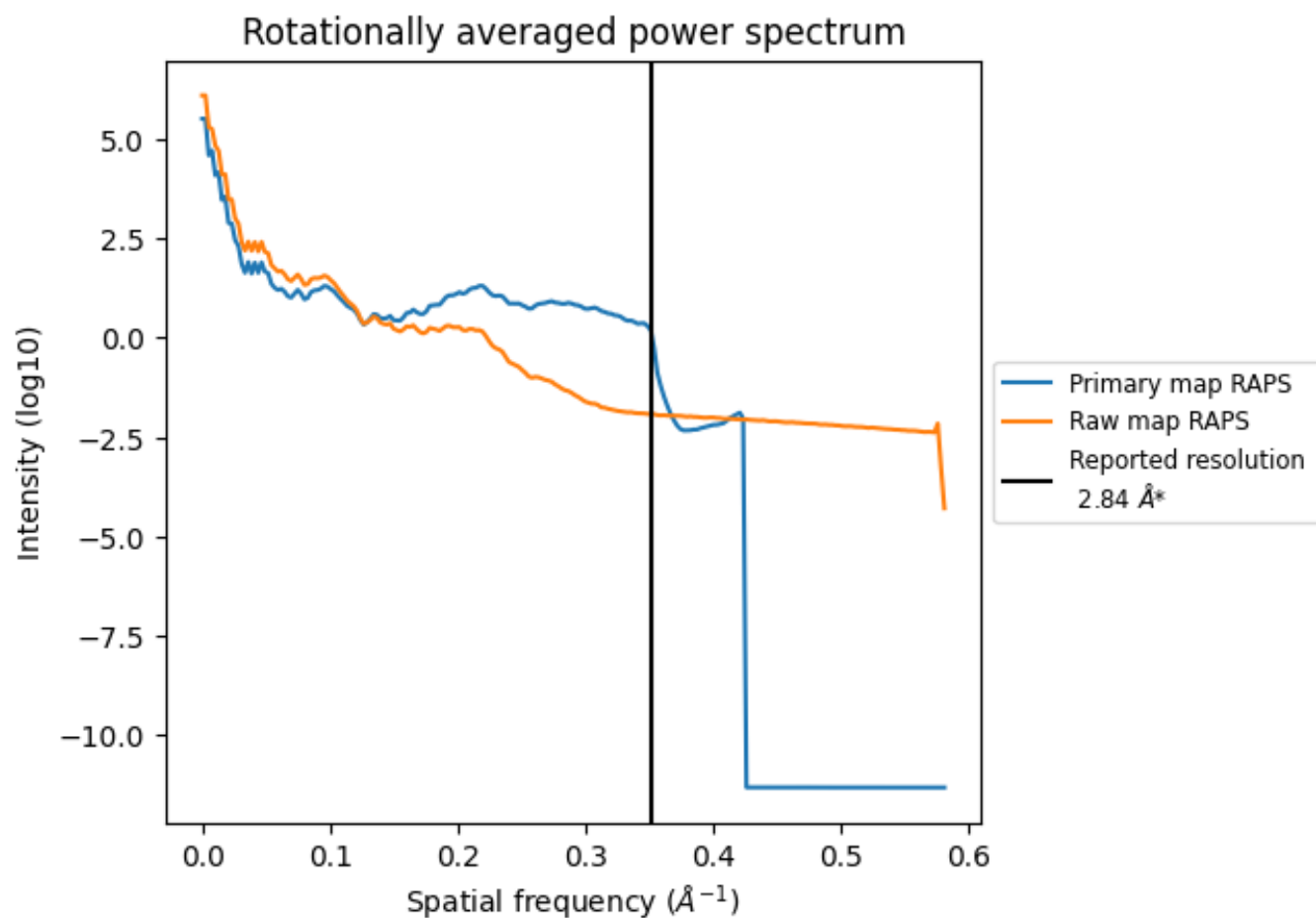


The volume at the recommended contour level is 769 nm<sup>3</sup>; this corresponds to an approximate mass of 695 kDa.

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 ⓘ



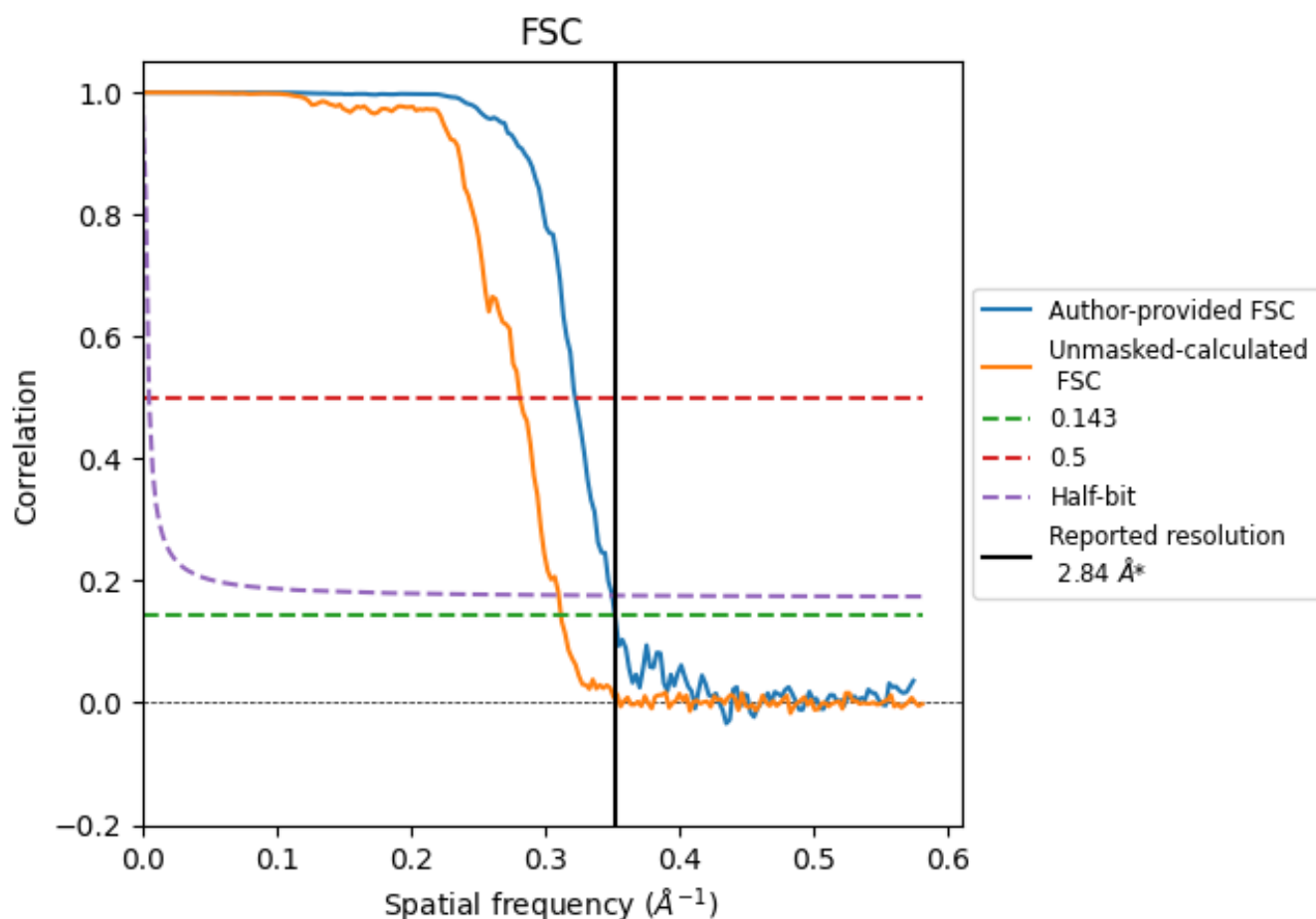
\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>



## 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 0.352  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

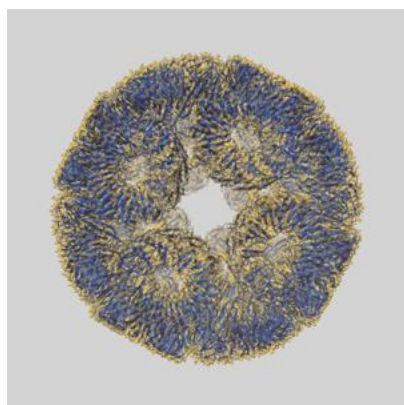
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.10	2.85
Unmasked-calculated*	3.20	3.55	3.22

\*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 2.84 by more than 10 %

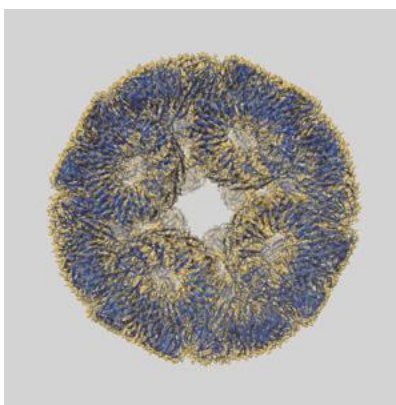
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18905 and PDB model 8R5A. Per-residue inclusion information can be found in section [3](#) on page [46](#).

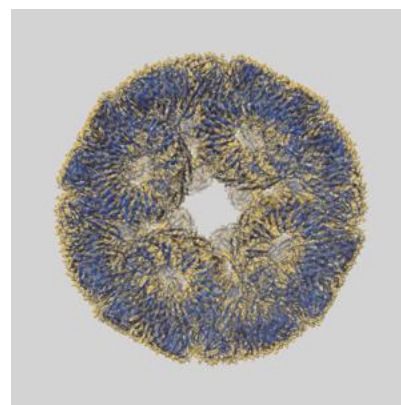
### 9.1 Map-model overlay [i](#)



X



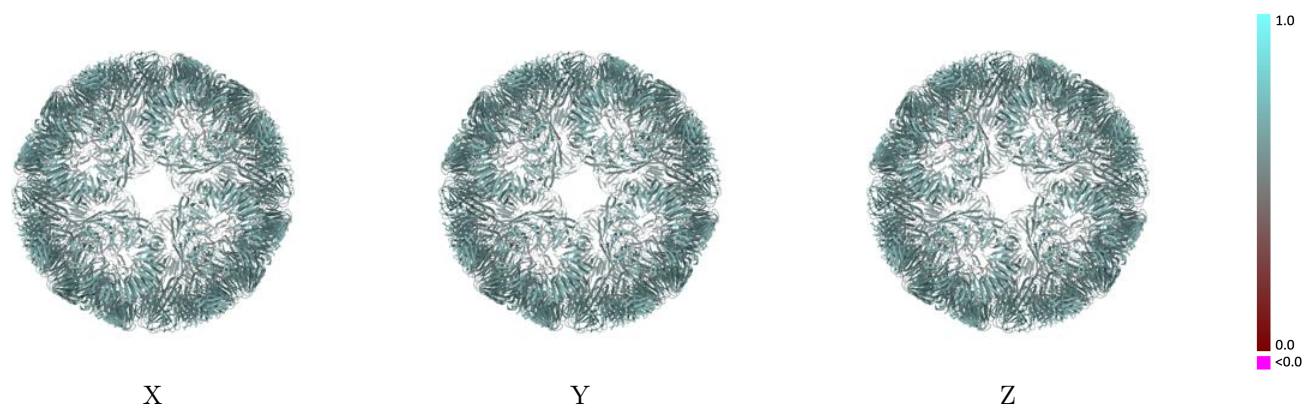
Y



Z

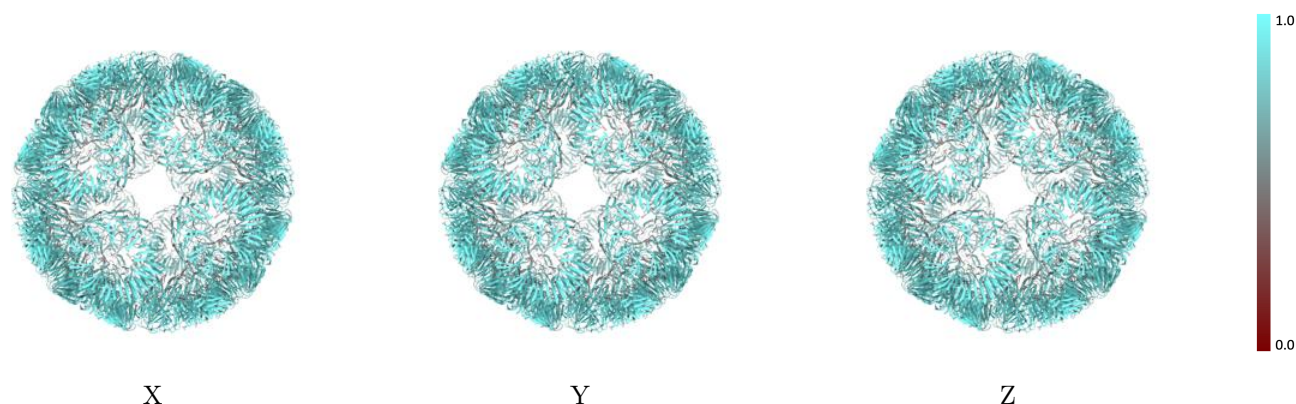
The images above show the 3D surface view of the map at the recommended contour level 0.976 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



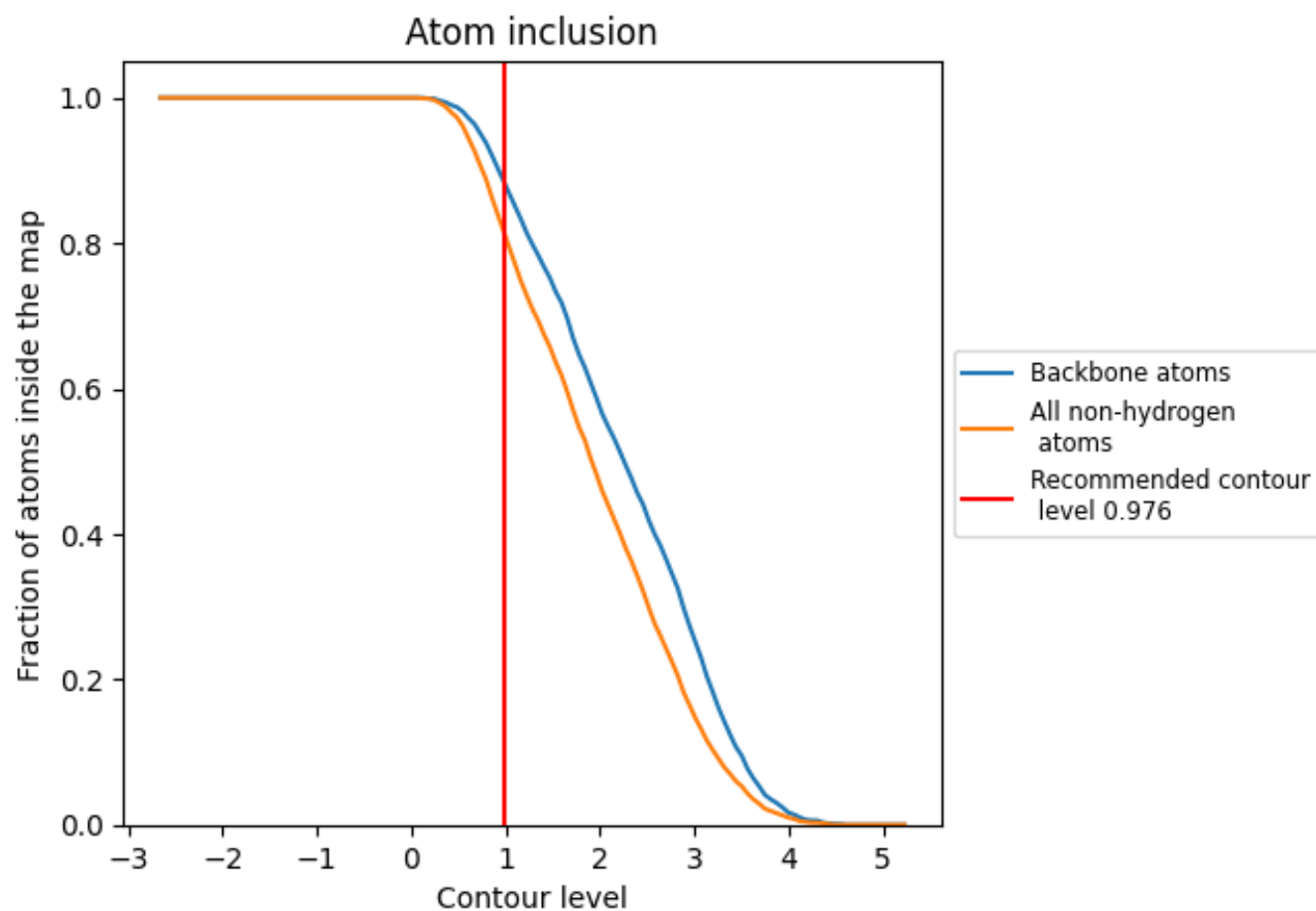
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.976).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.976) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.6050
0	 0.8440	 0.6130
0A	 0.8030	 0.6090
0B	 0.8050	 0.6030
0C	 0.8250	 0.6020
1	 0.8330	 0.6120
1A	 0.8030	 0.6020
1B	 0.8010	 0.5970
1C	 0.8220	 0.6040
2	 0.8220	 0.6040
2A	 0.8010	 0.6010
2B	 0.8030	 0.6000
2C	 0.8220	 0.5980
3	 0.8400	 0.6120
3A	 0.8050	 0.6070
3B	 0.8010	 0.5980
3C	 0.8270	 0.6010
4	 0.8380	 0.6140
4A	 0.8030	 0.6010
4B	 0.8050	 0.6010
4C	 0.8150	 0.6080
5	 0.8420	 0.6130
5A	 0.8030	 0.6090
5B	 0.8050	 0.5960
5C	 0.8160	 0.6070
6	 0.8330	 0.6040
6A	 0.8000	 0.6020
6B	 0.8030	 0.6010
6C	 0.8160	 0.6050
7	 0.8310	 0.6080
7A	 0.8010	 0.6060
7B	 0.8030	 0.5970
7C	 0.8150	 0.6130
8	 0.8370	 0.6050
8A	 0.8050	 0.6080























































































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Chain	Atom inclusion	Q-score
8B	 0.8010	 0.5980
8C	 0.8180	 0.6080
9	 0.8330	 0.6090
9A	 0.8030	 0.6070
9B	 0.7980	 0.5930
9C	 0.8150	 0.6160
A	 0.8440	 0.6110
AA	 0.8310	 0.6080
AB	 0.8030	 0.6020
AC	 0.8030	 0.6000
AD	 0.8160	 0.6130
B	 0.8400	 0.6100
BA	 0.8350	 0.6110
BB	 0.8050	 0.6050
BC	 0.8030	 0.5970
BD	 0.8160	 0.6120
C	 0.8330	 0.6050
CA	 0.8350	 0.6100
CB	 0.8030	 0.6080
CC	 0.7940	 0.5900
CD	 0.8160	 0.6100
D	 0.7860	 0.5930
DA	 0.8310	 0.6080
DB	 0.7940	 0.5920
DC	 0.8030	 0.5970
DD	 0.8160	 0.6120
E	 0.8050	 0.6050
EA	 0.8350	 0.6100
EB	 0.8000	 0.5970
EC	 0.8030	 0.6010
ED	 0.8180	 0.6120
F	 0.7940	 0.5960
FA	 0.8370	 0.6100
FB	 0.7960	 0.5940
FC	 0.8010	 0.6010
FD	 0.8160	 0.6100
G	 0.8200	 0.6090
GA	 0.8390	 0.6090
GB	 0.8000	 0.5960
GC	 0.8000	 0.5970
GD	 0.8160	 0.6060
H	 0.8030	 0.6000

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Chain	Atom inclusion	Q-score
HA	 0.8350	 0.6040
HB	 0.7940	 0.5930
HC	 0.8030	 0.5960
HD	 0.8160	 0.6090
I	 0.8230	 0.6150
IA	 0.8350	 0.6040
IB	 0.7960	 0.5980
IC	 0.8010	 0.5990
ID	 0.8160	 0.6050
J	 0.8200	 0.6050
JA	 0.8350	 0.6070
JB	 0.7960	 0.5990
JC	 0.8010	 0.5960
JD	 0.8150	 0.6130
K	 0.8150	 0.6100
KA	 0.8330	 0.6040
KB	 0.7980	 0.5960
KC	 0.8250	 0.6120
KD	 0.8160	 0.6100
L	 0.8460	 0.6050
LA	 0.8350	 0.6090
LB	 0.7940	 0.5920
LC	 0.8230	 0.6120
LD	 0.8160	 0.6120
M	 0.8480	 0.6090
MA	 0.8310	 0.6110
MB	 0.7960	 0.5950
MC	 0.8230	 0.6100
MD	 0.8160	 0.6120
N	 0.8480	 0.6050
NA	 0.8350	 0.6090
NB	 0.7960	 0.6000
NC	 0.8230	 0.6130
ND	 0.8150	 0.6120
O	 0.8440	 0.6140
OA	 0.8310	 0.6120
OB	 0.8070	 0.5920
OC	 0.8230	 0.6130
OD	 0.8150	 0.6110
P	 0.8440	 0.6150
PA	 0.8290	 0.6060
PB	 0.7980	 0.5940

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Chain	Atom inclusion	Q-score
PC	 0.8330	 0.6140
PD	 0.8160	 0.6140
Q	 0.8460	 0.6160
QA	 0.8350	 0.6080
QB	 0.7960	 0.5960
QC	 0.8250	 0.6140
QD	 0.8160	 0.6140
R	 0.8480	 0.6150
RA	 0.8350	 0.6070
RB	 0.7960	 0.5930
RC	 0.8230	 0.6090
S	 0.8460	 0.6140
SA	 0.8350	 0.6100
SB	 0.8010	 0.6010
SC	 0.8230	 0.6090
T	 0.8440	 0.6150
TA	 0.7900	 0.5930
TB	 0.7980	 0.5900
TC	 0.8250	 0.6140
U	 0.8440	 0.6170
UA	 0.7880	 0.5980
UB	 0.7940	 0.6000
UC	 0.8250	 0.6110
V	 0.8480	 0.6140
VA	 0.7880	 0.5960
VB	 0.7940	 0.5980
VC	 0.8310	 0.6130
W	 0.8460	 0.6090
WA	 0.7880	 0.5970
WB	 0.7960	 0.5980
WC	 0.8330	 0.6100
XA	 0.7880	 0.5960
XB	 0.7960	 0.5960
XC	 0.8250	 0.6140
Y	 0.8460	 0.6070
YA	 0.7920	 0.5980
YB	 0.7960	 0.5990
YC	 0.8290	 0.6100
Z	 0.8460	 0.6080
ZA	 0.7840	 0.5990
ZB	 0.7960	 0.6000
ZC	 0.8220	 0.6120





















































































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Chain	Atom inclusion	Q-score
a	 0.8460	 0.6100
aA	 0.7860	 0.5980
aB	 0.8200	 0.6040
aC	 0.8200	 0.6110
b	 0.8480	 0.6140
bA	 0.7860	 0.5940
bB	 0.8200	 0.6110
bC	 0.8250	 0.6140
c	 0.8480	 0.6150
cA	 0.7860	 0.5940
cB	 0.8180	 0.6040
cC	 0.8250	 0.6160
d	 0.8440	 0.6120
dA	 0.7860	 0.5970
dB	 0.8200	 0.6110
dC	 0.8250	 0.6090
e	 0.8440	 0.6170
eA	 0.7920	 0.5940
eB	 0.8200	 0.6080
eC	 0.8310	 0.6120
f	 0.8440	 0.6180
fA	 0.7900	 0.5920
fB	 0.8200	 0.6100
fC	 0.8250	 0.6130
g	 0.8440	 0.6150
gA	 0.7900	 0.5970
gB	 0.8200	 0.6090
gC	 0.8350	 0.6110
h	 0.8440	 0.6160
hA	 0.7860	 0.5940
hB	 0.8180	 0.6090
hC	 0.8220	 0.6020
i	 0.8480	 0.6120
iA	 0.7840	 0.5970
iB	 0.8200	 0.6080
iC	 0.8140	 0.5990
j	 0.8440	 0.6090
jA	 0.7880	 0.5970
jB	 0.8220	 0.6080
jC	 0.8200	 0.5990
k	 0.8400	 0.6100
kA	 0.7880	 0.5990









































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Chain	Atom inclusion	Q-score
kB	 0.8200	 0.6070
kC	 0.8200	 0.6020
l	 0.8270	 0.6010
lA	 0.7860	 0.5980
lB	 0.8200	 0.6070
lC	 0.8140	 0.5970
m	 0.8420	 0.6130
mA	 0.7880	 0.5960
mB	 0.8200	 0.6060
mC	 0.8160	 0.6010
n	 0.8400	 0.6140
nA	 0.7880	 0.5960
nB	 0.8200	 0.6080
nC	 0.8160	 0.5970
o	 0.8490	 0.6160
oA	 0.7840	 0.5960
oB	 0.8200	 0.6080
oC	 0.8160	 0.5970
p	 0.8380	 0.6150
pA	 0.7950	 0.6000
pB	 0.8200	 0.6120
pC	 0.8200	 0.6020
q	 0.8400	 0.6130
qA	 0.8030	 0.6020
qB	 0.8200	 0.6070
qC	 0.8230	 0.6020
r	 0.8400	 0.6130
rA	 0.8070	 0.6040
rB	 0.8200	 0.6090
rC	 0.8200	 0.5960
s	 0.8310	 0.6090
sA	 0.8000	 0.6020
sB	 0.8220	 0.6120
sC	 0.8230	 0.6020
t	 0.8310	 0.6110
tA	 0.8030	 0.6050
tB	 0.8200	 0.6090
tC	 0.8220	 0.5980
u	 0.8360	 0.6070
uA	 0.8050	 0.6040
uB	 0.8220	 0.6060
uC	 0.8230	 0.6020

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Chain	Atom inclusion	Q-score
v	 0.8420	 0.6070
vA	 0.8000	 0.6090
vB	 0.8200	 0.6110
vC	 0.8270	 0.6030
w	 0.8360	 0.6110
wA	 0.8030	 0.6060
wB	 0.8200	 0.6070
wC	 0.8220	 0.6040
x	 0.8460	 0.6120
xA	 0.8070	 0.6050
xB	 0.7990	 0.5990
xC	 0.8220	 0.6060
y	 0.8250	 0.6050
yA	 0.8030	 0.6030
yB	 0.8050	 0.6000
yC	 0.8120	 0.5980
z	 0.8420	 0.6130
zA	 0.8030	 0.6050
zB	 0.8050	 0.5980
zC	 0.8140	 0.6030