



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 6RVW / pdb_00006rvw
EMDB ID : EMD-4444
Title : Structure of right-handed protein cage consisting of 24 eleven-membered ring proteins held together by gold (I) bridges.
Authors : Malay, A.D.; Miyazaki, N.; Biela, A.P.; Iwasaki, K.; Heddle, J.G.
Deposited on : 2019-06-03
Resolution : 3.70 Å(reported)
Based on initial model : 4V4F

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

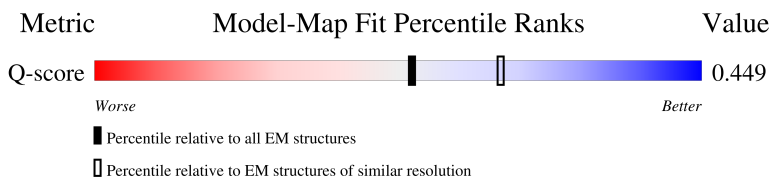
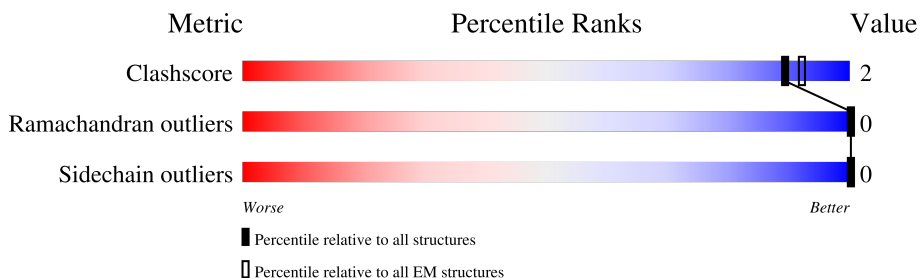
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	AA	74	11% 72% 26%
1	AB	74	5% 70% 26%
1	AC	74	11% 70% 26%
1	AD	74	72% 26%

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Mol	Chain	Length	Quality of chain
1	AE	74	
1	AF	74	
1	AG	74	
1	AH	74	
1	AI	74	
1	AJ	74	
1	AK	74	
1	BA	74	
1	BB	74	
1	BC	74	
1	BD	74	
1	BE	74	
1	BF	74	
1	BG	74	
1	BH	74	
1	BI	74	
1	BJ	74	
1	BK	74	
1	CA	74	
1	CB	74	
1	CC	74	
1	CD	74	
1	CE	74	
1	CF	74	
1	CG	74	

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Mol	Chain	Length	Quality of chain
1	CH	74	
1	CI	74	
1	CJ	74	
1	CK	74	
1	DA	74	
1	DB	74	
1	DC	74	
1	DD	74	
1	DE	74	
1	DF	74	
1	DG	74	
1	DH	74	
1	DI	74	
1	DJ	74	
1	DK	74	
1	EA	74	
1	EB	74	
1	EC	74	
1	ED	74	
1	EE	74	
1	EF	74	
1	EG	74	
1	EH	74	
1	EI	74	
1	EJ	74	

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Mol	Chain	Length	Quality of chain
1	EK	74	
1	FA	74	
1	FB	74	
1	FC	74	
1	FD	74	
1	FE	74	
1	FF	74	
1	FG	74	
1	FH	74	
1	FI	74	
1	FJ	74	
1	FK	74	
1	GA	74	
1	GB	74	
1	GC	74	
1	GD	74	
1	GE	74	
1	GF	74	
1	GG	74	
1	GH	74	
1	GI	74	
1	GJ	74	
1	GK	74	
1	HA	74	
1	HB	74	

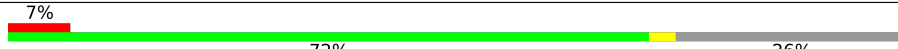
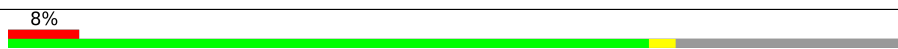
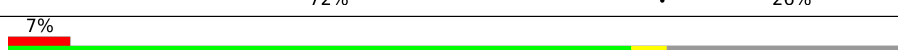
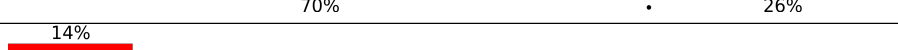
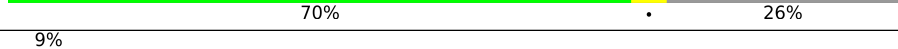
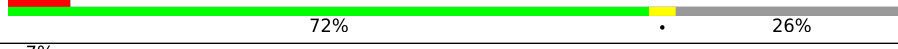
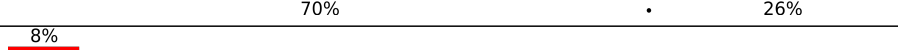
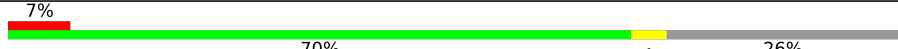
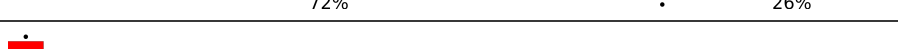
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Mol	Chain	Length	Quality of chain
1	HC	74	
1	HD	74	
1	HE	74	
1	HF	74	
1	HG	74	
1	HH	74	
1	HI	74	
1	HJ	74	
1	HK	74	
1	IA	74	
1	IB	74	
1	IC	74	
1	ID	74	
1	IE	74	
1	IF	74	
1	IG	74	
1	IH	74	
1	II	74	
1	IJ	74	
1	IK	74	
1	JA	74	
1	JB	74	
1	JC	74	
1	JD	74	
1	JE	74	

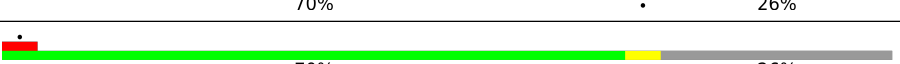
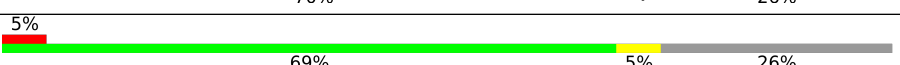
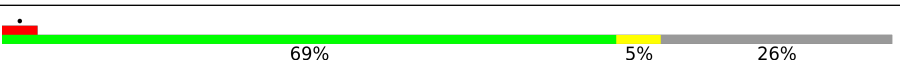
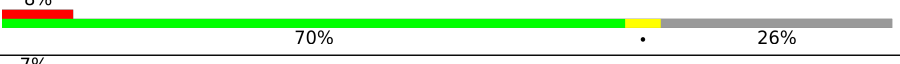
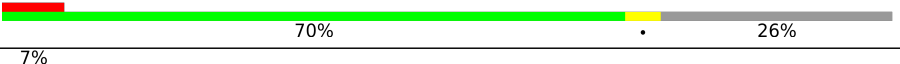
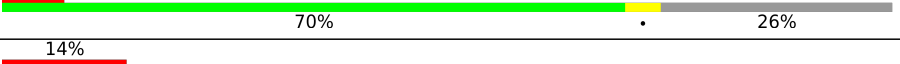
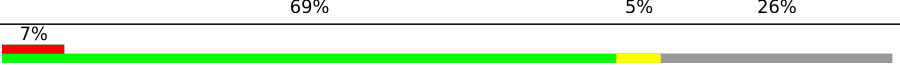
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Mol	Chain	Length	Quality of chain
1	JF	74	
1	JG	74	
1	JH	74	
1	JI	74	
1	JJ	74	
1	JK	74	
1	KA	74	
1	KB	74	
1	KC	74	
1	KD	74	
1	KE	74	
1	KF	74	
1	KG	74	
1	KH	74	
1	KI	74	
1	KJ	74	
1	KK	74	
1	LA	74	
1	LB	74	
1	LC	74	
1	LD	74	
1	LE	74	
1	LF	74	
1	LG	74	
1	LH	74	

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Mol	Chain	Length	Quality of chain
1	LI	74	
1	LJ	74	
1	LK	74	
1	MA	74	
1	MB	74	
1	MC	74	
1	MD	74	
1	ME	74	
1	MF	74	
1	MG	74	
1	MH	74	
1	MI	74	
1	MJ	74	
1	MK	74	
1	NA	74	
1	NB	74	
1	NC	74	
1	ND	74	
1	NE	74	
1	NF	74	
1	NG	74	
1	NH	74	
1	NI	74	
1	NJ	74	
1	NK	74	

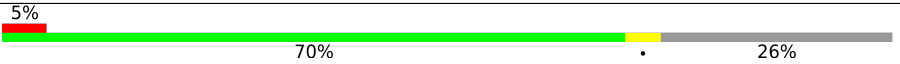
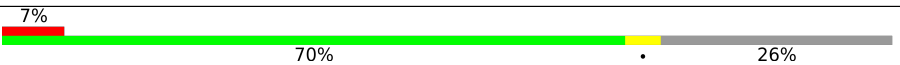
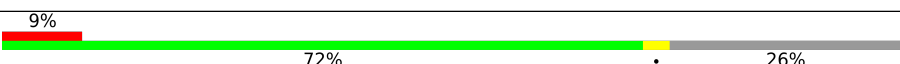
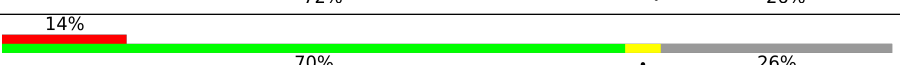
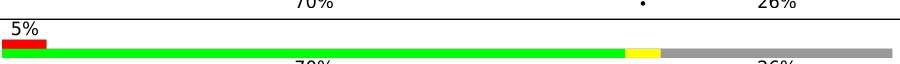
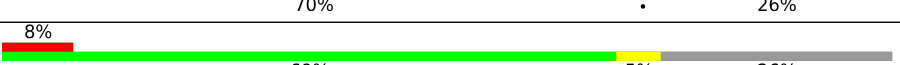
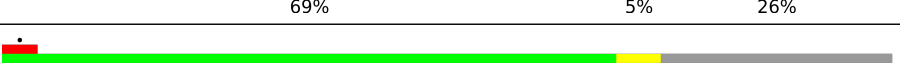
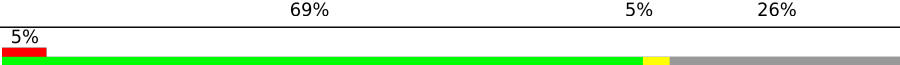
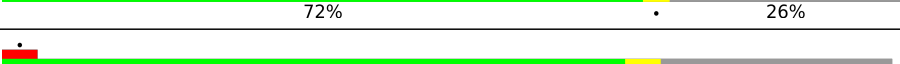
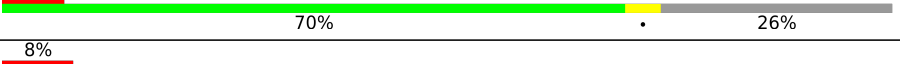
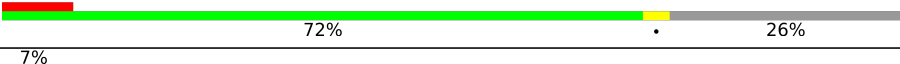
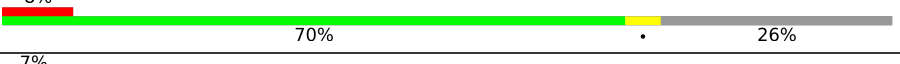
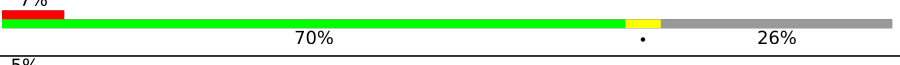
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Mol	Chain	Length	Quality of chain
1	OA	74	8% 70% 26%
1	OB	74	7% 70% 26%
1	OC	74	7% 69% 5% 26%
1	OD	74	• 68% 7% 26%
1	OE	74	7% 69% 5% 26%
1	OF	74	• 72% • 26%
1	OG	74	7% 72% • 26%
1	OH	74	8% 70% • 26%
1	OI	74	8% 70% • 26%
1	OJ	74	8% 72% • 26%
1	OK	74	12% 70% • 26%
1	PA	74	8% 70% • 26%
1	PB	74	8% 70% • 26%
1	PC	74	7% 70% • 26%
1	PD	74	• 70% • 26%
1	PE	74	• 70% • 26%
1	PF	74	5% 72% • 26%
1	PG	74	5% 72% • 26%
1	PH	74	8% 72% • 26%
1	PI	74	8% 70% • 26%
1	PJ	74	7% 70% • 26%
1	PK	74	12% 70% • 26%
1	QA	74	11% 70% • 26%
1	QB	74	8% 69% 5% 26%
1	QC	74	8% 69% 5% 26%

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Mol	Chain	Length	Quality of chain
1	QD	74	
1	QE	74	
1	QF	74	
1	QG	74	
1	QH	74	
1	QI	74	
1	QJ	74	
1	QK	74	
1	RA	74	
1	RB	74	
1	RC	74	
1	RD	74	
1	RE	74	
1	RF	74	
1	RG	74	
1	RH	74	
1	RI	74	
1	RJ	74	
1	RK	74	
1	SA	74	
1	SB	74	
1	SC	74	
1	SD	74	
1	SE	74	
1	SF	74	

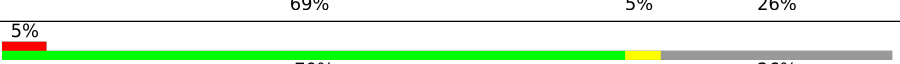
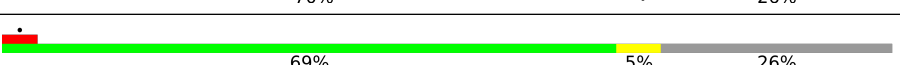
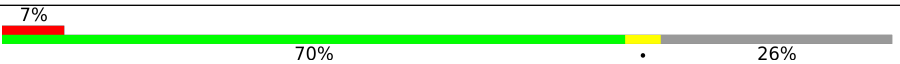
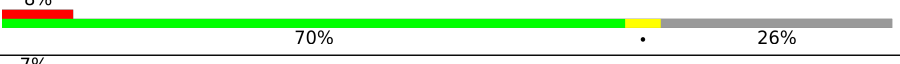
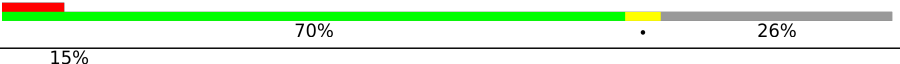
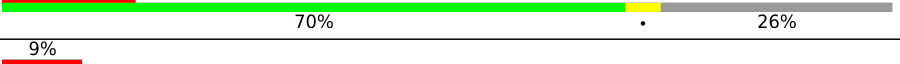
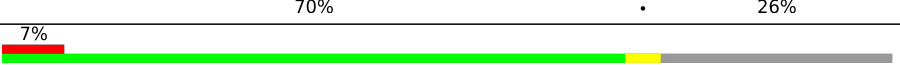
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Mol	Chain	Length	Quality of chain
1	SG	74	
1	SH	74	
1	SI	74	
1	SJ	74	
1	SK	74	
1	TA	74	
1	TB	74	
1	TC	74	
1	TD	74	
1	TE	74	
1	TF	74	
1	TG	74	
1	TH	74	
1	TI	74	
1	TJ	74	
1	TK	74	
1	UA	74	
1	UB	74	
1	UC	74	
1	UD	74	
1	UE	74	
1	UF	74	
1	UG	74	
1	UH	74	
1	UI	74	

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Mol	Chain	Length	Quality of chain
1	UJ	74	
1	UK	74	
1	VA	74	
1	VB	74	
1	VC	74	
1	VD	74	
1	VE	74	
1	VF	74	
1	VG	74	
1	VH	74	
1	VI	74	
1	VJ	74	
1	VK	74	
1	WA	74	
1	WB	74	
1	WC	74	
1	WD	74	
1	WE	74	
1	WF	74	
1	WG	74	
1	WH	74	
1	WI	74	
1	WJ	74	
1	WK	74	
1	XA	74	

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Mol	Chain	Length	Quality of chain
1	XB	74	
1	XC	74	
1	XD	74	
1	XE	74	
1	XF	74	
1	XG	74	
1	XH	74	
1	XI	74	
1	XJ	74	
1	XK	74	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 110208 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	AA	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AB	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AC	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AD	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AE	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AF	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AG	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AH	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AI	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AJ	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	AK	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BA	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BB	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BC	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BD	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BE	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	BF	55	Total	C	N	O	S	0	0
			417	263	69	84	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	BH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	BI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	BJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	BK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	CK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DE	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	DK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	ED	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	EK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FD	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	FK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	GK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HC	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	HK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	ID	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	II	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	IK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JB	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	JK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	KK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LA	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	LB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	LK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	ME	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	MK	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	ND	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	NK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	OJ	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	OK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	PK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QI	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	QJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	QK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	RK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SH	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	SI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	SK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	TK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UG	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	UH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	UK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VF	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VG	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VH	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VI	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VJ	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	VK	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WA	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WB	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WC	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WD	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WE	55	Total 417	C 263	N 69	O 84	S 1	0	0
1	WF	55	Total 417	C 263	N 69	O 84	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	WG	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	WH	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	WI	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	WJ	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	WK	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XA	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XB	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XC	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XD	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XE	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XF	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XG	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XH	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XI	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XJ	55	Total	C	N	O	S	0	0
			417	263	69	84	1		
1	XK	55	Total	C	N	O	S	0	0
			417	263	69	84	1		

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AA	64	SER	ARG	engineered mutation	UNP Q9X6J6
AB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AB	64	SER	ARG	engineered mutation	UNP Q9X6J6
AC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AC	64	SER	ARG	engineered mutation	UNP Q9X6J6
AD	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	64	SER	ARG	engineered mutation	UNP Q9X6J6
AE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AE	64	SER	ARG	engineered mutation	UNP Q9X6J6
AF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AF	64	SER	ARG	engineered mutation	UNP Q9X6J6
AG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AG	64	SER	ARG	engineered mutation	UNP Q9X6J6
AH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AH	64	SER	ARG	engineered mutation	UNP Q9X6J6
AI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AI	64	SER	ARG	engineered mutation	UNP Q9X6J6
AJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
AK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
AK	64	SER	ARG	engineered mutation	UNP Q9X6J6
BA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BA	64	SER	ARG	engineered mutation	UNP Q9X6J6
BB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BB	64	SER	ARG	engineered mutation	UNP Q9X6J6
BC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BC	64	SER	ARG	engineered mutation	UNP Q9X6J6
BD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BD	64	SER	ARG	engineered mutation	UNP Q9X6J6
BE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BE	64	SER	ARG	engineered mutation	UNP Q9X6J6
BF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BF	64	SER	ARG	engineered mutation	UNP Q9X6J6
BG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BG	64	SER	ARG	engineered mutation	UNP Q9X6J6
BH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BH	64	SER	ARG	engineered mutation	UNP Q9X6J6
BI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BI	64	SER	ARG	engineered mutation	UNP Q9X6J6
BJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
BK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
BK	64	SER	ARG	engineered mutation	UNP Q9X6J6
CA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CA	64	SER	ARG	engineered mutation	UNP Q9X6J6
CB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CB	64	SER	ARG	engineered mutation	UNP Q9X6J6
CC	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	64	SER	ARG	engineered mutation	UNP Q9X6J6
CD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CD	64	SER	ARG	engineered mutation	UNP Q9X6J6
CE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CE	64	SER	ARG	engineered mutation	UNP Q9X6J6
CF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CF	64	SER	ARG	engineered mutation	UNP Q9X6J6
CG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CG	64	SER	ARG	engineered mutation	UNP Q9X6J6
CH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CH	64	SER	ARG	engineered mutation	UNP Q9X6J6
CI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CI	64	SER	ARG	engineered mutation	UNP Q9X6J6
CJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
CK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
CK	64	SER	ARG	engineered mutation	UNP Q9X6J6
DA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DA	64	SER	ARG	engineered mutation	UNP Q9X6J6
DB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DB	64	SER	ARG	engineered mutation	UNP Q9X6J6
DC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DC	64	SER	ARG	engineered mutation	UNP Q9X6J6
DD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DD	64	SER	ARG	engineered mutation	UNP Q9X6J6
DE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DE	64	SER	ARG	engineered mutation	UNP Q9X6J6
DF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DF	64	SER	ARG	engineered mutation	UNP Q9X6J6
DG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DG	64	SER	ARG	engineered mutation	UNP Q9X6J6
DH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DH	64	SER	ARG	engineered mutation	UNP Q9X6J6
DI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DI	64	SER	ARG	engineered mutation	UNP Q9X6J6
DJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
DK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
DK	64	SER	ARG	engineered mutation	UNP Q9X6J6
EA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EA	64	SER	ARG	engineered mutation	UNP Q9X6J6
EB	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	64	SER	ARG	engineered mutation	UNP Q9X6J6
EC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EC	64	SER	ARG	engineered mutation	UNP Q9X6J6
ED	35	CYS	LYS	engineered mutation	UNP Q9X6J6
ED	64	SER	ARG	engineered mutation	UNP Q9X6J6
EE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EE	64	SER	ARG	engineered mutation	UNP Q9X6J6
EF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EF	64	SER	ARG	engineered mutation	UNP Q9X6J6
EG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EG	64	SER	ARG	engineered mutation	UNP Q9X6J6
EH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EH	64	SER	ARG	engineered mutation	UNP Q9X6J6
EI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EI	64	SER	ARG	engineered mutation	UNP Q9X6J6
EJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
EK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
EK	64	SER	ARG	engineered mutation	UNP Q9X6J6
FA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FA	64	SER	ARG	engineered mutation	UNP Q9X6J6
FB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FB	64	SER	ARG	engineered mutation	UNP Q9X6J6
FC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FC	64	SER	ARG	engineered mutation	UNP Q9X6J6
FD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FD	64	SER	ARG	engineered mutation	UNP Q9X6J6
FE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FE	64	SER	ARG	engineered mutation	UNP Q9X6J6
FF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FF	64	SER	ARG	engineered mutation	UNP Q9X6J6
FG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FG	64	SER	ARG	engineered mutation	UNP Q9X6J6
FH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FH	64	SER	ARG	engineered mutation	UNP Q9X6J6
FI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FI	64	SER	ARG	engineered mutation	UNP Q9X6J6
FJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
FK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
FK	64	SER	ARG	engineered mutation	UNP Q9X6J6
GA	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	64	SER	ARG	engineered mutation	UNP Q9X6J6
GB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GB	64	SER	ARG	engineered mutation	UNP Q9X6J6
GC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GC	64	SER	ARG	engineered mutation	UNP Q9X6J6
GD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GD	64	SER	ARG	engineered mutation	UNP Q9X6J6
GE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GE	64	SER	ARG	engineered mutation	UNP Q9X6J6
GF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GF	64	SER	ARG	engineered mutation	UNP Q9X6J6
GG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GG	64	SER	ARG	engineered mutation	UNP Q9X6J6
GH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GH	64	SER	ARG	engineered mutation	UNP Q9X6J6
GI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GI	64	SER	ARG	engineered mutation	UNP Q9X6J6
GJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
GK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
GK	64	SER	ARG	engineered mutation	UNP Q9X6J6
HA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HA	64	SER	ARG	engineered mutation	UNP Q9X6J6
HB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HB	64	SER	ARG	engineered mutation	UNP Q9X6J6
HC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HC	64	SER	ARG	engineered mutation	UNP Q9X6J6
HD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HD	64	SER	ARG	engineered mutation	UNP Q9X6J6
HE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HE	64	SER	ARG	engineered mutation	UNP Q9X6J6
HF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HF	64	SER	ARG	engineered mutation	UNP Q9X6J6
HG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HG	64	SER	ARG	engineered mutation	UNP Q9X6J6
HH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HH	64	SER	ARG	engineered mutation	UNP Q9X6J6
HI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HI	64	SER	ARG	engineered mutation	UNP Q9X6J6
HJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
HJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
HK	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
HK	64	SER	ARG	engineered mutation	UNP Q9X6J6
IA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IA	64	SER	ARG	engineered mutation	UNP Q9X6J6
IB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IB	64	SER	ARG	engineered mutation	UNP Q9X6J6
IC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IC	64	SER	ARG	engineered mutation	UNP Q9X6J6
ID	35	CYS	LYS	engineered mutation	UNP Q9X6J6
ID	64	SER	ARG	engineered mutation	UNP Q9X6J6
IE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IE	64	SER	ARG	engineered mutation	UNP Q9X6J6
IF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IF	64	SER	ARG	engineered mutation	UNP Q9X6J6
IG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IG	64	SER	ARG	engineered mutation	UNP Q9X6J6
IH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IH	64	SER	ARG	engineered mutation	UNP Q9X6J6
II	35	CYS	LYS	engineered mutation	UNP Q9X6J6
II	64	SER	ARG	engineered mutation	UNP Q9X6J6
IJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
IK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
IK	64	SER	ARG	engineered mutation	UNP Q9X6J6
JA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JA	64	SER	ARG	engineered mutation	UNP Q9X6J6
JB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JB	64	SER	ARG	engineered mutation	UNP Q9X6J6
JC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JC	64	SER	ARG	engineered mutation	UNP Q9X6J6
JD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JD	64	SER	ARG	engineered mutation	UNP Q9X6J6
JE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JE	64	SER	ARG	engineered mutation	UNP Q9X6J6
JF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JF	64	SER	ARG	engineered mutation	UNP Q9X6J6
JG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JG	64	SER	ARG	engineered mutation	UNP Q9X6J6
JH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JH	64	SER	ARG	engineered mutation	UNP Q9X6J6
JI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JI	64	SER	ARG	engineered mutation	UNP Q9X6J6
JJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
JJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
JK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
JK	64	SER	ARG	engineered mutation	UNP Q9X6J6
KA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KA	64	SER	ARG	engineered mutation	UNP Q9X6J6
KB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KB	64	SER	ARG	engineered mutation	UNP Q9X6J6
KC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KC	64	SER	ARG	engineered mutation	UNP Q9X6J6
KD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KD	64	SER	ARG	engineered mutation	UNP Q9X6J6
KE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KE	64	SER	ARG	engineered mutation	UNP Q9X6J6
KF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KF	64	SER	ARG	engineered mutation	UNP Q9X6J6
KG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KG	64	SER	ARG	engineered mutation	UNP Q9X6J6
KH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KH	64	SER	ARG	engineered mutation	UNP Q9X6J6
KI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KI	64	SER	ARG	engineered mutation	UNP Q9X6J6
KJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
KK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
KK	64	SER	ARG	engineered mutation	UNP Q9X6J6
LA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LA	64	SER	ARG	engineered mutation	UNP Q9X6J6
LB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LB	64	SER	ARG	engineered mutation	UNP Q9X6J6
LC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LC	64	SER	ARG	engineered mutation	UNP Q9X6J6
LD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LD	64	SER	ARG	engineered mutation	UNP Q9X6J6
LE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LE	64	SER	ARG	engineered mutation	UNP Q9X6J6
LF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LF	64	SER	ARG	engineered mutation	UNP Q9X6J6
LG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LG	64	SER	ARG	engineered mutation	UNP Q9X6J6
LH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LH	64	SER	ARG	engineered mutation	UNP Q9X6J6
LI	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
LI	64	SER	ARG	engineered mutation	UNP Q9X6J6
LJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
LK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
LK	64	SER	ARG	engineered mutation	UNP Q9X6J6
MA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MA	64	SER	ARG	engineered mutation	UNP Q9X6J6
MB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MB	64	SER	ARG	engineered mutation	UNP Q9X6J6
MC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MC	64	SER	ARG	engineered mutation	UNP Q9X6J6
MD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MD	64	SER	ARG	engineered mutation	UNP Q9X6J6
ME	35	CYS	LYS	engineered mutation	UNP Q9X6J6
ME	64	SER	ARG	engineered mutation	UNP Q9X6J6
MF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MF	64	SER	ARG	engineered mutation	UNP Q9X6J6
MG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MG	64	SER	ARG	engineered mutation	UNP Q9X6J6
MH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MH	64	SER	ARG	engineered mutation	UNP Q9X6J6
MI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MI	64	SER	ARG	engineered mutation	UNP Q9X6J6
MJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
MK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
MK	64	SER	ARG	engineered mutation	UNP Q9X6J6
NA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NA	64	SER	ARG	engineered mutation	UNP Q9X6J6
NB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NB	64	SER	ARG	engineered mutation	UNP Q9X6J6
NC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NC	64	SER	ARG	engineered mutation	UNP Q9X6J6
ND	35	CYS	LYS	engineered mutation	UNP Q9X6J6
ND	64	SER	ARG	engineered mutation	UNP Q9X6J6
NE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NE	64	SER	ARG	engineered mutation	UNP Q9X6J6
NF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NF	64	SER	ARG	engineered mutation	UNP Q9X6J6
NG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NG	64	SER	ARG	engineered mutation	UNP Q9X6J6
NH	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
NH	64	SER	ARG	engineered mutation	UNP Q9X6J6
NI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NI	64	SER	ARG	engineered mutation	UNP Q9X6J6
NJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
NK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
NK	64	SER	ARG	engineered mutation	UNP Q9X6J6
OA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OA	64	SER	ARG	engineered mutation	UNP Q9X6J6
OB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OB	64	SER	ARG	engineered mutation	UNP Q9X6J6
OC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OC	64	SER	ARG	engineered mutation	UNP Q9X6J6
OD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OD	64	SER	ARG	engineered mutation	UNP Q9X6J6
OE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OE	64	SER	ARG	engineered mutation	UNP Q9X6J6
OF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OF	64	SER	ARG	engineered mutation	UNP Q9X6J6
OG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OG	64	SER	ARG	engineered mutation	UNP Q9X6J6
OH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OH	64	SER	ARG	engineered mutation	UNP Q9X6J6
OI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OI	64	SER	ARG	engineered mutation	UNP Q9X6J6
OJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
OK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
OK	64	SER	ARG	engineered mutation	UNP Q9X6J6
PA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PA	64	SER	ARG	engineered mutation	UNP Q9X6J6
PB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PB	64	SER	ARG	engineered mutation	UNP Q9X6J6
PC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PC	64	SER	ARG	engineered mutation	UNP Q9X6J6
PD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PD	64	SER	ARG	engineered mutation	UNP Q9X6J6
PE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PE	64	SER	ARG	engineered mutation	UNP Q9X6J6
PF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PF	64	SER	ARG	engineered mutation	UNP Q9X6J6
PG	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
PG	64	SER	ARG	engineered mutation	UNP Q9X6J6
PH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PH	64	SER	ARG	engineered mutation	UNP Q9X6J6
PI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PI	64	SER	ARG	engineered mutation	UNP Q9X6J6
PJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
PK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
PK	64	SER	ARG	engineered mutation	UNP Q9X6J6
QA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QA	64	SER	ARG	engineered mutation	UNP Q9X6J6
QB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QB	64	SER	ARG	engineered mutation	UNP Q9X6J6
QC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QC	64	SER	ARG	engineered mutation	UNP Q9X6J6
QD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QD	64	SER	ARG	engineered mutation	UNP Q9X6J6
QE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QE	64	SER	ARG	engineered mutation	UNP Q9X6J6
QF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QF	64	SER	ARG	engineered mutation	UNP Q9X6J6
QG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QG	64	SER	ARG	engineered mutation	UNP Q9X6J6
QH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QH	64	SER	ARG	engineered mutation	UNP Q9X6J6
QI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QI	64	SER	ARG	engineered mutation	UNP Q9X6J6
QJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
QK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
QK	64	SER	ARG	engineered mutation	UNP Q9X6J6
RA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RA	64	SER	ARG	engineered mutation	UNP Q9X6J6
RB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RB	64	SER	ARG	engineered mutation	UNP Q9X6J6
RC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RC	64	SER	ARG	engineered mutation	UNP Q9X6J6
RD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RD	64	SER	ARG	engineered mutation	UNP Q9X6J6
RE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RE	64	SER	ARG	engineered mutation	UNP Q9X6J6
RF	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
RF	64	SER	ARG	engineered mutation	UNP Q9X6J6
RG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RG	64	SER	ARG	engineered mutation	UNP Q9X6J6
RH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RH	64	SER	ARG	engineered mutation	UNP Q9X6J6
RI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RI	64	SER	ARG	engineered mutation	UNP Q9X6J6
RJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
RK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
RK	64	SER	ARG	engineered mutation	UNP Q9X6J6
SA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SA	64	SER	ARG	engineered mutation	UNP Q9X6J6
SB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SB	64	SER	ARG	engineered mutation	UNP Q9X6J6
SC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SC	64	SER	ARG	engineered mutation	UNP Q9X6J6
SD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SD	64	SER	ARG	engineered mutation	UNP Q9X6J6
SE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SE	64	SER	ARG	engineered mutation	UNP Q9X6J6
SF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SF	64	SER	ARG	engineered mutation	UNP Q9X6J6
SG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SG	64	SER	ARG	engineered mutation	UNP Q9X6J6
SH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SH	64	SER	ARG	engineered mutation	UNP Q9X6J6
SI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SI	64	SER	ARG	engineered mutation	UNP Q9X6J6
SJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
SK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
SK	64	SER	ARG	engineered mutation	UNP Q9X6J6
TA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TA	64	SER	ARG	engineered mutation	UNP Q9X6J6
TB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TB	64	SER	ARG	engineered mutation	UNP Q9X6J6
TC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TC	64	SER	ARG	engineered mutation	UNP Q9X6J6
TD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TD	64	SER	ARG	engineered mutation	UNP Q9X6J6
TE	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
TE	64	SER	ARG	engineered mutation	UNP Q9X6J6
TF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TF	64	SER	ARG	engineered mutation	UNP Q9X6J6
TG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TG	64	SER	ARG	engineered mutation	UNP Q9X6J6
TH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TH	64	SER	ARG	engineered mutation	UNP Q9X6J6
TI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TI	64	SER	ARG	engineered mutation	UNP Q9X6J6
TJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
TK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
TK	64	SER	ARG	engineered mutation	UNP Q9X6J6
UA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UA	64	SER	ARG	engineered mutation	UNP Q9X6J6
UB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UB	64	SER	ARG	engineered mutation	UNP Q9X6J6
UC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UC	64	SER	ARG	engineered mutation	UNP Q9X6J6
UD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UD	64	SER	ARG	engineered mutation	UNP Q9X6J6
UE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UE	64	SER	ARG	engineered mutation	UNP Q9X6J6
UF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UF	64	SER	ARG	engineered mutation	UNP Q9X6J6
UG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UG	64	SER	ARG	engineered mutation	UNP Q9X6J6
UH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UH	64	SER	ARG	engineered mutation	UNP Q9X6J6
UI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UI	64	SER	ARG	engineered mutation	UNP Q9X6J6
UJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
UK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
UK	64	SER	ARG	engineered mutation	UNP Q9X6J6
VA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VA	64	SER	ARG	engineered mutation	UNP Q9X6J6
VB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VB	64	SER	ARG	engineered mutation	UNP Q9X6J6
VC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VC	64	SER	ARG	engineered mutation	UNP Q9X6J6
VD	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
VD	64	SER	ARG	engineered mutation	UNP Q9X6J6
VE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VE	64	SER	ARG	engineered mutation	UNP Q9X6J6
VF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VF	64	SER	ARG	engineered mutation	UNP Q9X6J6
VG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VG	64	SER	ARG	engineered mutation	UNP Q9X6J6
VH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VH	64	SER	ARG	engineered mutation	UNP Q9X6J6
VI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VI	64	SER	ARG	engineered mutation	UNP Q9X6J6
VJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
VK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
VK	64	SER	ARG	engineered mutation	UNP Q9X6J6
WA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WA	64	SER	ARG	engineered mutation	UNP Q9X6J6
WB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WB	64	SER	ARG	engineered mutation	UNP Q9X6J6
WC	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WC	64	SER	ARG	engineered mutation	UNP Q9X6J6
WD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WD	64	SER	ARG	engineered mutation	UNP Q9X6J6
WE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WE	64	SER	ARG	engineered mutation	UNP Q9X6J6
WF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WF	64	SER	ARG	engineered mutation	UNP Q9X6J6
WG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WG	64	SER	ARG	engineered mutation	UNP Q9X6J6
WH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WH	64	SER	ARG	engineered mutation	UNP Q9X6J6
WI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WI	64	SER	ARG	engineered mutation	UNP Q9X6J6
WJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
WK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
WK	64	SER	ARG	engineered mutation	UNP Q9X6J6
XA	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XA	64	SER	ARG	engineered mutation	UNP Q9X6J6
XB	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XB	64	SER	ARG	engineered mutation	UNP Q9X6J6
XC	35	CYS	LYS	engineered mutation	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
XC	64	SER	ARG	engineered mutation	UNP Q9X6J6
XD	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XD	64	SER	ARG	engineered mutation	UNP Q9X6J6
XE	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XE	64	SER	ARG	engineered mutation	UNP Q9X6J6
XF	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XF	64	SER	ARG	engineered mutation	UNP Q9X6J6
XG	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XG	64	SER	ARG	engineered mutation	UNP Q9X6J6
XH	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XH	64	SER	ARG	engineered mutation	UNP Q9X6J6
XI	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XI	64	SER	ARG	engineered mutation	UNP Q9X6J6
XJ	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XJ	64	SER	ARG	engineered mutation	UNP Q9X6J6
XK	35	CYS	LYS	engineered mutation	UNP Q9X6J6
XK	64	SER	ARG	engineered mutation	UNP Q9X6J6

- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	AA	1	Total Au 1 1	0
2	AB	1	Total Au 1 1	0
2	AC	1	Total Au 1 1	0
2	AD	1	Total Au 1 1	0
2	AE	1	Total Au 1 1	0
2	AF	1	Total Au 1 1	0
2	AG	1	Total Au 1 1	0
2	AH	1	Total Au 1 1	0
2	AI	1	Total Au 1 1	0
2	AJ	1	Total Au 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	BA	1	Total 1	Au 1	0
2	BB	1	Total 1	Au 1	0
2	BC	1	Total 1	Au 1	0
2	BD	1	Total 1	Au 1	0
2	BE	1	Total 1	Au 1	0
2	BF	1	Total 1	Au 1	0
2	BG	1	Total 1	Au 1	0
2	BH	1	Total 1	Au 1	0
2	BI	1	Total 1	Au 1	0
2	BJ	1	Total 1	Au 1	0
2	CA	1	Total 1	Au 1	0
2	CB	1	Total 1	Au 1	0
2	CC	1	Total 1	Au 1	0
2	CD	1	Total 1	Au 1	0
2	CE	1	Total 1	Au 1	0
2	CF	1	Total 1	Au 1	0
2	CI	1	Total 1	Au 1	0
2	CJ	1	Total 1	Au 1	0
2	DA	1	Total 1	Au 1	0
2	DB	1	Total 1	Au 1	0
2	DC	1	Total 1	Au 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	DD	1	Total 1	Au 1	0
2	DE	1	Total 1	Au 1	0
2	DF	1	Total 1	Au 1	0
2	DG	1	Total 1	Au 1	0
2	DH	1	Total 1	Au 1	0
2	DI	1	Total 1	Au 1	0
2	DJ	1	Total 1	Au 1	0
2	EE	1	Total 1	Au 1	0
2	EF	1	Total 1	Au 1	0
2	EG	1	Total 1	Au 1	0
2	EH	1	Total 1	Au 1	0
2	EI	1	Total 1	Au 1	0
2	EJ	1	Total 1	Au 1	0
2	FA	1	Total 1	Au 1	0
2	FB	1	Total 1	Au 1	0
2	FE	1	Total 1	Au 1	0
2	FF	1	Total 1	Au 1	0
2	FG	1	Total 1	Au 1	0
2	FH	1	Total 1	Au 1	0
2	FI	1	Total 1	Au 1	0
2	FJ	1	Total 1	Au 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	GC	1	Total 1	Au 1	0
2	GD	1	Total 1	Au 1	0
2	GG	1	Total 1	Au 1	0
2	GH	1	Total 1	Au 1	0
2	GI	1	Total 1	Au 1	0
2	GJ	1	Total 1	Au 1	0
2	HA	1	Total 1	Au 1	0
2	HB	1	Total 1	Au 1	0
2	HC	1	Total 1	Au 1	0
2	HD	1	Total 1	Au 1	0
2	HG	1	Total 1	Au 1	0
2	HH	1	Total 1	Au 1	0
2	HI	1	Total 1	Au 1	0
2	HJ	1	Total 1	Au 1	0
2	IA	1	Total 1	Au 1	0
2	IB	1	Total 1	Au 1	0
2	IE	1	Total 1	Au 1	0
2	IF	1	Total 1	Au 1	0
2	IG	1	Total 1	Au 1	0
2	IH	1	Total 1	Au 1	0
2	II	1	Total 1	Au 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	IJ	1	Total 1	Au 1	0
2	JC	1	Total 1	Au 1	0
2	JD	1	Total 1	Au 1	0
2	JE	1	Total 1	Au 1	0
2	JF	1	Total 1	Au 1	0
2	KC	1	Total 1	Au 1	0
2	KD	1	Total 1	Au 1	0
2	KE	1	Total 1	Au 1	0
2	KF	1	Total 1	Au 1	0
2	LA	1	Total 1	Au 1	0
2	LB	1	Total 1	Au 1	0
2	LC	1	Total 1	Au 1	0
2	LD	1	Total 1	Au 1	0
2	LI	1	Total 1	Au 1	0
2	LJ	1	Total 1	Au 1	0
2	ME	1	Total 1	Au 1	0
2	MF	1	Total 1	Au 1	0
2	NA	1	Total 1	Au 1	0
2	NB	1	Total 1	Au 1	0
2	NC	1	Total 1	Au 1	0
2	ND	1	Total 1	Au 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	OE	1	Total 1	Au 1	0
2	OF	1	Total 1	Au 1	0
2	OG	1	Total 1	Au 1	0
2	OH	1	Total 1	Au 1	0
2	OI	1	Total 1	Au 1	0
2	OJ	1	Total 1	Au 1	0
2	PC	1	Total 1	Au 1	0
2	PD	1	Total 1	Au 1	0
2	PE	1	Total 1	Au 1	0
2	PF	1	Total 1	Au 1	0
2	PG	1	Total 1	Au 1	0
2	PH	1	Total 1	Au 1	0
2	QG	1	Total 1	Au 1	0
2	QH	1	Total 1	Au 1	0
2	RA	1	Total 1	Au 1	0
2	RB	1	Total 1	Au 1	0
2	RC	1	Total 1	Au 1	0
2	RD	1	Total 1	Au 1	0
2	SE	1	Total 1	Au 1	0
2	SF	1	Total 1	Au 1	0
2	TA	1	Total 1	Au 1	0

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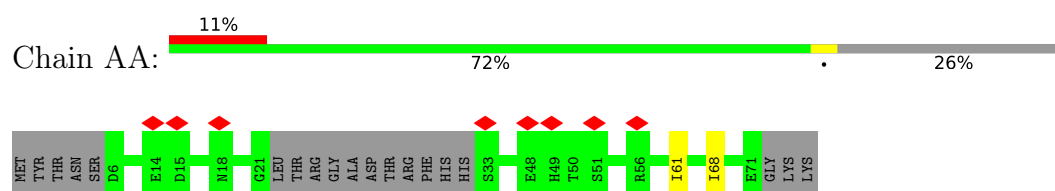
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Mol	Chain	Residues	Atoms		AltConf
2	TB	1	Total 1	Au 1	0
2	TI	1	Total 1	Au 1	0
2	TJ	1	Total 1	Au 1	0
2	WI	1	Total 1	Au 1	0
2	WJ	1	Total 1	Au 1	0

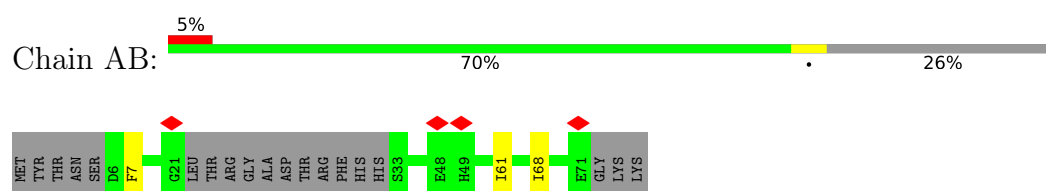
3 Residue-property plots [i](#)

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.

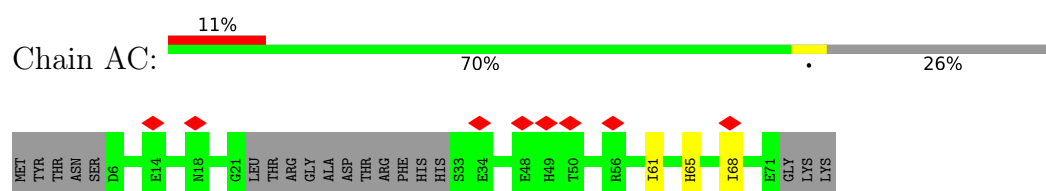
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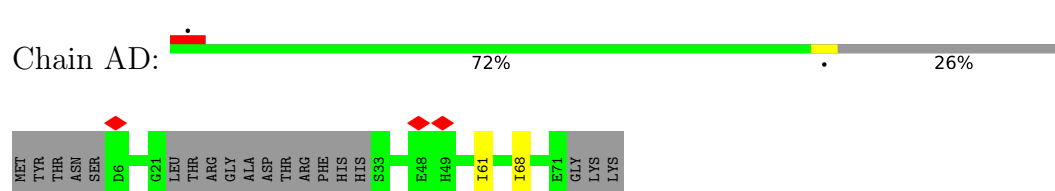
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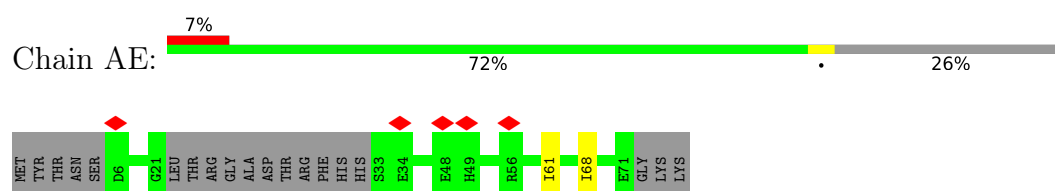
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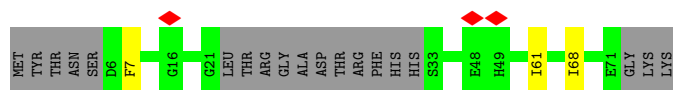
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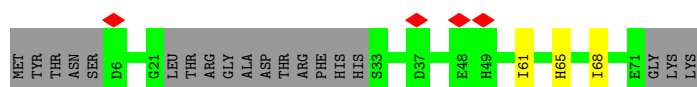
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• Molecule 1: Transcription attenuation protein MtrB

Chain AF:  70% 26%

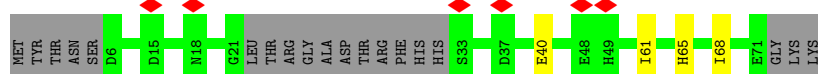
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Chain AG:  5% 70% 26%

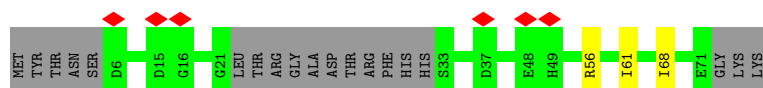
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Chain AH:  7% 70% 26%

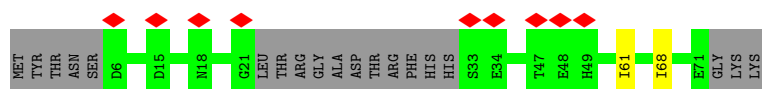
• Molecule 1: Transcription attenuation protein MtrB

Chain AI:  8% 69% 5% 26%

• Molecule 1: Transcription attenuation protein MtrB

Chain AJ:  8% 70% 26%

• Molecule 1: Transcription attenuation protein MtrB

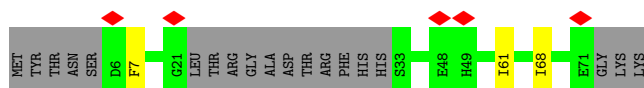
Chain AK:  12% 72% 26%

• Molecule 1: Transcription attenuation protein MtrB

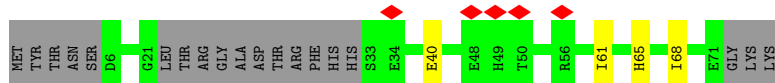
Chain BA:  11% 72% 26%



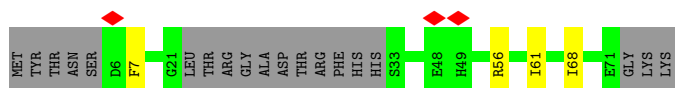
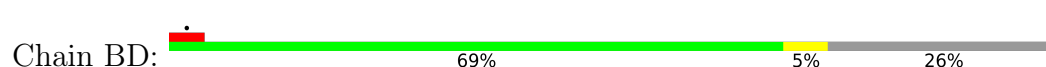
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



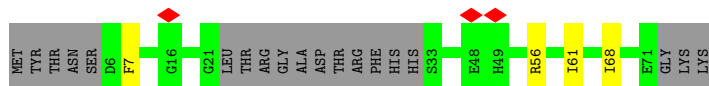
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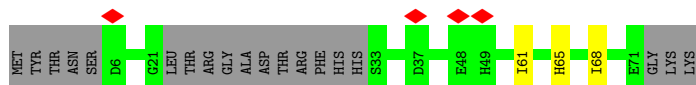
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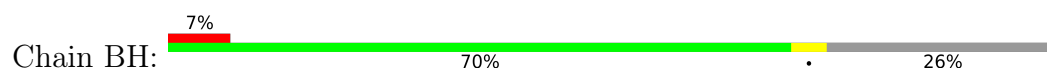
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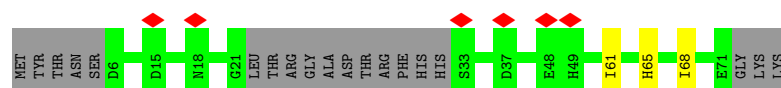
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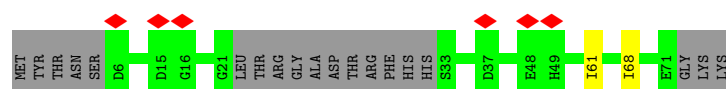
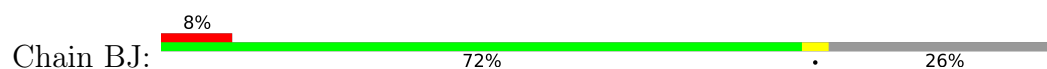
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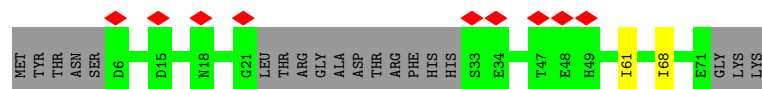
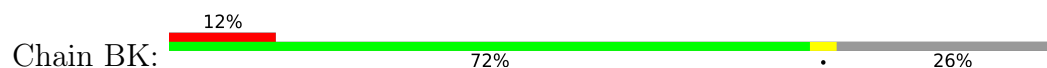
- Molecule 1: Transcription attenuation protein MtrB



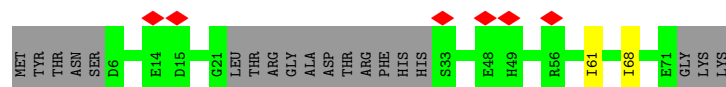
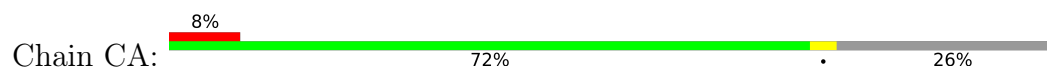
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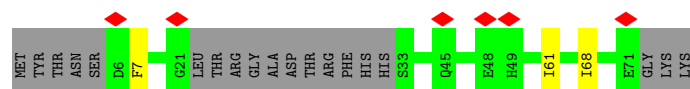
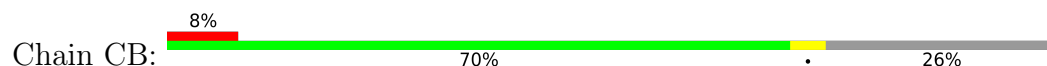
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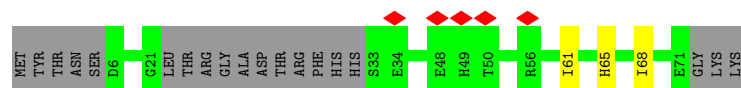
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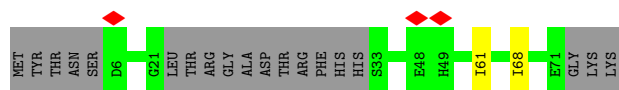
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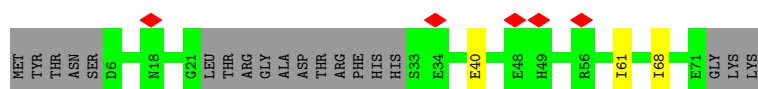
- Molecule 1: Transcription attenuation protein MtrB



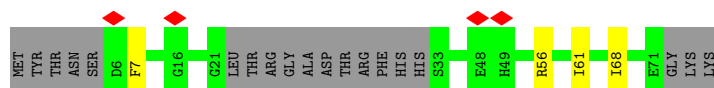
• Molecule 1: Transcription attenuation protein MtrB

Chain CD:  72% 26%

• Molecule 1: Transcription attenuation protein MtrB

Chain CE:  7% 70% 26%

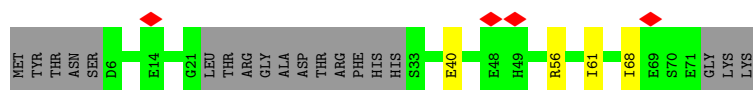
• Molecule 1: Transcription attenuation protein MtrB

Chain CF:  5% 69% 5% 26%

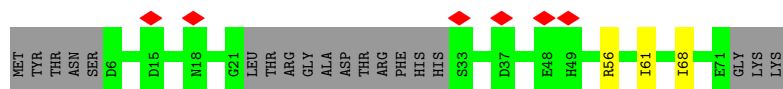
• Molecule 1: Transcription attenuation protein MtrB

Chain CG:  5% 69% 5% 26%

• Molecule 1: Transcription attenuation protein MtrB

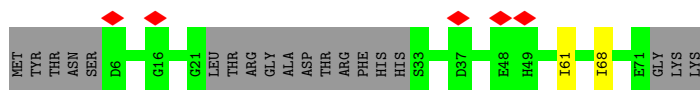
Chain CH:  5% 69% 5% 26%

• Molecule 1: Transcription attenuation protein MtrB

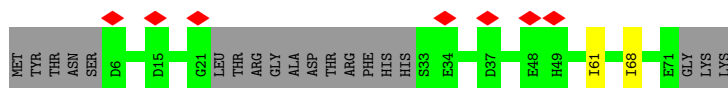
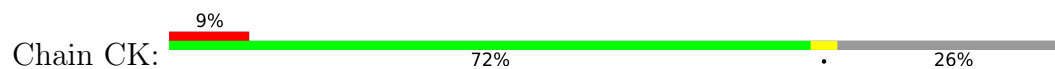
Chain CI:  8% 70% 26%

• Molecule 1: Transcription attenuation protein MtrB

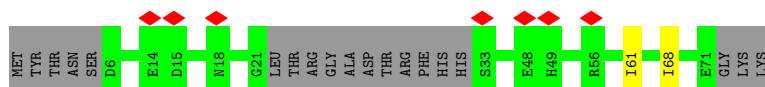
Chain CJ:  7% 72% 26%



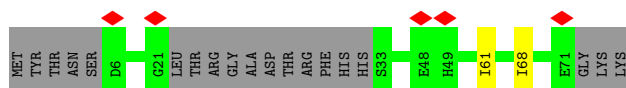
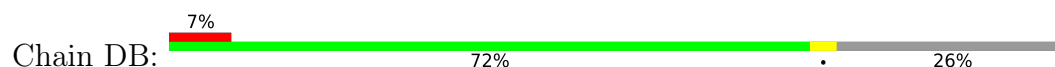
- Molecule 1: Transcription attenuation protein MtrB



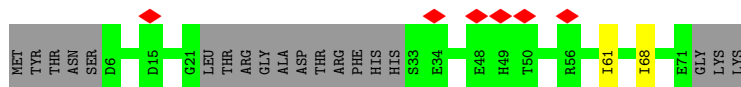
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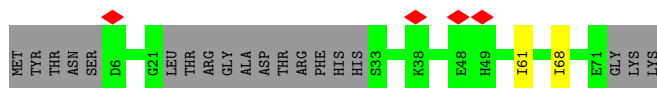
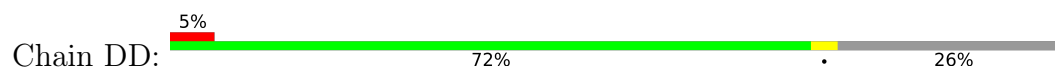
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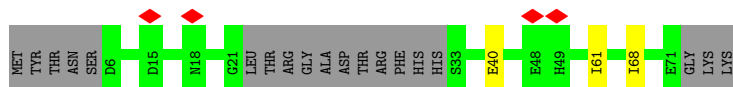
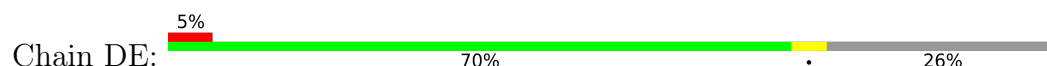
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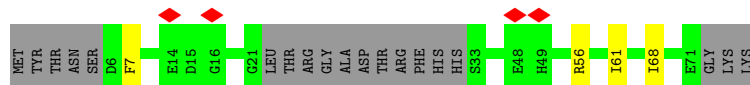
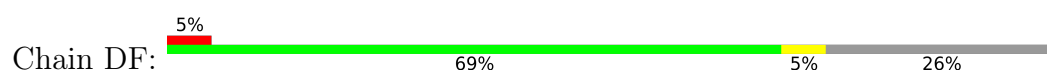
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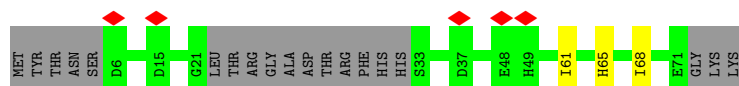
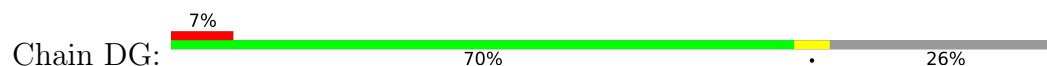
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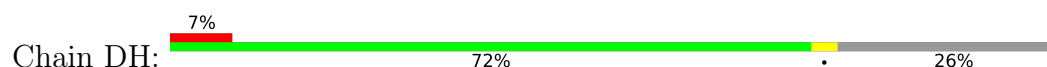
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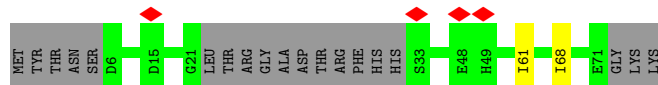
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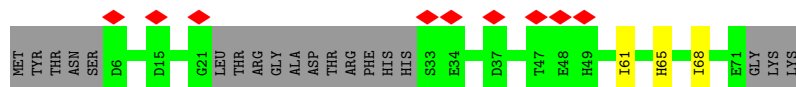
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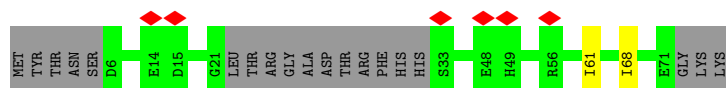
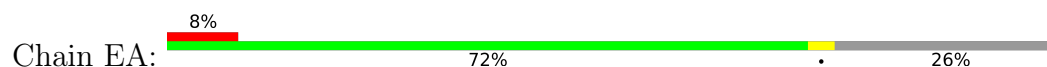
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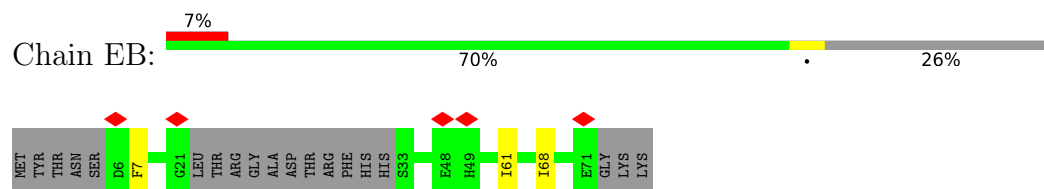
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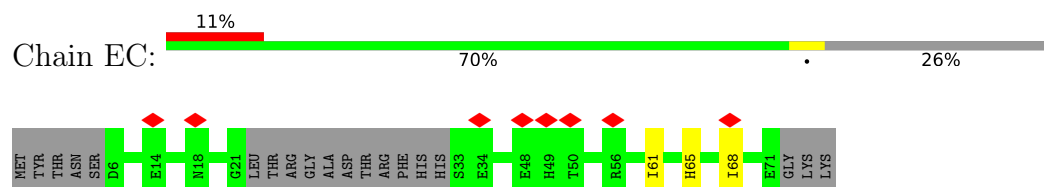
- Molecule 1: Transcription attenuation protein MtrB



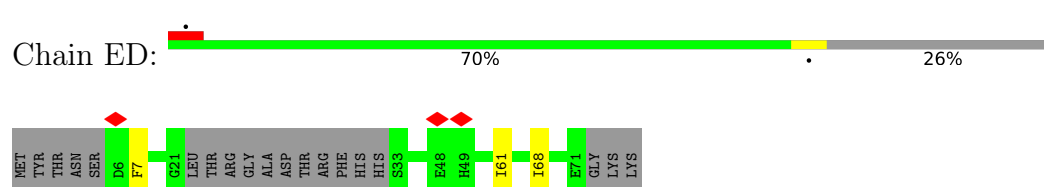
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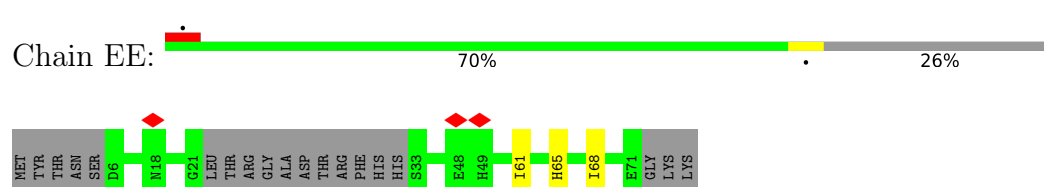
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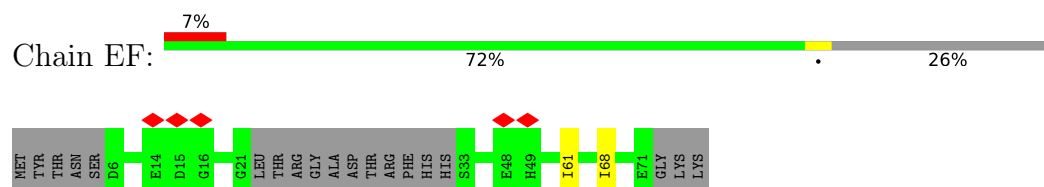
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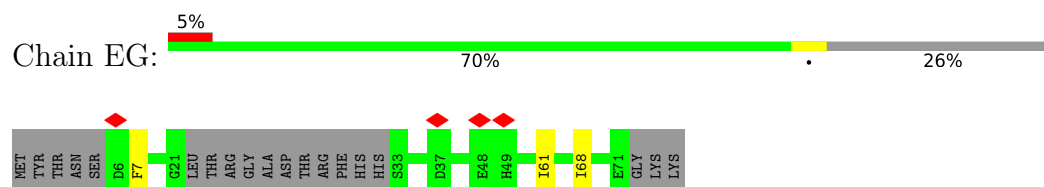
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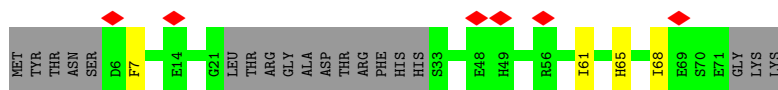


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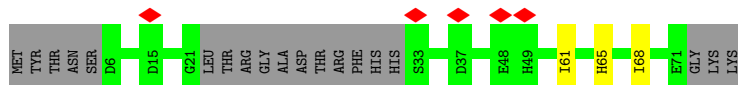


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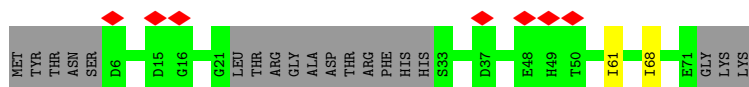




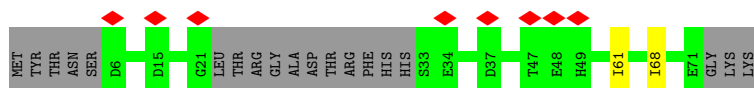
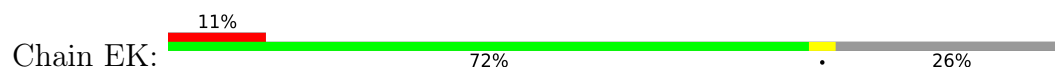
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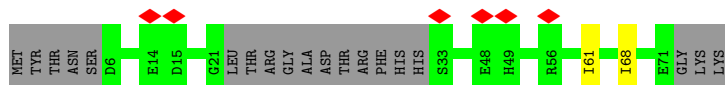
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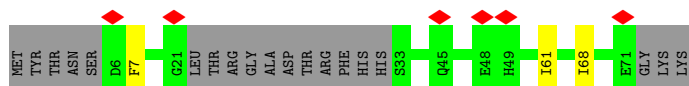
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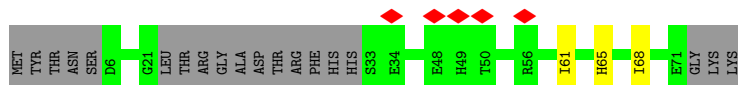
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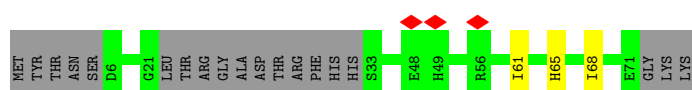
- Molecule 1: Transcription attenuation protein MtrB

Chain FD:  70% 26%



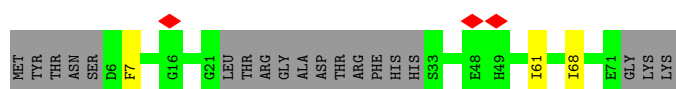
- Molecule 1: Transcription attenuation protein MtrB

Chain FE:  70% 26%



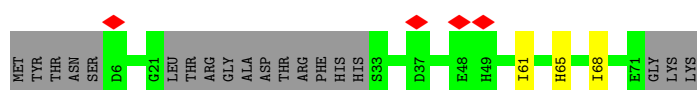
- Molecule 1: Transcription attenuation protein MtrB

Chain FF:  70% 26%



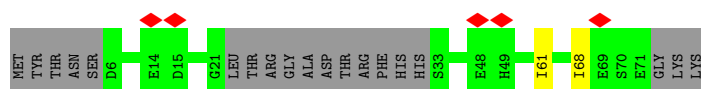
- Molecule 1: Transcription attenuation protein MtrB

Chain FG:  70% 26% 5%



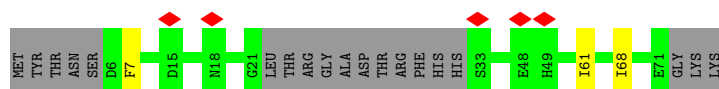
- Molecule 1: Transcription attenuation protein MtrB

Chain FH:  72% 26% 7%



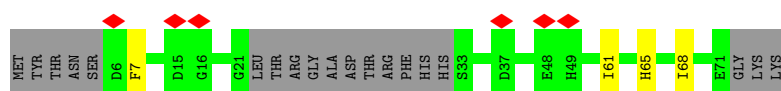
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Chain FI:  70% 26% 7%

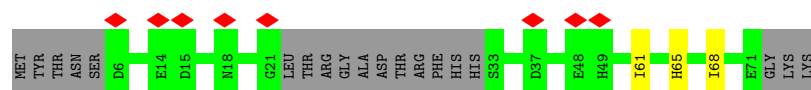
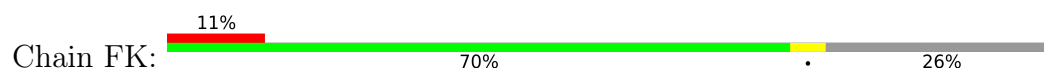


- Molecule 1: Transcription attenuation protein MtrB

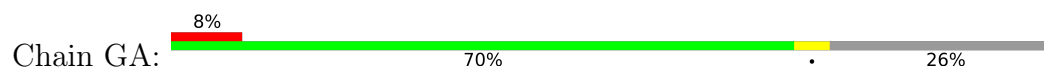
Chain FJ:  69% 26% 8% 5%



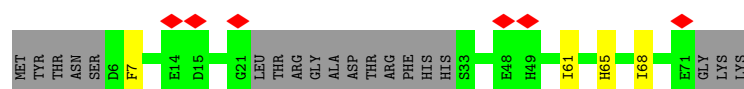
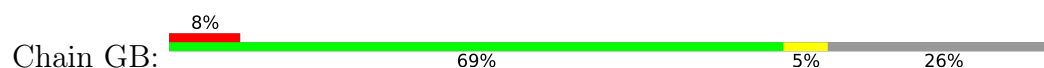
• Molecule 1: Transcription attenuation protein MtrB



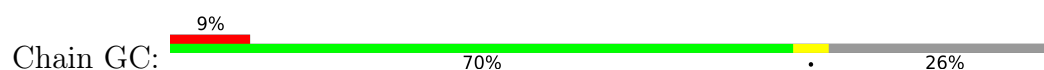
• Molecule 1: Transcription attenuation protein MtrB



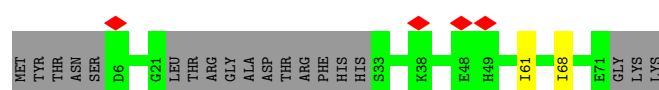
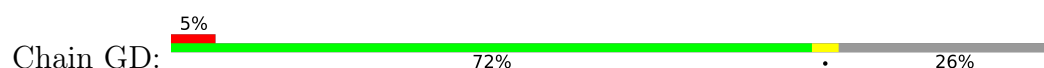
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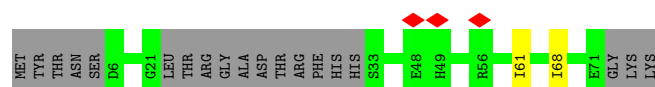
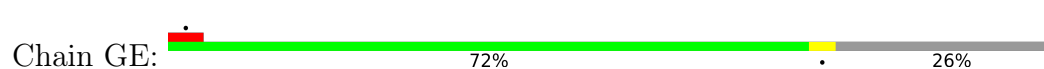
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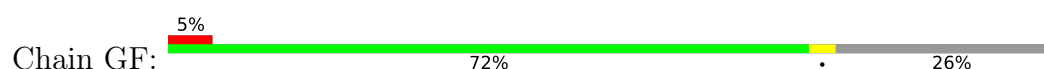
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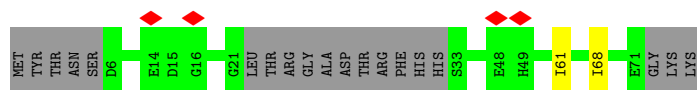


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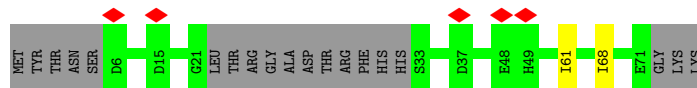
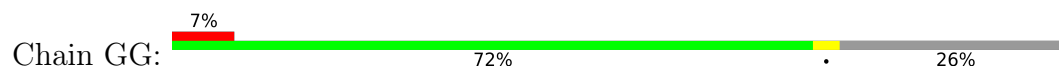


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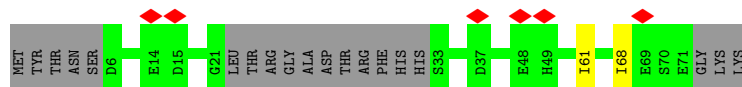




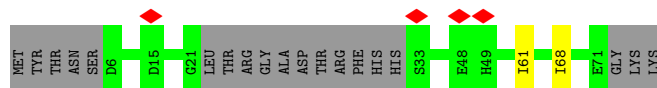
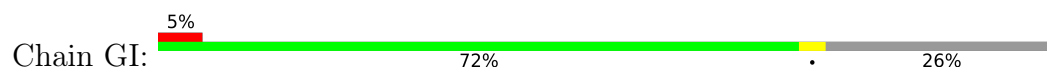
- Molecule 1: Transcription attenuation protein MtrB



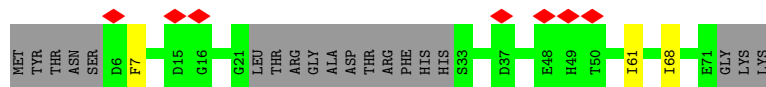
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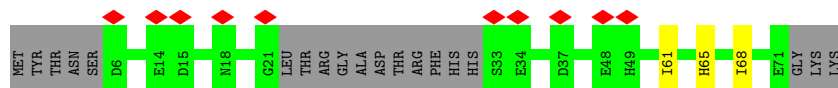
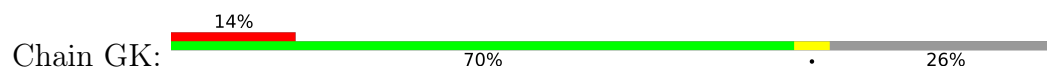
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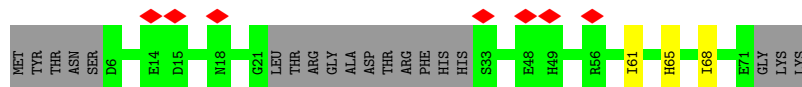
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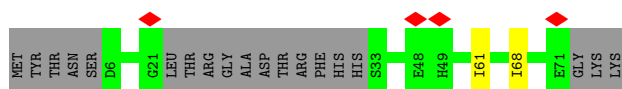
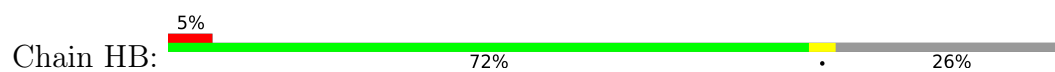
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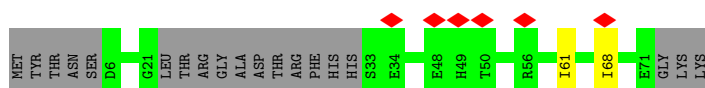
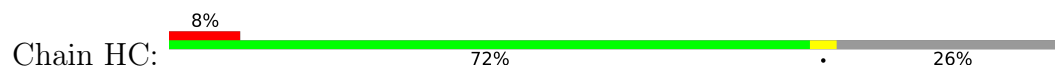
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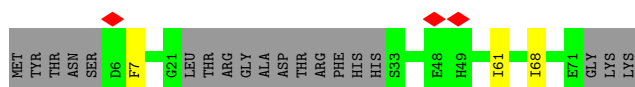
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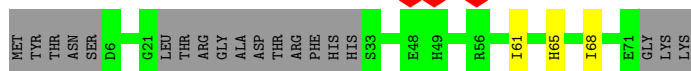
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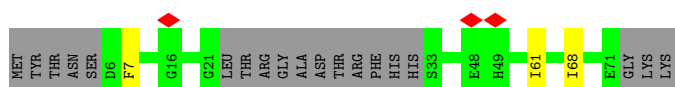
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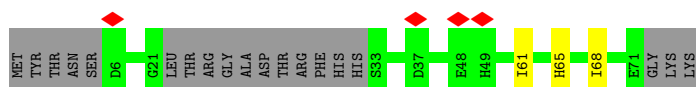
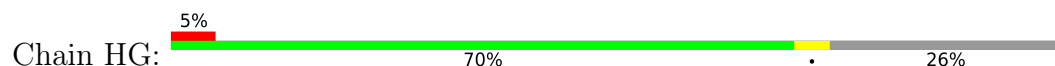
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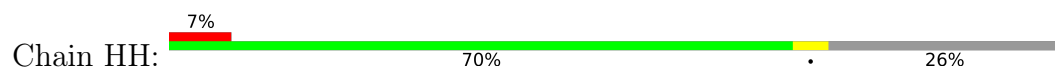
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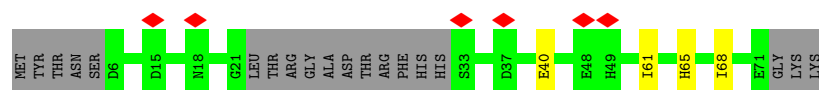
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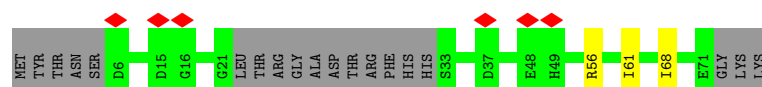
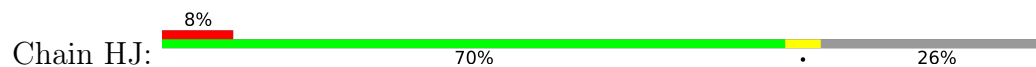
- Molecule 1: Transcription attenuation protein MtrB



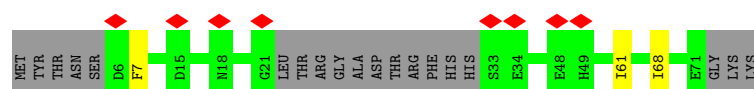
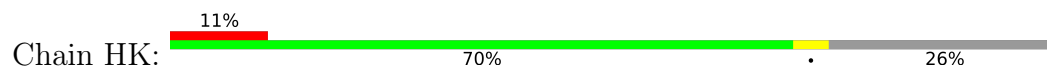
• Molecule 1: Transcription attenuation protein MtrB



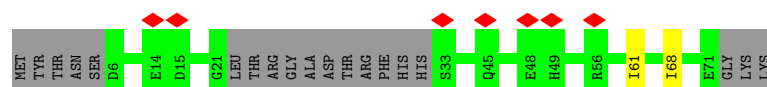
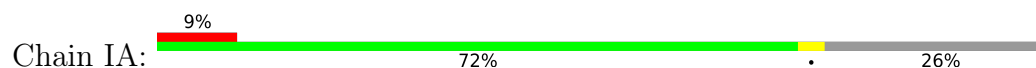
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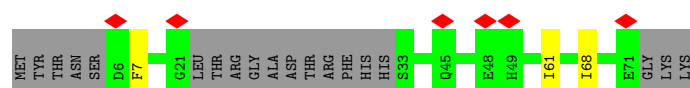
• Molecule 1: Transcription attenuation protein MtrB



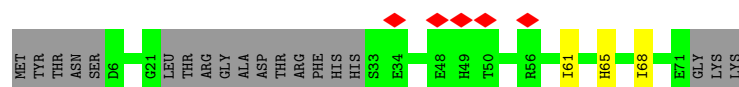
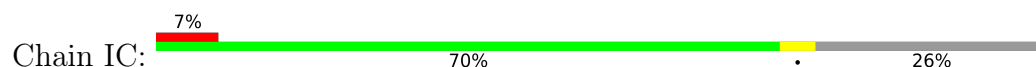
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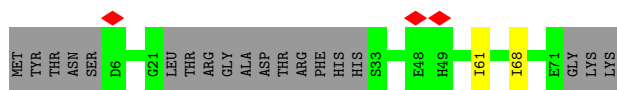


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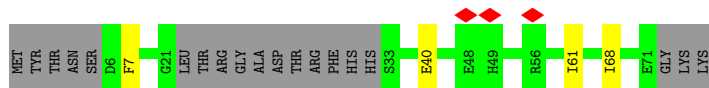


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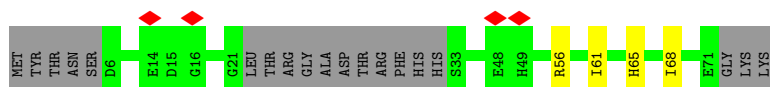




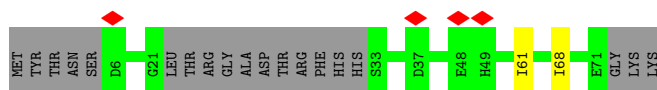
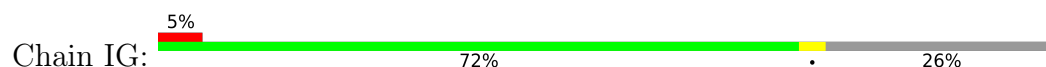
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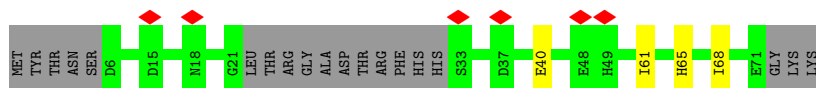
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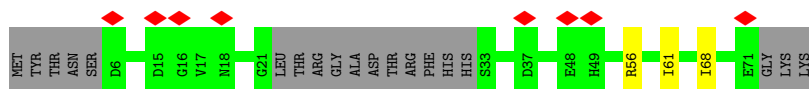
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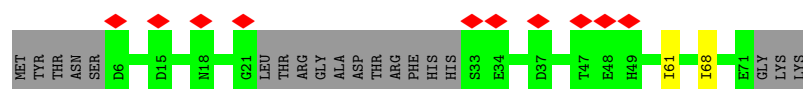
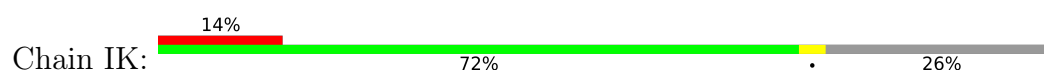
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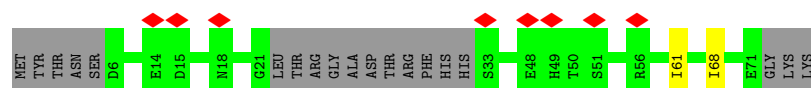
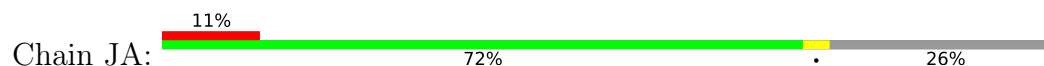
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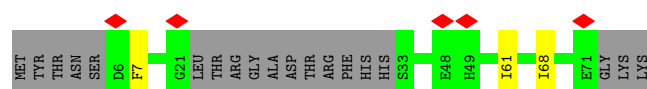
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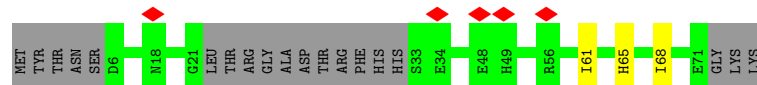
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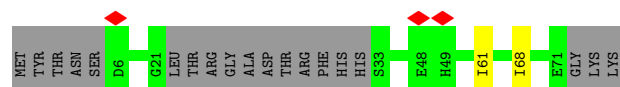
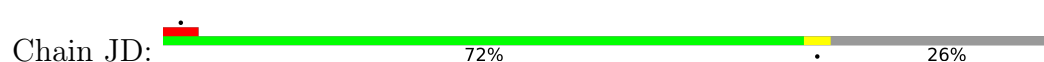
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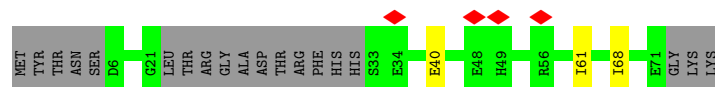
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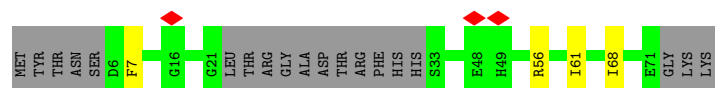
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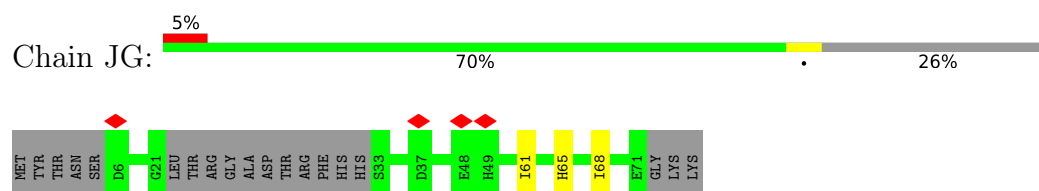
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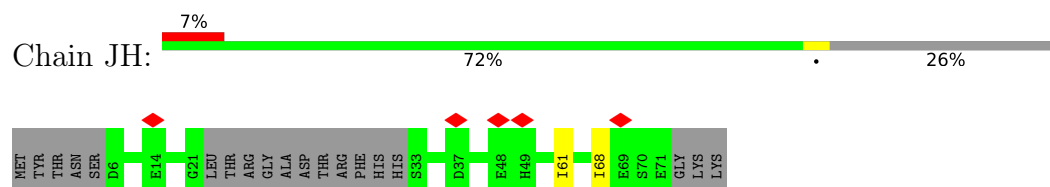
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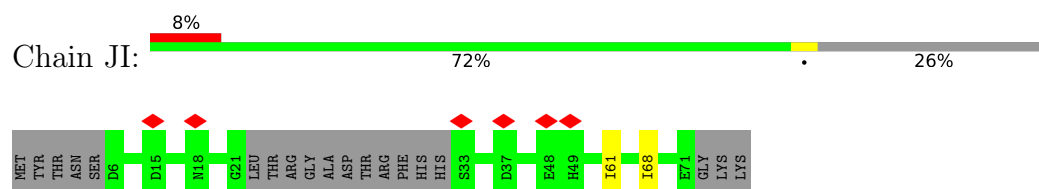
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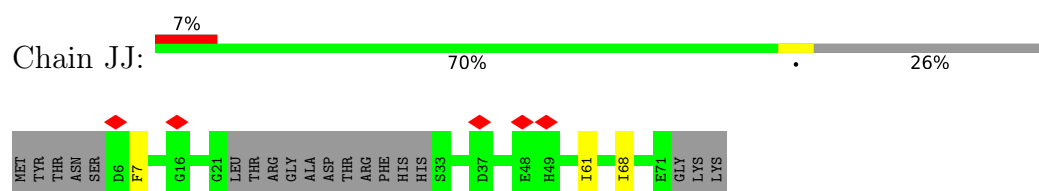
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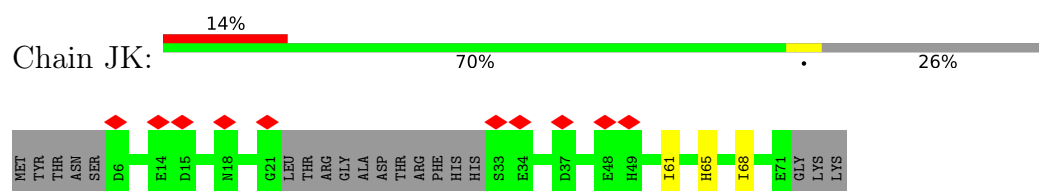
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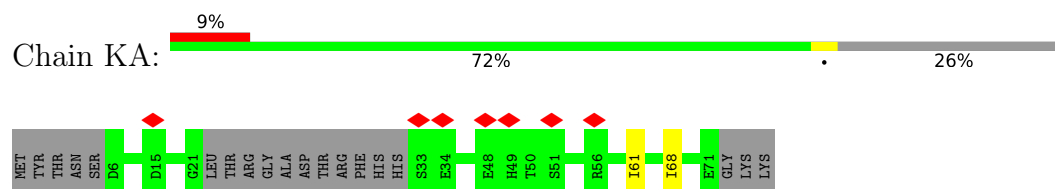
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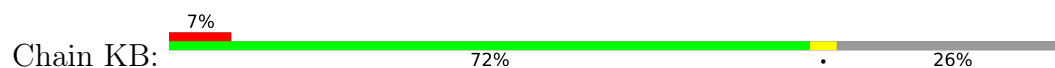
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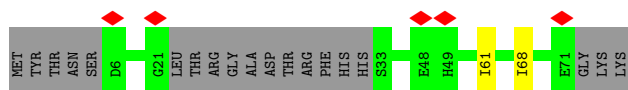


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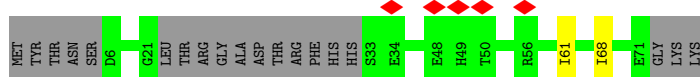
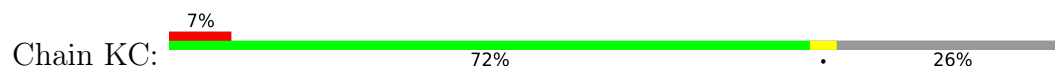


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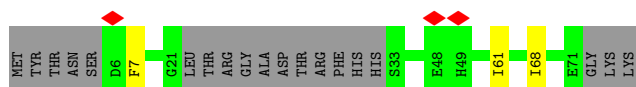




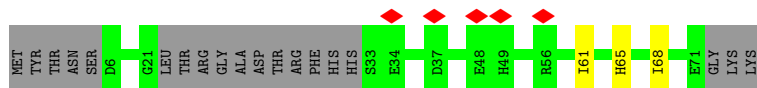
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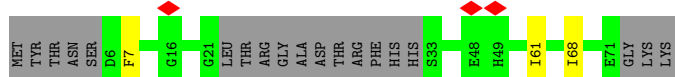
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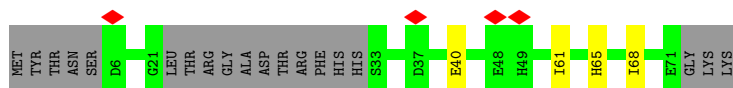
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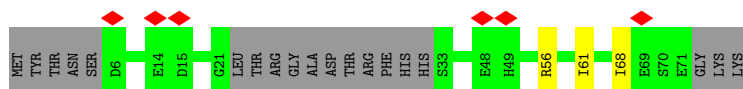
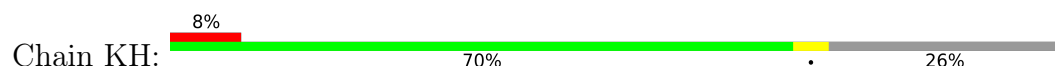
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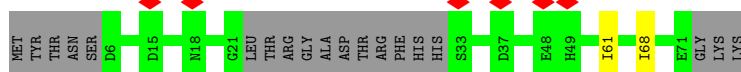
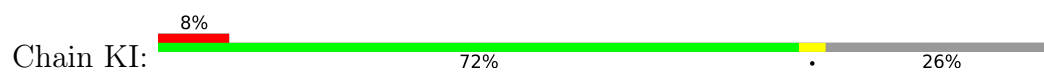
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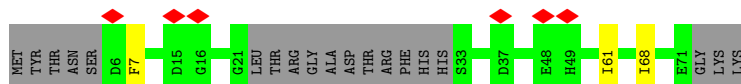
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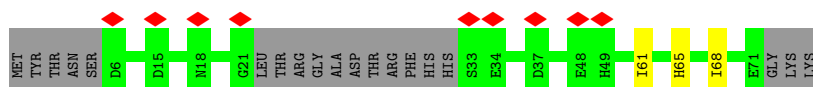
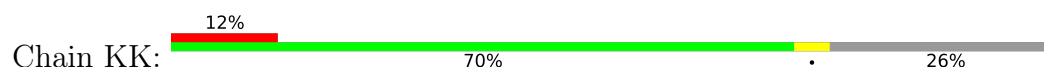
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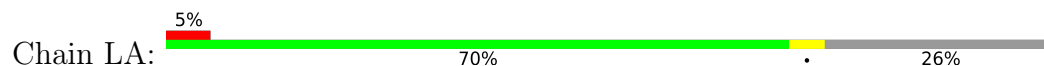
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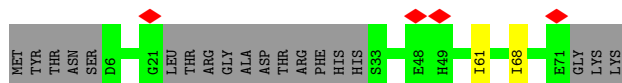
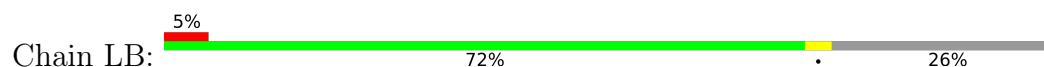
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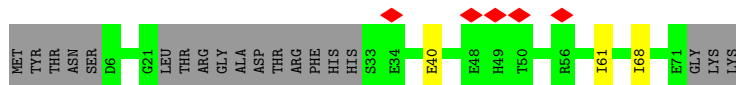
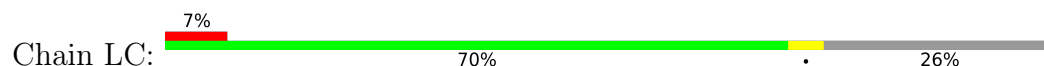
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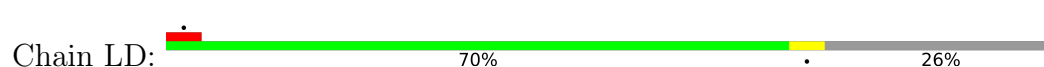
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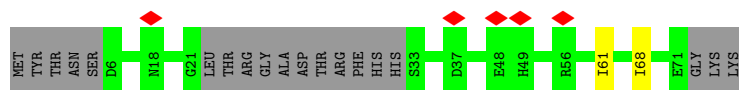
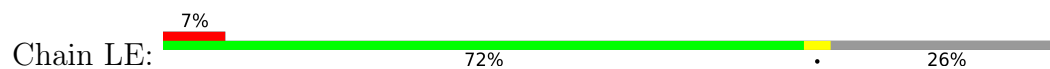
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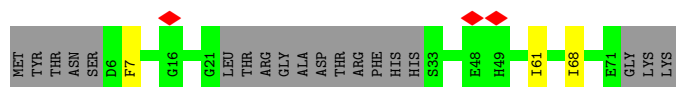
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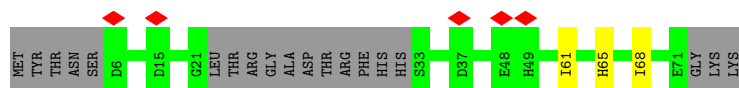
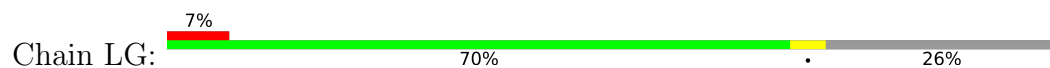
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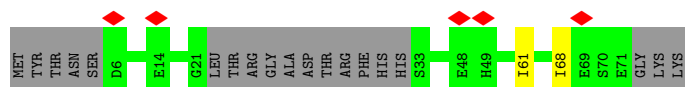
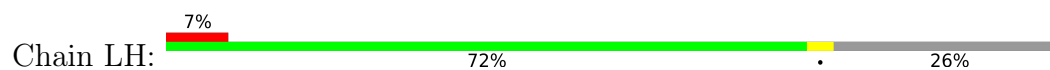
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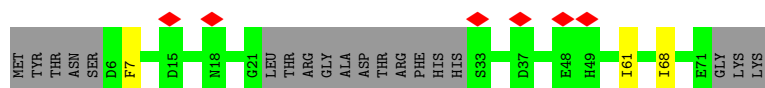
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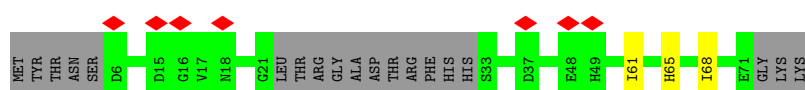
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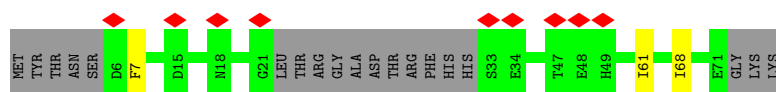


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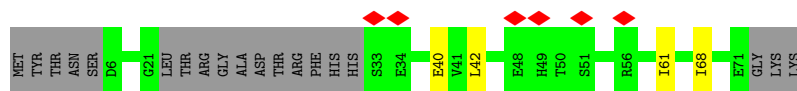
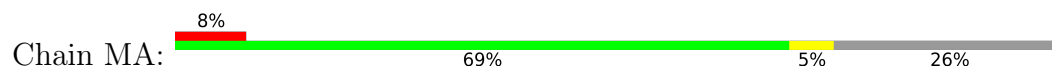


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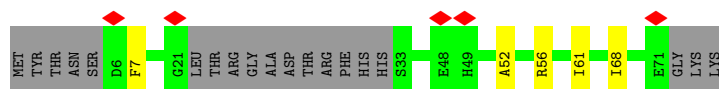




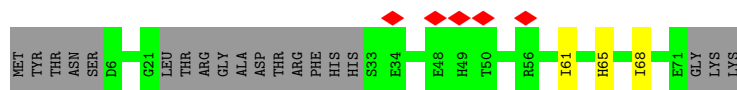
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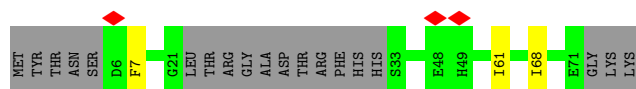
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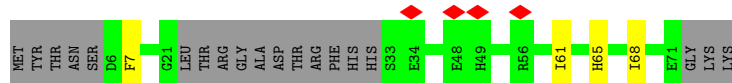
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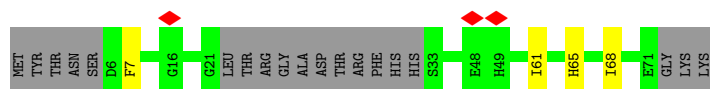
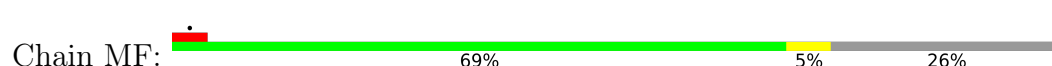
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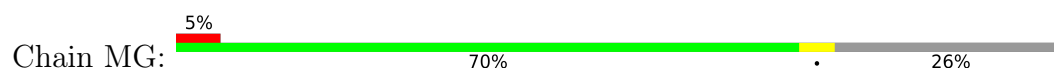
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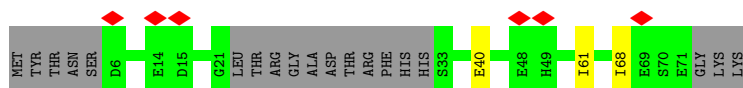
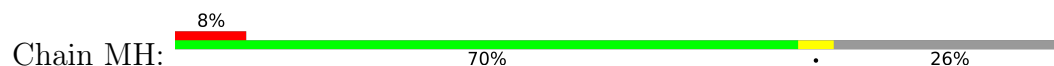
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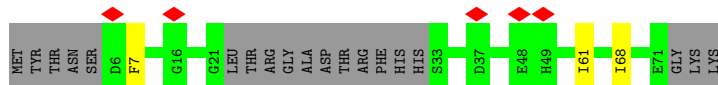
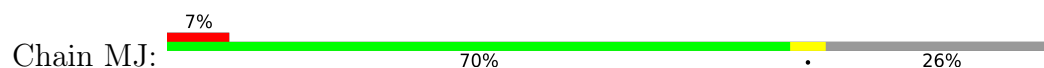
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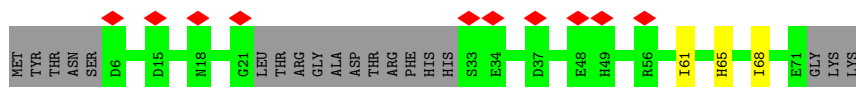
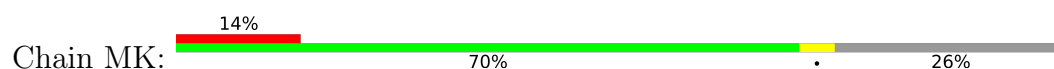
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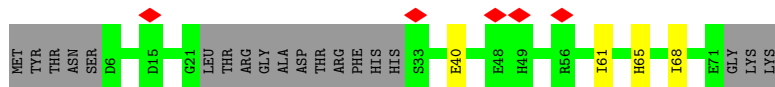
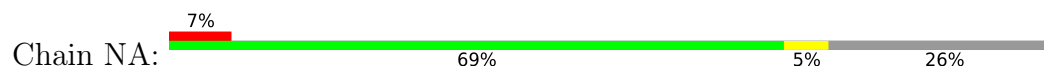
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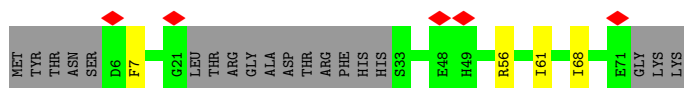
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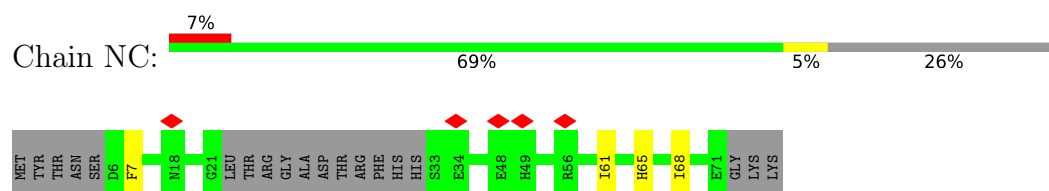
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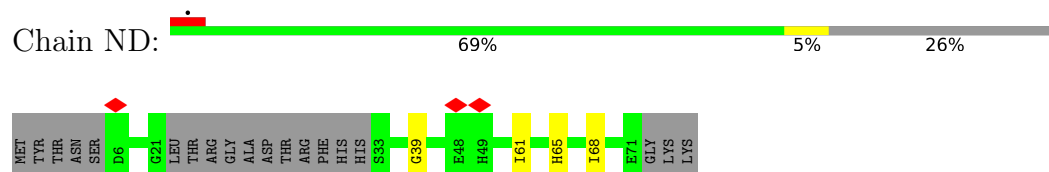
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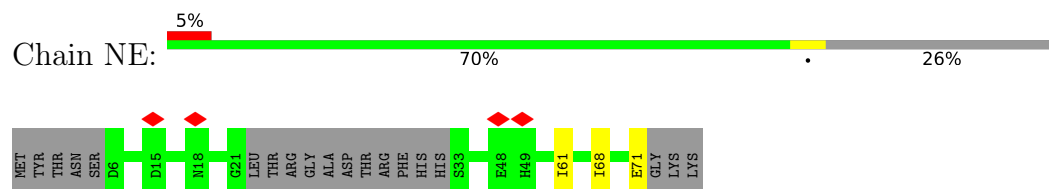
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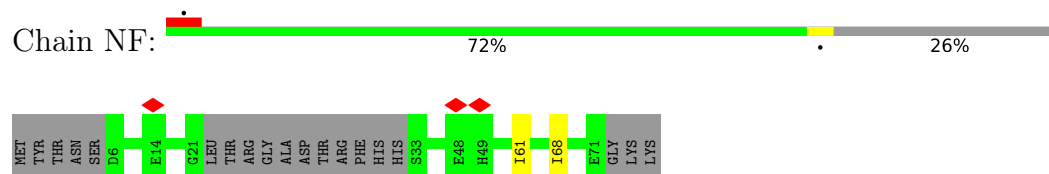
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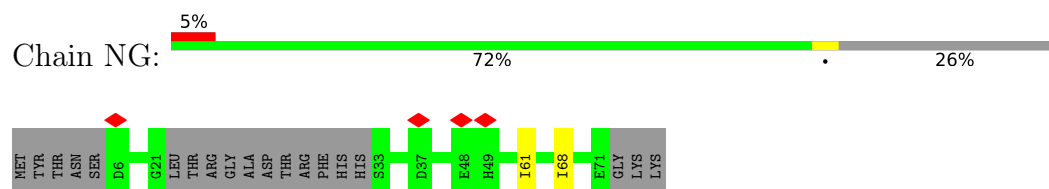
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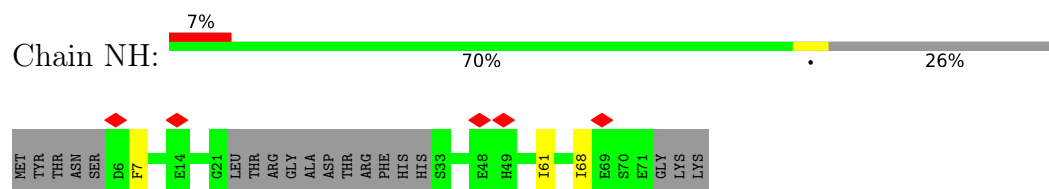
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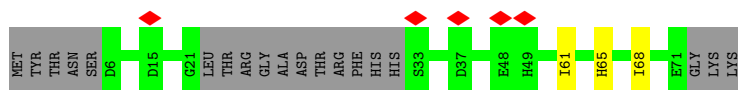


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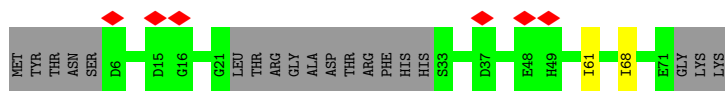
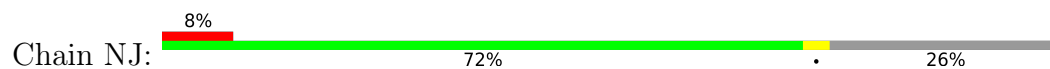


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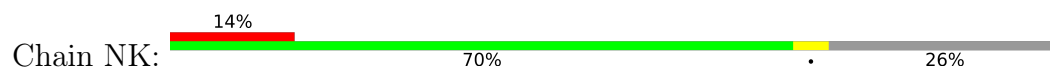




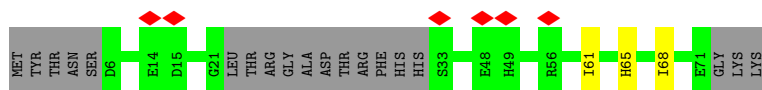
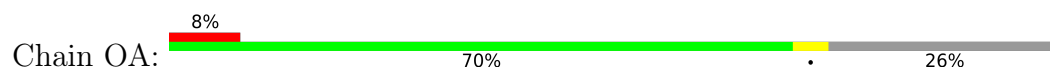
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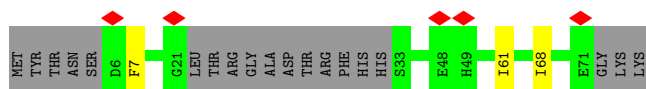
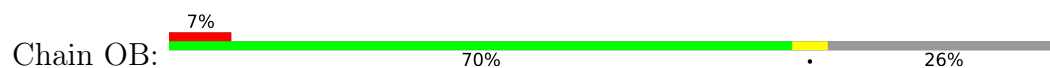
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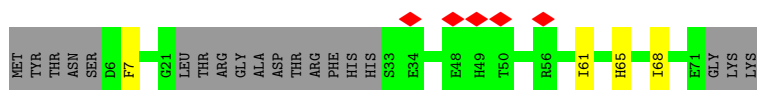
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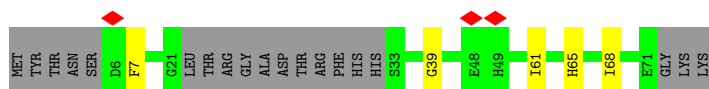
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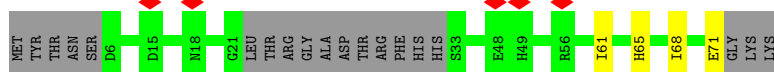
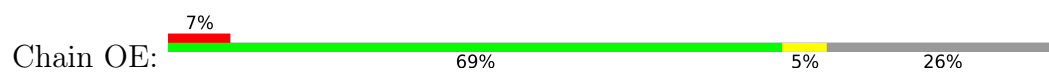
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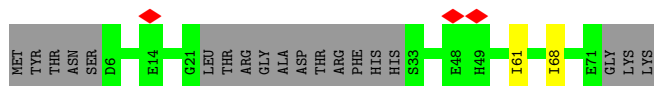
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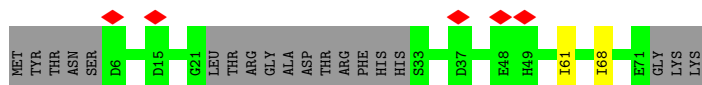
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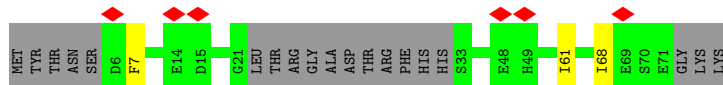
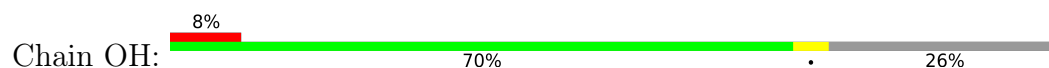
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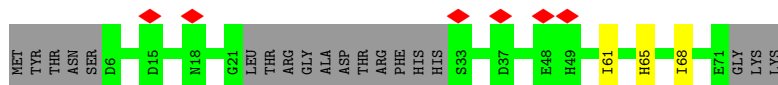
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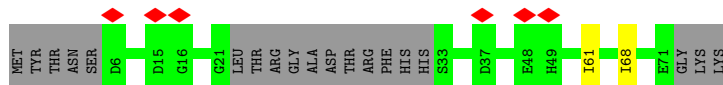
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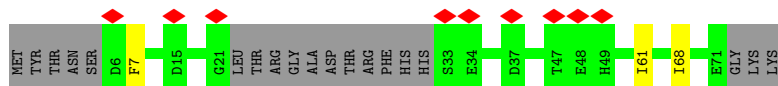
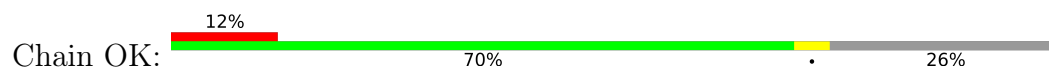
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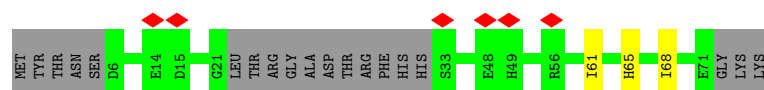
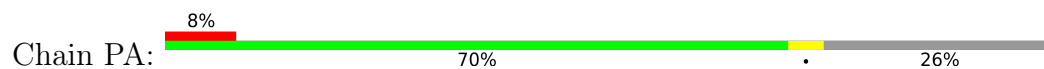
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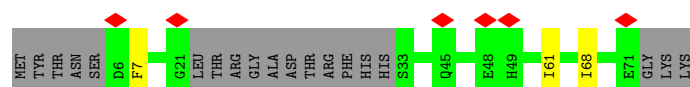
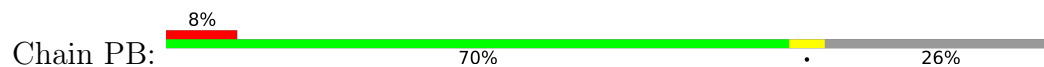
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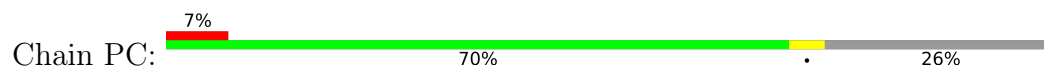
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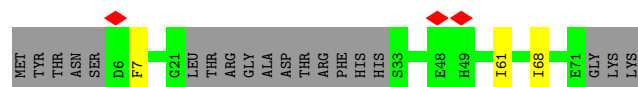
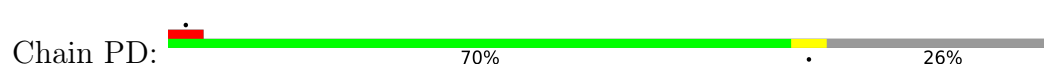
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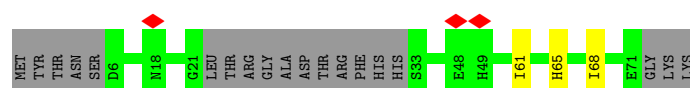
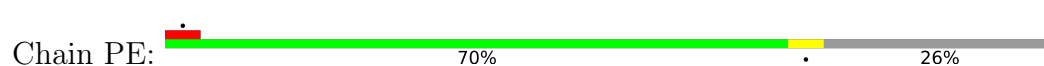
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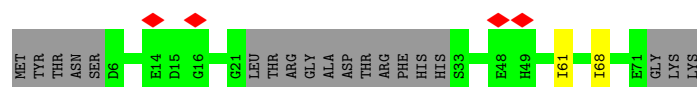
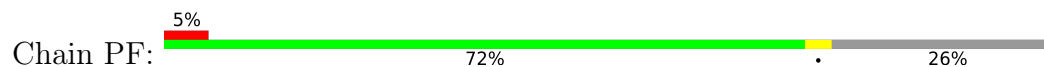
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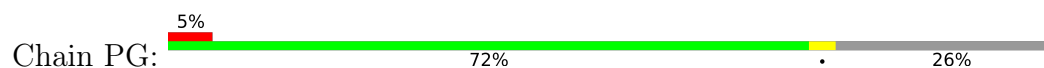
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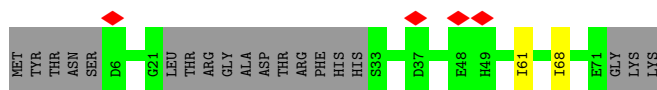


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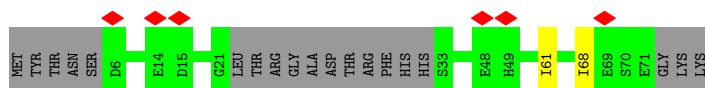
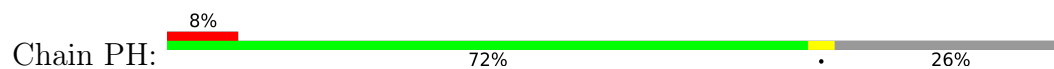


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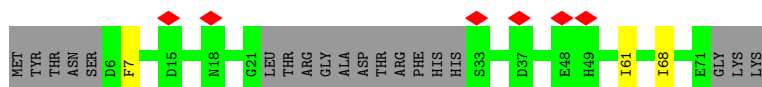




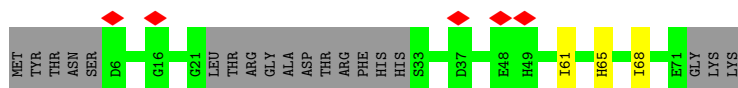
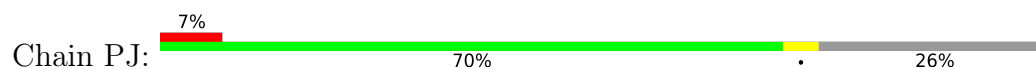
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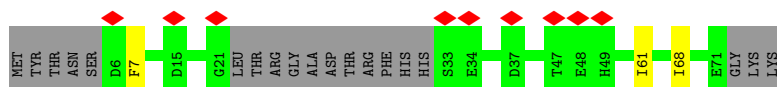
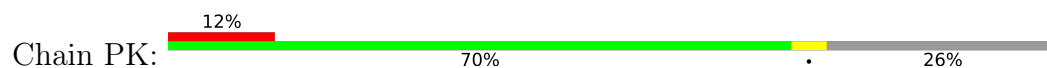
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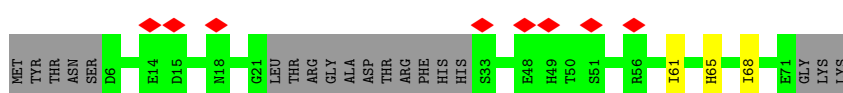
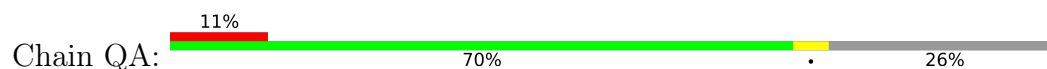
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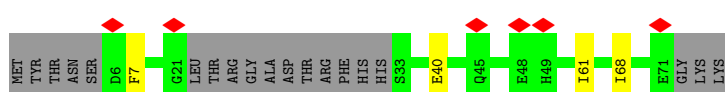
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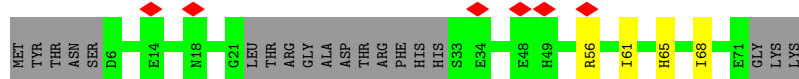
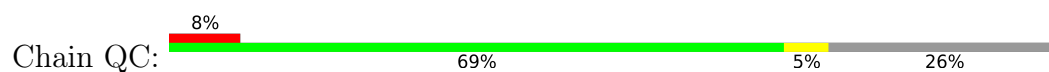
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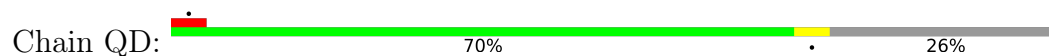
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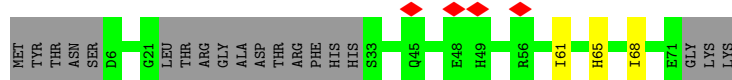
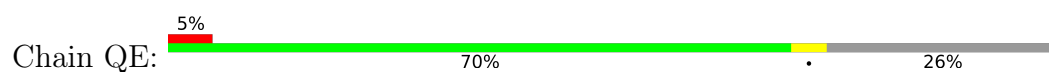
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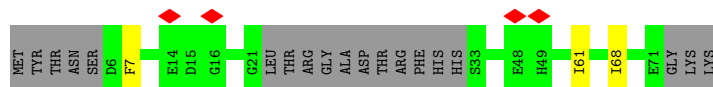
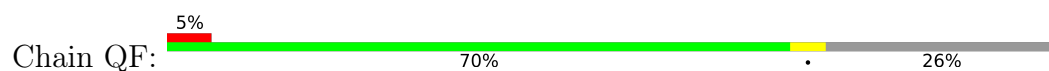
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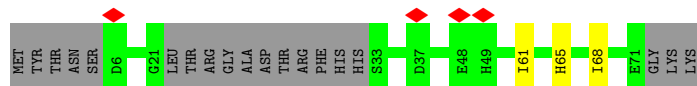
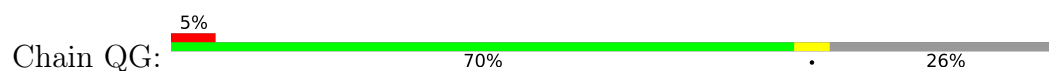
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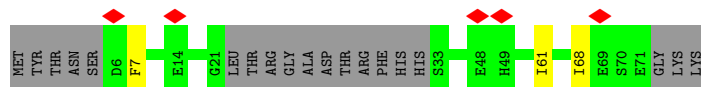
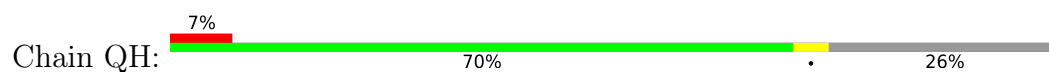
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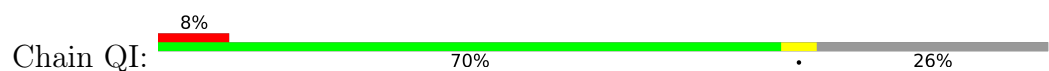
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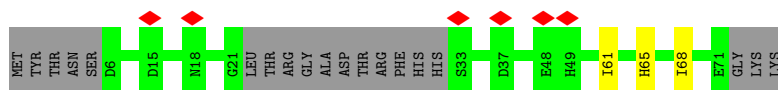


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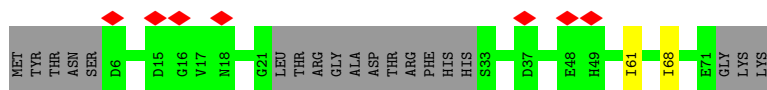
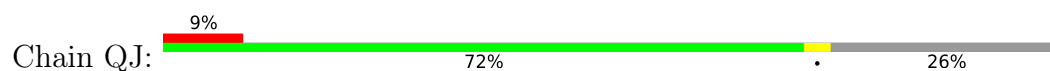


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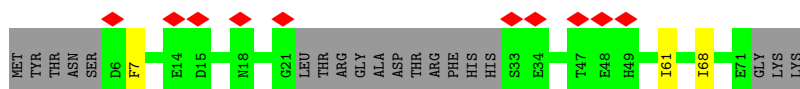
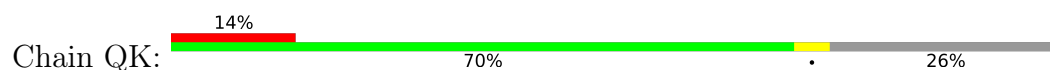




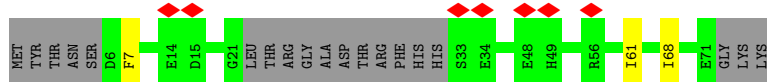
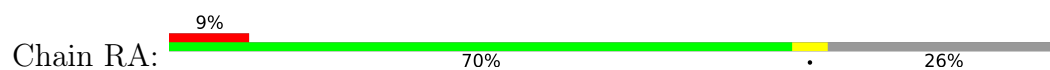
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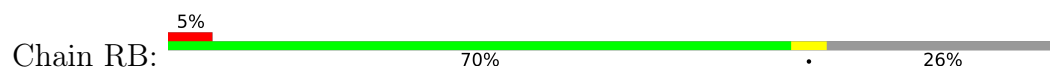
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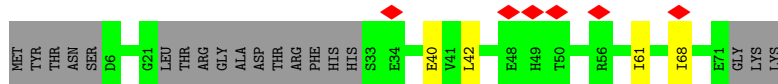
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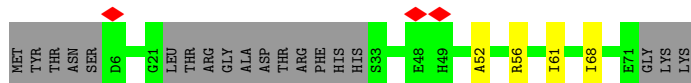
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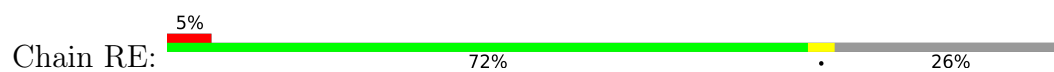
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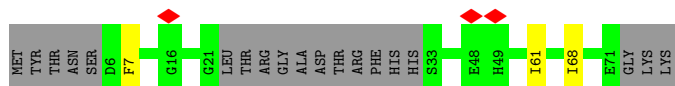
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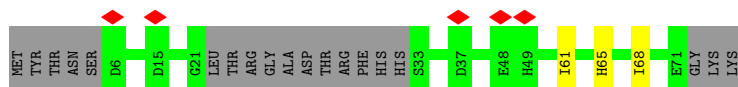
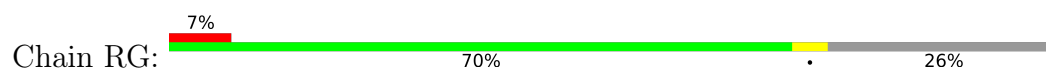
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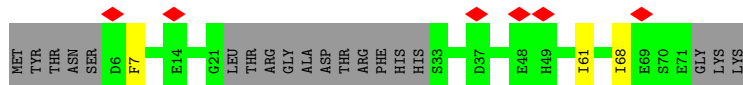
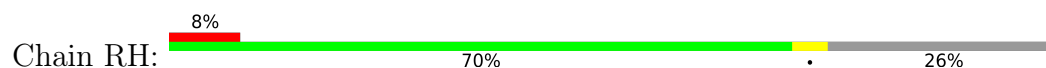
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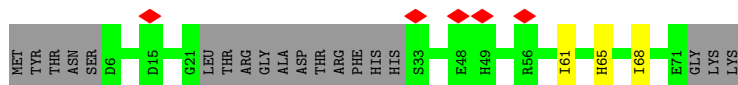
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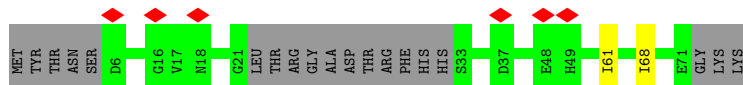
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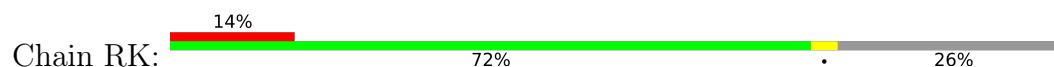
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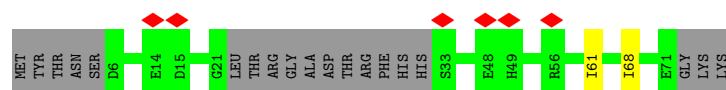
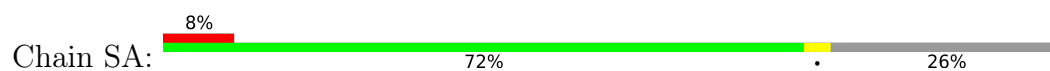
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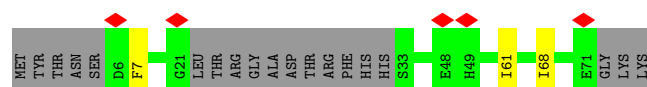
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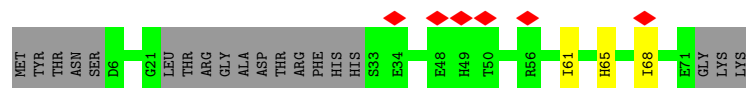
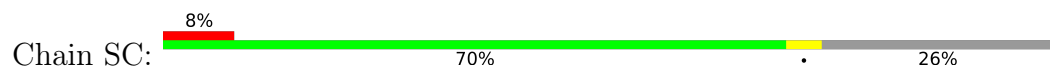
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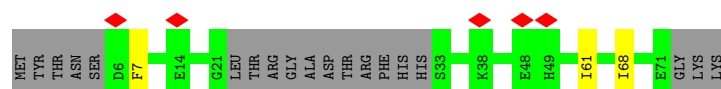
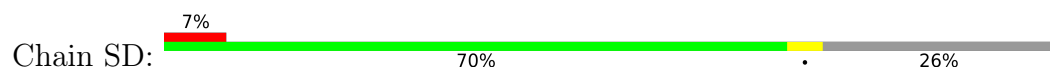
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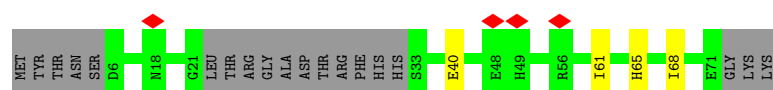
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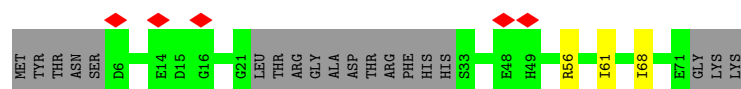
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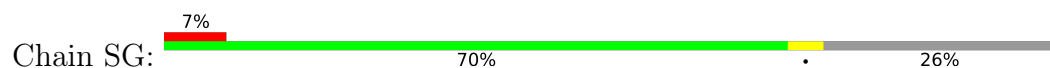
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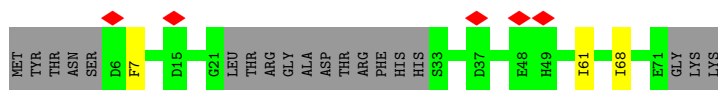


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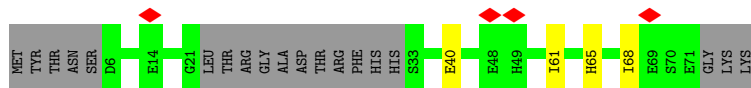


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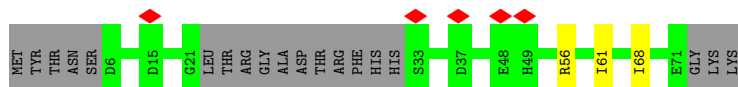




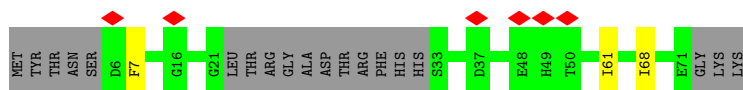
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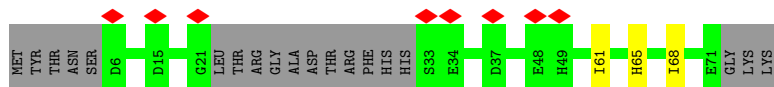
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- Molecule 1: Transcription attenuation protein MtrB



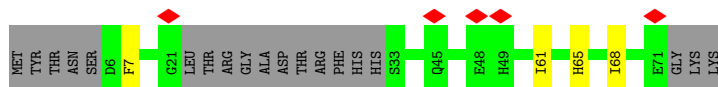
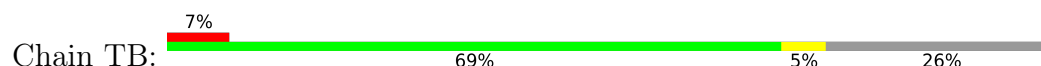
- Molecule 1: Transcription attenuation protein MtrB



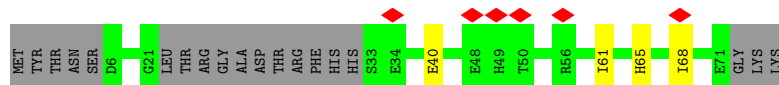
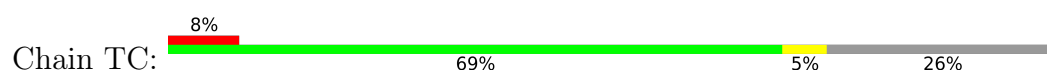
- Molecule 1: Transcription attenuation protein MtrB



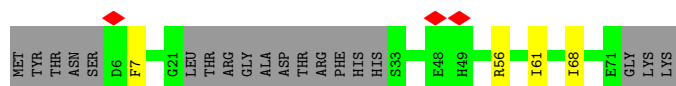
- Molecule 1: Transcription attenuation protein MtrB



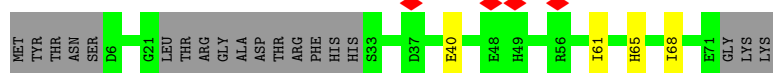
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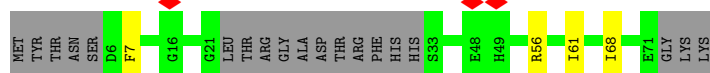
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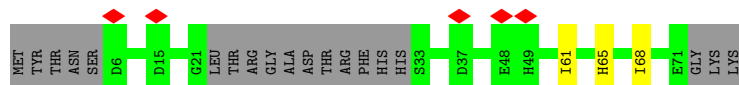
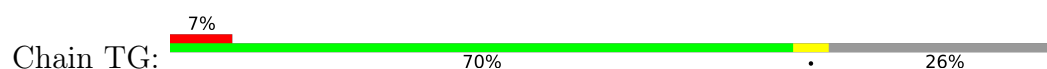
- Molecule 1: Transcription attenuation protein MtrB



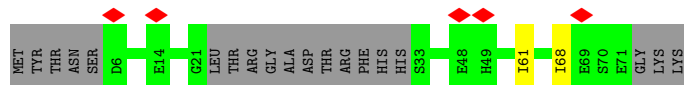
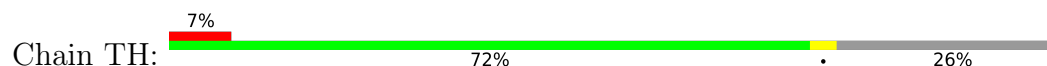
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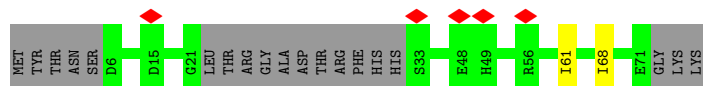
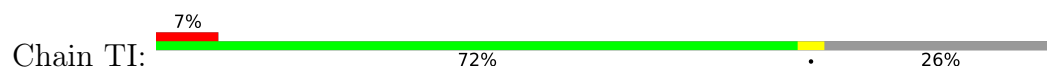
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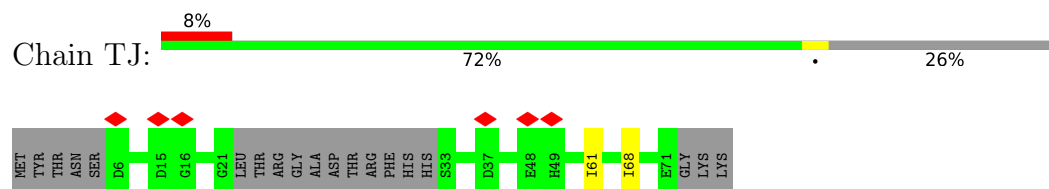
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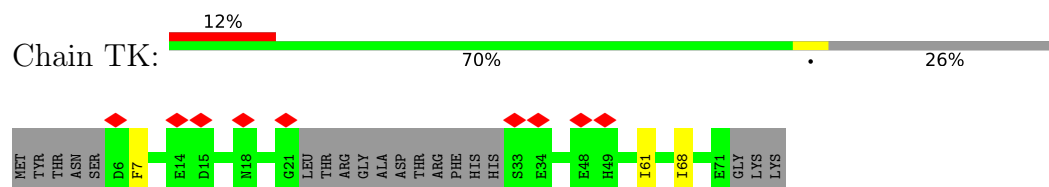
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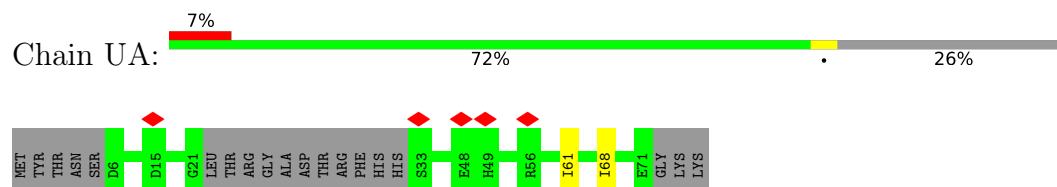
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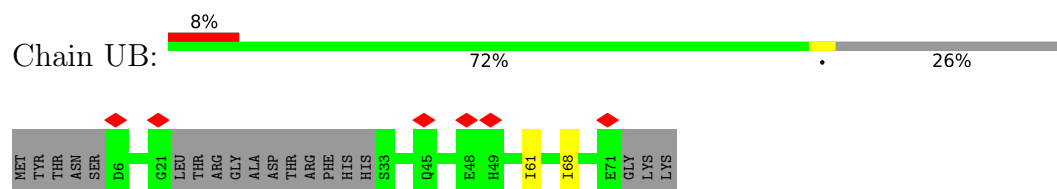
- Molecule 1: Transcription attenuation protein MtrB



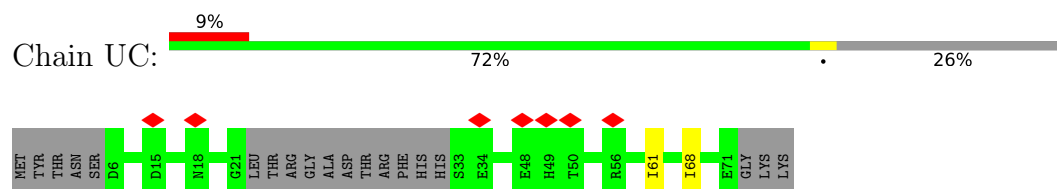
- Molecule 1: Transcription attenuation protein MtrB



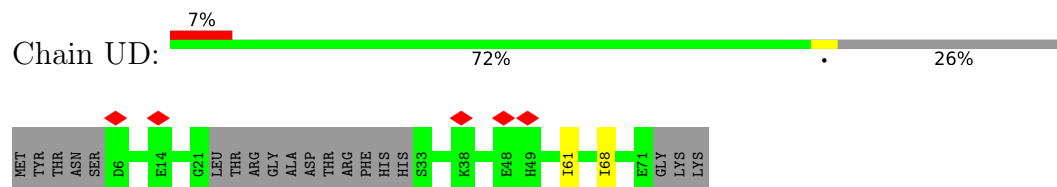
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

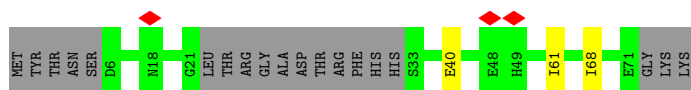


- Molecule 1: Transcription attenuation protein MtrB

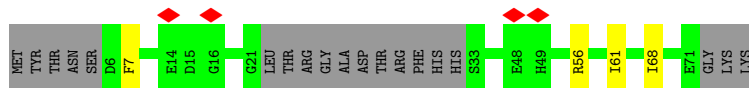


- Molecule 1: Transcription attenuation protein MtrB

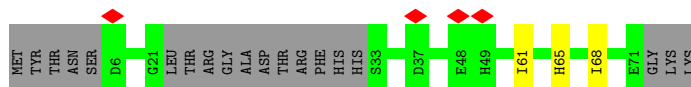




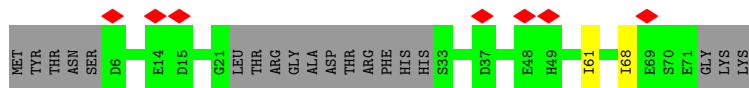
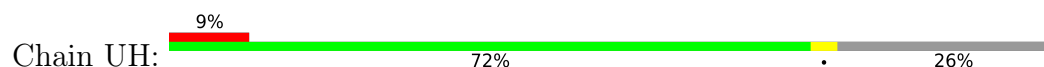
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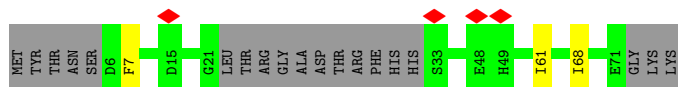
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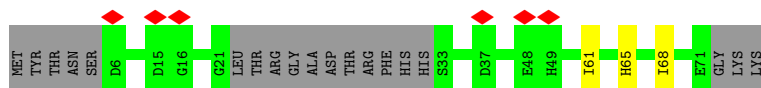
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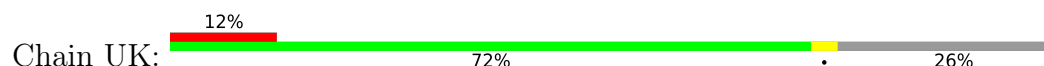
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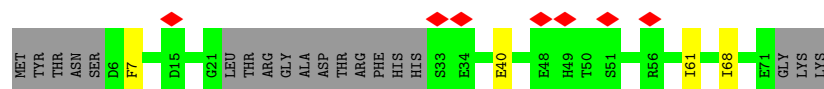
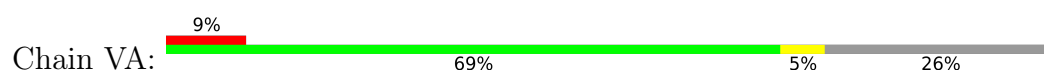
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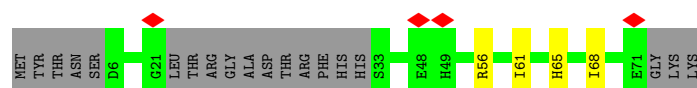
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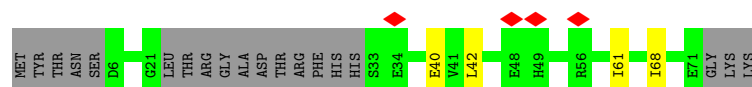
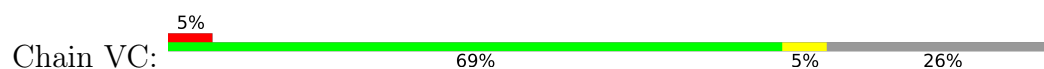
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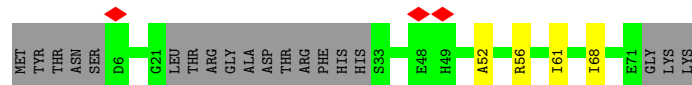
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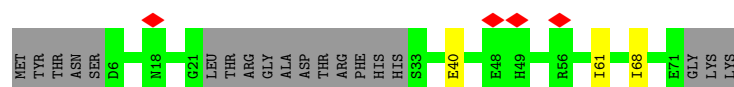
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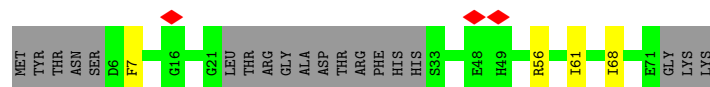
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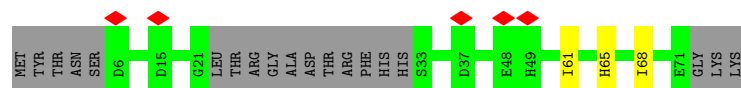
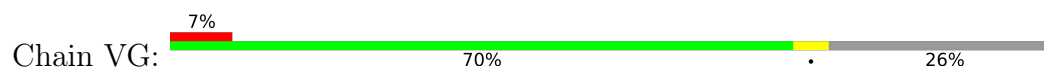
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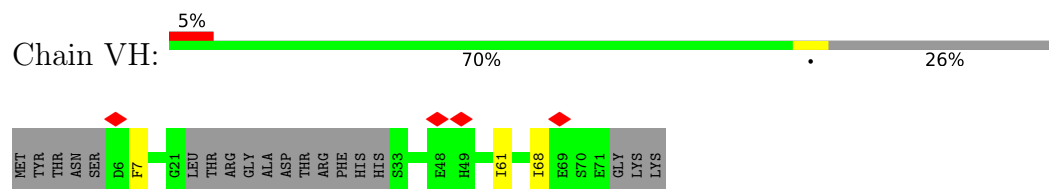
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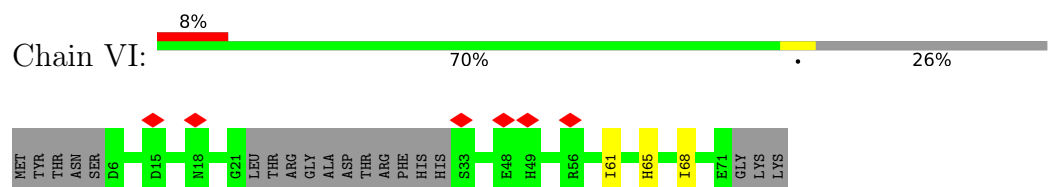
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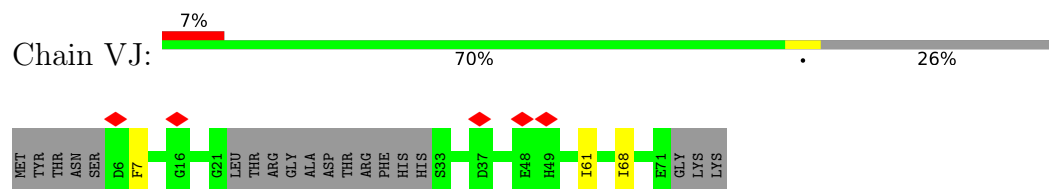
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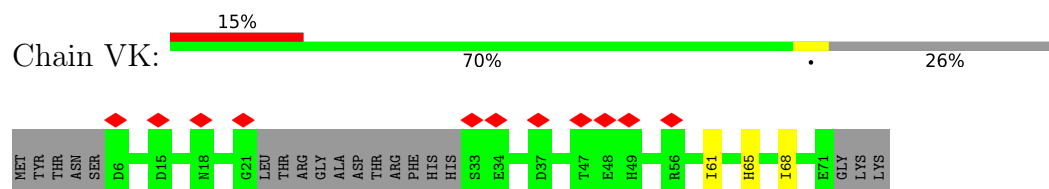
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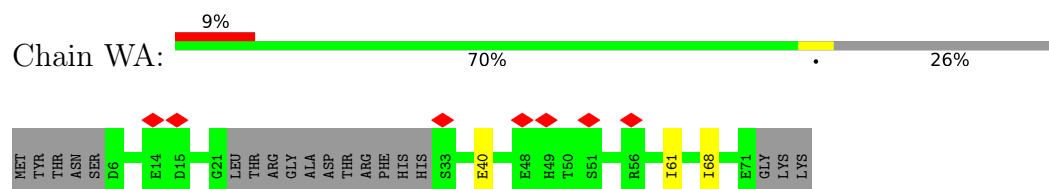
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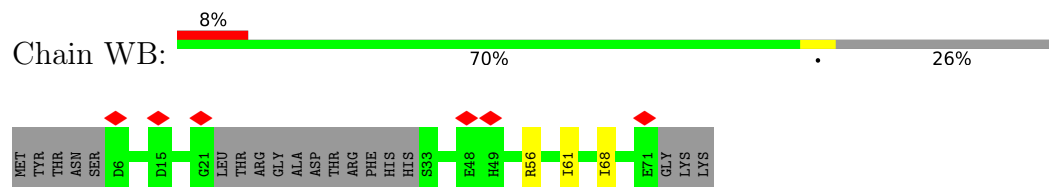
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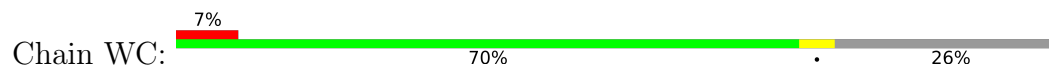
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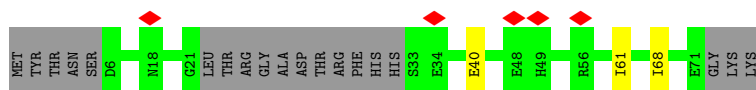


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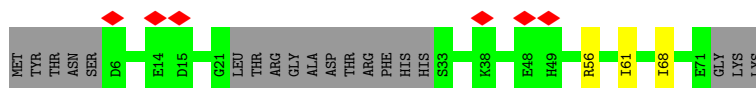
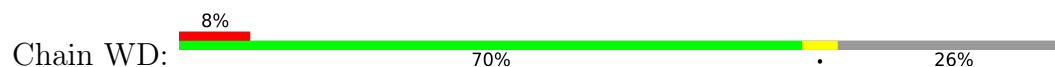


- Molecule 1: Transcription attenuation protein MtrB

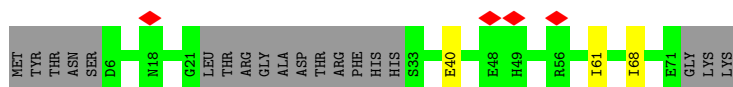




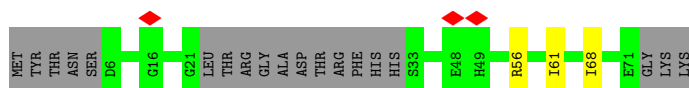
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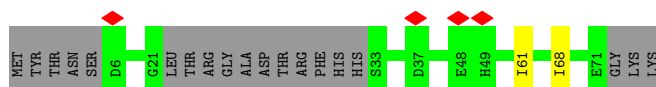
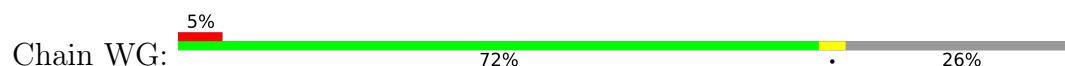
- Molecule 1: Transcription attenuation protein MtrB



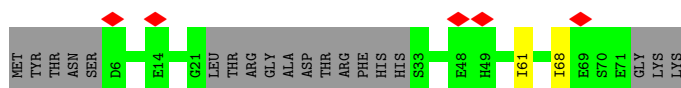
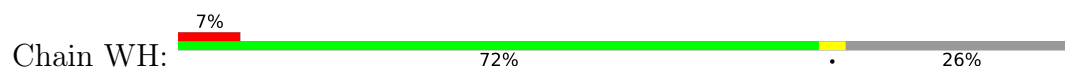
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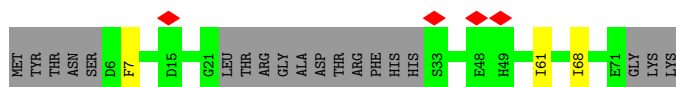
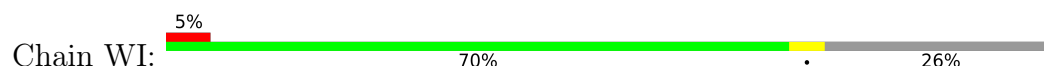
- Molecule 1: Transcription attenuation protein MtrB



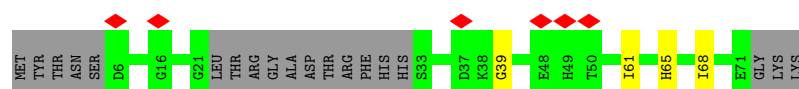
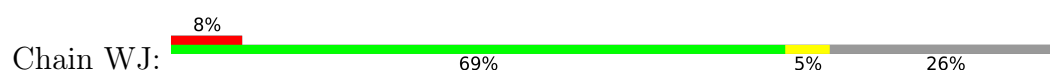
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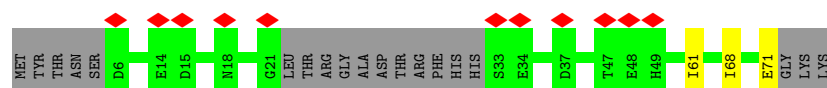
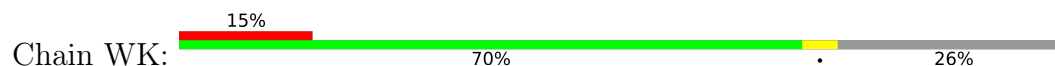
- Molecule 1: Transcription attenuation protein MtrB



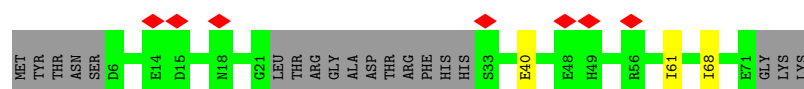
- Molecule 1: Transcription attenuation protein MtrB



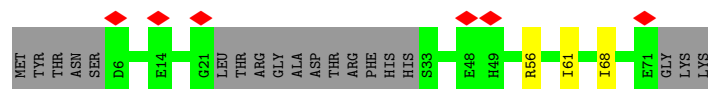
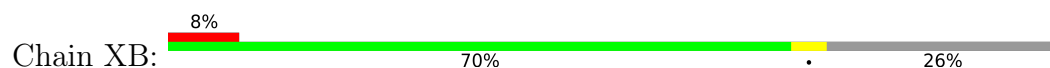
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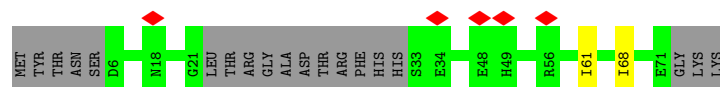
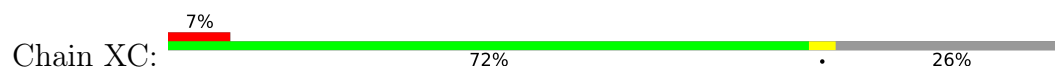
- Molecule 1: Transcription attenuation protein MtrB



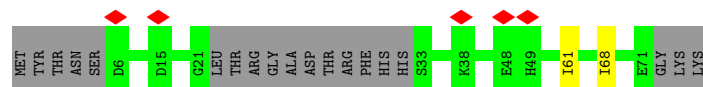
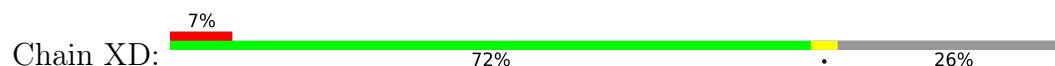
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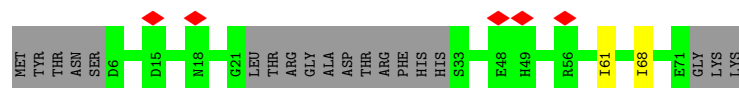
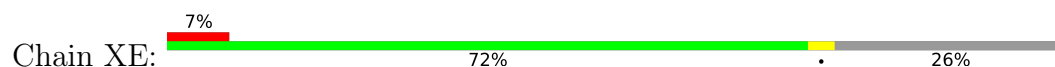
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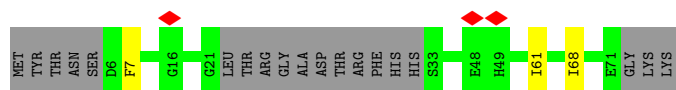
- Molecule 1: Transcription attenuation protein MtrB



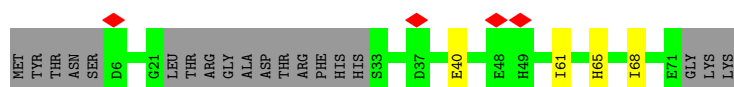
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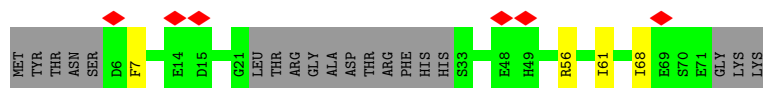
● Molecule 1: Transcription attenuation protein MtrB

Chain XF:  70% 26%

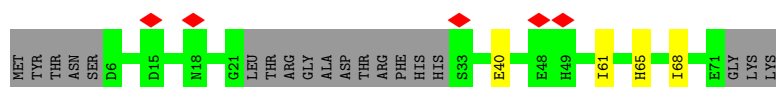
● Molecule 1: Transcription attenuation protein MtrB

Chain XG:  5% 69% 5% 26%

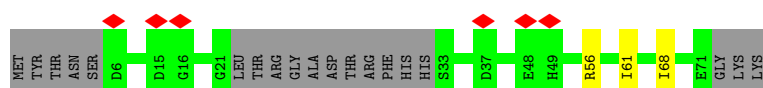
● Molecule 1: Transcription attenuation protein MtrB

Chain XH:  8% 69% 5% 26%

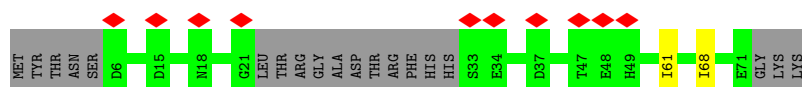
● Molecule 1: Transcription attenuation protein MtrB

Chain XI:  7% 69% 5% 26%

● Molecule 1: Transcription attenuation protein MtrB

Chain XJ:  8% 70% 26%

● Molecule 1: Transcription attenuation protein MtrB

Chain XK:  14% 72% 26%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94388	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.115	Depositor
Map size (Å)	382.8, 382.8, 382.8	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7399999, 1.7399999, 1.7399999	Depositor

5 Model quality

5.1 Standard geometry

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

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	AA	0.34	0/420	0.43	0/564
1	AB	0.34	0/420	0.43	0/564
1	AC	0.34	0/420	0.43	0/564
1	AD	0.34	0/420	0.43	0/564
1	AE	0.34	0/420	0.43	0/564
1	AF	0.34	0/420	0.43	0/564
1	AG	0.35	0/420	0.43	0/564
1	AH	0.34	0/420	0.43	0/564
1	AI	0.34	0/420	0.43	0/564
1	AJ	0.34	0/420	0.43	0/564
1	AK	0.34	0/420	0.44	0/564
1	BA	0.34	0/420	0.43	0/564
1	BB	0.34	0/420	0.44	0/564
1	BC	0.34	0/420	0.43	0/564
1	BD	0.34	0/420	0.43	0/564
1	BE	0.34	0/420	0.43	0/564
1	BF	0.34	0/420	0.43	0/564
1	BG	0.34	0/420	0.43	0/564
1	BH	0.34	0/420	0.43	0/564
1	BI	0.34	0/420	0.43	0/564
1	BJ	0.34	0/420	0.43	0/564
1	BK	0.34	0/420	0.43	0/564
1	CA	0.34	0/420	0.43	0/564
1	CB	0.34	0/420	0.43	0/564
1	CC	0.34	0/420	0.43	0/564
1	CD	0.34	0/420	0.43	0/564
1	CE	0.34	0/420	0.43	0/564
1	CF	0.34	0/420	0.43	0/564
1	CG	0.34	0/420	0.43	0/564
1	CH	0.34	0/420	0.43	0/564
1	CI	0.34	0/420	0.43	0/564
1	CJ	0.34	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CK	0.35	0/420	0.43	0/564
1	DA	0.34	0/420	0.43	0/564
1	DB	0.34	0/420	0.43	0/564
1	DC	0.34	0/420	0.43	0/564
1	DD	0.34	0/420	0.43	0/564
1	DE	0.34	0/420	0.43	0/564
1	DF	0.34	0/420	0.43	0/564
1	DG	0.34	0/420	0.43	0/564
1	DH	0.34	0/420	0.43	0/564
1	DI	0.34	0/420	0.43	0/564
1	DJ	0.34	0/420	0.43	0/564
1	DK	0.34	0/420	0.43	0/564
1	EA	0.34	0/420	0.43	0/564
1	EB	0.34	0/420	0.43	0/564
1	EC	0.34	0/420	0.43	0/564
1	ED	0.34	0/420	0.43	0/564
1	EE	0.34	0/420	0.43	0/564
1	EF	0.34	0/420	0.43	0/564
1	EG	0.34	0/420	0.43	0/564
1	EH	0.35	0/420	0.43	0/564
1	EI	0.34	0/420	0.43	0/564
1	EJ	0.34	0/420	0.43	0/564
1	EK	0.34	0/420	0.43	0/564
1	FA	0.34	0/420	0.43	0/564
1	FB	0.34	0/420	0.43	0/564
1	FC	0.34	0/420	0.43	0/564
1	FD	0.34	0/420	0.43	0/564
1	FE	0.34	0/420	0.43	0/564
1	FF	0.34	0/420	0.43	0/564
1	FG	0.34	0/420	0.43	0/564
1	FH	0.34	0/420	0.43	0/564
1	FI	0.34	0/420	0.43	0/564
1	FJ	0.35	0/420	0.43	0/564
1	FK	0.34	0/420	0.43	0/564
1	GA	0.34	0/420	0.43	0/564
1	GB	0.34	0/420	0.43	0/564
1	GC	0.34	0/420	0.43	0/564
1	GD	0.34	0/420	0.43	0/564
1	GE	0.34	0/420	0.43	0/564
1	GF	0.34	0/420	0.43	0/564
1	GG	0.34	0/420	0.43	0/564
1	GH	0.34	0/420	0.43	0/564
1	GI	0.34	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GJ	0.34	0/420	0.43	0/564
1	GK	0.34	0/420	0.43	0/564
1	HA	0.34	0/420	0.43	0/564
1	HB	0.34	0/420	0.43	0/564
1	HC	0.34	0/420	0.43	0/564
1	HD	0.34	0/420	0.43	0/564
1	HE	0.34	0/420	0.43	0/564
1	HF	0.34	0/420	0.43	0/564
1	HG	0.34	0/420	0.43	0/564
1	HH	0.34	0/420	0.43	0/564
1	HI	0.34	0/420	0.43	0/564
1	HJ	0.34	0/420	0.43	0/564
1	HK	0.34	0/420	0.43	0/564
1	IA	0.34	0/420	0.43	0/564
1	IB	0.34	0/420	0.43	0/564
1	IC	0.34	0/420	0.43	0/564
1	ID	0.34	0/420	0.44	0/564
1	IE	0.34	0/420	0.43	0/564
1	IF	0.34	0/420	0.43	0/564
1	IG	0.34	0/420	0.43	0/564
1	IH	0.34	0/420	0.43	0/564
1	II	0.34	0/420	0.43	0/564
1	IJ	0.34	0/420	0.43	0/564
1	IK	0.34	0/420	0.43	0/564
1	JA	0.34	0/420	0.43	0/564
1	JB	0.34	0/420	0.43	0/564
1	JC	0.34	0/420	0.43	0/564
1	JD	0.34	0/420	0.43	0/564
1	JE	0.34	0/420	0.43	0/564
1	JF	0.34	0/420	0.43	0/564
1	JG	0.34	0/420	0.43	0/564
1	JH	0.34	0/420	0.43	0/564
1	JI	0.34	0/420	0.43	0/564
1	JJ	0.34	0/420	0.43	0/564
1	JK	0.34	0/420	0.43	0/564
1	KA	0.34	0/420	0.43	0/564
1	KB	0.34	0/420	0.43	0/564
1	KC	0.34	0/420	0.43	0/564
1	KD	0.34	0/420	0.43	0/564
1	KE	0.34	0/420	0.43	0/564
1	KF	0.34	0/420	0.43	0/564
1	KG	0.34	0/420	0.43	0/564
1	KH	0.34	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	KI	0.35	0/420	0.43	0/564
1	KJ	0.34	0/420	0.43	0/564
1	KK	0.34	0/420	0.43	0/564
1	LA	0.34	0/420	0.43	0/564
1	LB	0.34	0/420	0.43	0/564
1	LC	0.34	0/420	0.43	0/564
1	LD	0.34	0/420	0.43	0/564
1	LE	0.34	0/420	0.43	0/564
1	LF	0.34	0/420	0.43	0/564
1	LG	0.34	0/420	0.43	0/564
1	LH	0.34	0/420	0.43	0/564
1	LI	0.34	0/420	0.43	0/564
1	LJ	0.34	0/420	0.43	0/564
1	LK	0.34	0/420	0.43	0/564
1	MA	0.34	0/420	0.43	0/564
1	MB	0.34	0/420	0.43	0/564
1	MC	0.34	0/420	0.43	0/564
1	MD	0.34	0/420	0.43	0/564
1	ME	0.34	0/420	0.43	0/564
1	MF	0.34	0/420	0.43	0/564
1	MG	0.34	0/420	0.43	0/564
1	MH	0.34	0/420	0.43	0/564
1	MI	0.34	0/420	0.43	0/564
1	MJ	0.34	0/420	0.43	0/564
1	MK	0.34	0/420	0.43	0/564
1	NA	0.34	0/420	0.43	0/564
1	NB	0.34	0/420	0.43	0/564
1	NC	0.34	0/420	0.43	0/564
1	ND	0.34	0/420	0.43	0/564
1	NE	0.34	0/420	0.43	0/564
1	NF	0.34	0/420	0.43	0/564
1	NG	0.34	0/420	0.43	0/564
1	NH	0.34	0/420	0.43	0/564
1	NI	0.35	0/420	0.43	0/564
1	NJ	0.34	0/420	0.43	0/564
1	NK	0.34	0/420	0.43	0/564
1	OA	0.34	0/420	0.43	0/564
1	OB	0.34	0/420	0.43	0/564
1	OC	0.34	0/420	0.43	0/564
1	OD	0.34	0/420	0.43	0/564
1	OE	0.35	0/420	0.43	0/564
1	OF	0.34	0/420	0.43	0/564
1	OG	0.35	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	OH	0.34	0/420	0.43	0/564
1	OI	0.34	0/420	0.43	0/564
1	OJ	0.34	0/420	0.43	0/564
1	OK	0.34	0/420	0.43	0/564
1	PA	0.34	0/420	0.43	0/564
1	PB	0.34	0/420	0.43	0/564
1	PC	0.34	0/420	0.43	0/564
1	PD	0.34	0/420	0.43	0/564
1	PE	0.34	0/420	0.43	0/564
1	PF	0.34	0/420	0.43	0/564
1	PG	0.34	0/420	0.43	0/564
1	PH	0.34	0/420	0.43	0/564
1	PI	0.34	0/420	0.43	0/564
1	PJ	0.34	0/420	0.43	0/564
1	PK	0.34	0/420	0.43	0/564
1	QA	0.34	0/420	0.43	0/564
1	QB	0.34	0/420	0.43	0/564
1	QC	0.34	0/420	0.43	0/564
1	QD	0.34	0/420	0.43	0/564
1	QE	0.34	0/420	0.43	0/564
1	QF	0.34	0/420	0.43	0/564
1	QG	0.34	0/420	0.43	0/564
1	QH	0.34	0/420	0.43	0/564
1	QI	0.34	0/420	0.43	0/564
1	QJ	0.34	0/420	0.43	0/564
1	QK	0.34	0/420	0.43	0/564
1	RA	0.35	0/420	0.43	0/564
1	RB	0.34	0/420	0.43	0/564
1	RC	0.34	0/420	0.43	0/564
1	RD	0.34	0/420	0.43	0/564
1	RE	0.34	0/420	0.43	0/564
1	RF	0.34	0/420	0.43	0/564
1	RG	0.34	0/420	0.43	0/564
1	RH	0.34	0/420	0.43	0/564
1	RI	0.34	0/420	0.43	0/564
1	RJ	0.34	0/420	0.43	0/564
1	RK	0.34	0/420	0.43	0/564
1	SA	0.35	0/420	0.43	0/564
1	SB	0.34	0/420	0.43	0/564
1	SC	0.34	0/420	0.43	0/564
1	SD	0.34	0/420	0.43	0/564
1	SE	0.34	0/420	0.43	0/564
1	SF	0.34	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	SG	0.34	0/420	0.43	0/564
1	SH	0.34	0/420	0.43	0/564
1	SI	0.34	0/420	0.43	0/564
1	SJ	0.34	0/420	0.43	0/564
1	SK	0.34	0/420	0.43	0/564
1	TA	0.34	0/420	0.43	0/564
1	TB	0.34	0/420	0.43	0/564
1	TC	0.34	0/420	0.43	0/564
1	TD	0.34	0/420	0.43	0/564
1	TE	0.35	0/420	0.43	0/564
1	TF	0.35	0/420	0.43	0/564
1	TG	0.34	0/420	0.43	0/564
1	TH	0.34	0/420	0.43	0/564
1	TI	0.34	0/420	0.43	0/564
1	TJ	0.34	0/420	0.43	0/564
1	TK	0.34	0/420	0.43	0/564
1	UA	0.34	0/420	0.43	0/564
1	UB	0.34	0/420	0.43	0/564
1	UC	0.34	0/420	0.43	0/564
1	UD	0.34	0/420	0.43	0/564
1	UE	0.34	0/420	0.43	0/564
1	UF	0.34	0/420	0.43	0/564
1	UG	0.34	0/420	0.44	0/564
1	UH	0.34	0/420	0.43	0/564
1	UI	0.35	0/420	0.43	0/564
1	UJ	0.34	0/420	0.43	0/564
1	UK	0.34	0/420	0.43	0/564
1	VA	0.34	0/420	0.43	0/564
1	VB	0.34	0/420	0.43	0/564
1	VC	0.34	0/420	0.43	0/564
1	VD	0.34	0/420	0.43	0/564
1	VE	0.34	0/420	0.43	0/564
1	VF	0.34	0/420	0.43	0/564
1	VG	0.34	0/420	0.43	0/564
1	VH	0.34	0/420	0.43	0/564
1	VI	0.34	0/420	0.43	0/564
1	VJ	0.34	0/420	0.43	0/564
1	VK	0.34	0/420	0.43	0/564
1	WA	0.34	0/420	0.43	0/564
1	WB	0.34	0/420	0.43	0/564
1	WC	0.34	0/420	0.43	0/564
1	WD	0.34	0/420	0.43	0/564
1	WE	0.35	0/420	0.43	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	WF	0.34	0/420	0.43	0/564
1	WG	0.34	0/420	0.43	0/564
1	WH	0.34	0/420	0.43	0/564
1	WI	0.34	0/420	0.43	0/564
1	WJ	0.34	0/420	0.43	0/564
1	WK	0.34	0/420	0.43	0/564
1	XA	0.34	0/420	0.43	0/564
1	XB	0.34	0/420	0.43	0/564
1	XC	0.34	0/420	0.43	0/564
1	XD	0.34	0/420	0.43	0/564
1	XE	0.34	0/420	0.43	0/564
1	XF	0.34	0/420	0.43	0/564
1	XG	0.34	0/420	0.43	0/564
1	XH	0.34	0/420	0.43	0/564
1	XI	0.34	0/420	0.43	0/564
1	XJ	0.34	0/420	0.43	0/564
1	XK	0.34	0/420	0.43	0/564
All	All	0.34	0/110880	0.43	0/148896

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	417	0	416	1	0
1	AB	417	0	416	2	0
1	AC	417	0	416	2	0
1	AD	417	0	416	1	0
1	AE	417	0	416	1	0
1	AF	417	0	417	2	0
1	AG	417	0	417	2	0
1	AH	417	0	416	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	417	0	416	3	0
1	AJ	417	0	416	2	0
1	AK	417	0	417	1	0
1	BA	417	0	416	1	0
1	BB	417	0	416	2	0
1	BC	417	0	416	3	0
1	BD	417	0	416	3	0
1	BE	417	0	417	3	0
1	BF	417	0	416	3	0
1	BG	417	0	416	2	0
1	BH	417	0	416	2	0
1	BI	417	0	416	2	0
1	BJ	417	0	417	1	0
1	BK	417	0	417	1	0
1	CA	417	0	417	1	0
1	CB	417	0	416	2	0
1	CC	417	0	417	2	0
1	CD	417	0	416	1	0
1	CE	417	0	417	2	0
1	CF	417	0	417	3	0
1	CG	417	0	416	3	0
1	CH	417	0	417	3	0
1	CI	417	0	416	2	0
1	CJ	417	0	416	1	0
1	CK	417	0	417	1	0
1	DA	417	0	416	1	0
1	DB	417	0	416	1	0
1	DC	417	0	417	1	0
1	DD	417	0	417	1	0
1	DE	417	0	417	2	0
1	DF	417	0	417	3	0
1	DG	417	0	417	2	0
1	DH	417	0	417	1	0
1	DI	417	0	416	1	0
1	DJ	417	0	416	2	0
1	DK	417	0	417	2	0
1	EA	417	0	416	1	0
1	EB	417	0	416	2	0
1	EC	417	0	416	2	0
1	ED	417	0	416	2	0
1	EE	417	0	417	2	0
1	EF	417	0	417	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EG	417	0	416	2	0
1	EH	417	0	417	3	0
1	EI	417	0	416	2	0
1	EJ	417	0	416	1	0
1	EK	417	0	417	1	0
1	FA	417	0	416	1	0
1	FB	417	0	416	2	0
1	FC	417	0	417	2	0
1	FD	417	0	417	2	0
1	FE	417	0	416	2	0
1	FF	417	0	417	2	0
1	FG	417	0	417	2	0
1	FH	417	0	417	1	0
1	FI	417	0	416	2	0
1	FJ	417	0	416	3	0
1	FK	417	0	417	2	0
1	GA	417	0	416	2	0
1	GB	417	0	416	3	0
1	GC	417	0	416	2	0
1	GD	417	0	416	1	0
1	GE	417	0	417	1	0
1	GF	417	0	417	1	0
1	GG	417	0	416	1	0
1	GH	417	0	416	1	0
1	GI	417	0	416	1	0
1	GJ	417	0	417	2	0
1	GK	417	0	417	2	0
1	HA	417	0	416	2	0
1	HB	417	0	416	1	0
1	HC	417	0	416	1	0
1	HD	417	0	416	2	0
1	HE	417	0	417	2	0
1	HF	417	0	417	2	0
1	HG	417	0	417	2	0
1	HH	417	0	416	2	0
1	HI	417	0	416	3	0
1	HJ	417	0	417	2	0
1	HK	417	0	417	2	0
1	IA	417	0	416	1	0
1	IB	417	0	416	2	0
1	IC	417	0	416	2	0
1	ID	417	0	416	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IE	417	0	417	3	0
1	IF	417	0	417	3	0
1	IG	417	0	417	1	0
1	IH	417	0	416	2	0
1	II	417	0	416	3	0
1	IJ	417	0	417	2	0
1	IK	417	0	417	1	0
1	JA	417	0	416	1	0
1	JB	417	0	416	2	0
1	JC	417	0	416	2	0
1	JD	417	0	416	1	0
1	JE	417	0	417	2	0
1	JF	417	0	416	3	0
1	JG	417	0	417	2	0
1	JH	417	0	417	1	0
1	JI	417	0	416	1	0
1	JJ	417	0	416	2	0
1	JK	417	0	417	2	0
1	KA	417	0	417	1	0
1	KB	417	0	416	1	0
1	KC	417	0	416	1	0
1	KD	417	0	416	2	0
1	KE	417	0	416	2	0
1	KF	417	0	416	2	0
1	KG	417	0	417	3	0
1	KH	417	0	416	2	0
1	KI	417	0	416	1	0
1	KJ	417	0	416	2	0
1	KK	417	0	417	2	0
1	LA	417	0	416	2	0
1	LB	417	0	417	1	0
1	LC	417	0	416	2	0
1	LD	417	0	417	2	0
1	LE	417	0	416	1	0
1	LF	417	0	416	2	0
1	LG	417	0	417	2	0
1	LH	417	0	417	1	0
1	LI	417	0	416	2	0
1	LJ	417	0	417	2	0
1	LK	417	0	417	2	0
1	MA	417	0	417	3	0
1	MB	417	0	416	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MC	417	0	417	2	0
1	MD	417	0	416	2	0
1	ME	417	0	416	3	0
1	MF	417	0	417	3	0
1	MG	417	0	417	2	0
1	MH	417	0	417	2	0
1	MI	417	0	416	2	0
1	MJ	417	0	416	2	0
1	MK	417	0	417	2	0
1	NA	417	0	416	3	0
1	NB	417	0	416	3	0
1	NC	417	0	416	3	0
1	ND	417	0	416	3	0
1	NE	417	0	416	2	0
1	NF	417	0	416	1	0
1	NG	417	0	417	1	0
1	NH	417	0	417	2	0
1	NI	417	0	416	2	0
1	NJ	417	0	416	1	0
1	NK	417	0	417	2	0
1	OA	417	0	416	2	0
1	OB	417	0	416	2	0
1	OC	417	0	416	3	0
1	OD	417	0	416	4	0
1	OE	417	0	416	3	0
1	OF	417	0	417	1	0
1	OG	417	0	417	1	0
1	OH	417	0	417	2	0
1	OI	417	0	416	2	0
1	OJ	417	0	416	1	0
1	OK	417	0	417	2	0
1	PA	417	0	416	2	0
1	PB	417	0	416	2	0
1	PC	417	0	416	2	0
1	PD	417	0	416	2	0
1	PE	417	0	416	2	0
1	PF	417	0	417	1	0
1	PG	417	0	417	1	0
1	PH	417	0	417	1	0
1	PI	417	0	416	2	0
1	PJ	417	0	416	2	0
1	PK	417	0	417	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	417	0	416	2	0
1	QB	417	0	416	3	0
1	QC	417	0	416	3	0
1	QD	417	0	416	2	0
1	QE	417	0	417	2	0
1	QF	417	0	417	2	0
1	QG	417	0	417	2	0
1	QH	417	0	417	2	0
1	QI	417	0	416	2	0
1	QJ	417	0	417	1	0
1	QK	417	0	417	2	0
1	RA	417	0	416	2	0
1	RB	417	0	417	2	0
1	RC	417	0	417	3	0
1	RD	417	0	416	3	0
1	RE	417	0	416	1	0
1	RF	417	0	417	2	0
1	RG	417	0	417	2	0
1	RH	417	0	416	2	0
1	RI	417	0	417	2	0
1	RJ	417	0	416	1	0
1	RK	417	0	417	1	0
1	SA	417	0	417	1	0
1	SB	417	0	416	2	0
1	SC	417	0	416	2	0
1	SD	417	0	417	2	0
1	SE	417	0	417	3	0
1	SF	417	0	416	2	0
1	SG	417	0	417	2	0
1	SH	417	0	416	3	0
1	SI	417	0	416	2	0
1	SJ	417	0	416	2	0
1	SK	417	0	417	2	0
1	TA	417	0	416	3	0
1	TB	417	0	417	3	0
1	TC	417	0	416	3	0
1	TD	417	0	416	3	0
1	TE	417	0	416	3	0
1	TF	417	0	417	3	0
1	TG	417	0	416	2	0
1	TH	417	0	416	1	0
1	TI	417	0	417	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TJ	417	0	417	1	0
1	TK	417	0	417	2	0
1	UA	417	0	417	1	0
1	UB	417	0	417	1	0
1	UC	417	0	416	1	0
1	UD	417	0	417	1	0
1	UE	417	0	416	2	0
1	UF	417	0	417	3	0
1	UG	417	0	416	2	0
1	UH	417	0	416	1	0
1	UI	417	0	416	2	0
1	UJ	417	0	416	2	0
1	UK	417	0	417	1	0
1	VA	417	0	416	3	0
1	VB	417	0	416	3	0
1	VC	417	0	416	3	0
1	VD	417	0	416	3	0
1	VE	417	0	417	2	0
1	VF	417	0	417	3	0
1	VG	417	0	416	2	0
1	VH	417	0	417	2	0
1	VI	417	0	417	2	0
1	VJ	417	0	416	2	0
1	VK	417	0	417	2	0
1	WA	417	0	417	2	0
1	WB	417	0	416	2	0
1	WC	417	0	416	2	0
1	WD	417	0	417	2	0
1	WE	417	0	417	2	0
1	WF	417	0	417	2	0
1	WG	417	0	417	1	0
1	WH	417	0	416	1	0
1	WI	417	0	416	2	0
1	WJ	417	0	416	3	0
1	WK	417	0	417	2	0
1	XA	417	0	416	2	0
1	XB	417	0	416	2	0
1	XC	417	0	416	1	0
1	XD	417	0	416	1	0
1	XE	417	0	417	1	0
1	XF	417	0	417	2	0
1	XG	417	0	416	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XH	417	0	417	3	0
1	XI	417	0	417	3	0
1	XJ	417	0	416	2	0
1	XK	417	0	417	1	0
2	AA	1	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AD	1	0	0	0	0
2	AE	1	0	0	0	0
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AH	1	0	0	0	0
2	AI	1	0	0	0	0
2	AJ	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BC	1	0	0	0	0
2	BD	1	0	0	0	0
2	BE	1	0	0	0	0
2	BF	1	0	0	0	0
2	BG	1	0	0	0	0
2	BH	1	0	0	0	0
2	BI	1	0	0	0	0
2	BJ	1	0	0	0	0
2	CA	1	0	0	0	0
2	CB	1	0	0	0	0
2	CC	1	0	0	0	0
2	CD	1	0	0	0	0
2	CE	1	0	0	0	0
2	CF	1	0	0	0	0
2	CI	1	0	0	0	0
2	CJ	1	0	0	0	0
2	DA	1	0	0	0	0
2	DB	1	0	0	0	0
2	DC	1	0	0	0	0
2	DD	1	0	0	0	0
2	DE	1	0	0	0	0
2	DF	1	0	0	0	0
2	DG	1	0	0	0	0
2	DH	1	0	0	0	0
2	DI	1	0	0	0	0
2	DJ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EE	1	0	0	0	0
2	EF	1	0	0	0	0
2	EG	1	0	0	0	0
2	EH	1	0	0	0	0
2	EI	1	0	0	0	0
2	EJ	1	0	0	0	0
2	FA	1	0	0	0	0
2	FB	1	0	0	0	0
2	FE	1	0	0	0	0
2	FF	1	0	0	0	0
2	FG	1	0	0	0	0
2	FH	1	0	0	0	0
2	FI	1	0	0	0	0
2	FJ	1	0	0	0	0
2	GC	1	0	0	0	0
2	GD	1	0	0	0	0
2	GG	1	0	0	0	0
2	GH	1	0	0	0	0
2	GI	1	0	0	0	0
2	GJ	1	0	0	0	0
2	HA	1	0	0	0	0
2	HB	1	0	0	0	0
2	HC	1	0	0	0	0
2	HD	1	0	0	0	0
2	HG	1	0	0	0	0
2	HH	1	0	0	0	0
2	HI	1	0	0	0	0
2	HJ	1	0	0	0	0
2	IA	1	0	0	0	0
2	IB	1	0	0	0	0
2	IE	1	0	0	0	0
2	IF	1	0	0	0	0
2	IG	1	0	0	0	0
2	IH	1	0	0	0	0
2	II	1	0	0	0	0
2	IJ	1	0	0	0	0
2	JC	1	0	0	0	0
2	JD	1	0	0	0	0
2	JE	1	0	0	0	0
2	JF	1	0	0	0	0
2	KC	1	0	0	0	0
2	KD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	KE	1	0	0	0	0
2	KF	1	0	0	0	0
2	LA	1	0	0	0	0
2	LB	1	0	0	0	0
2	LC	1	0	0	0	0
2	LD	1	0	0	0	0
2	LI	1	0	0	0	0
2	LJ	1	0	0	0	0
2	ME	1	0	0	0	0
2	MF	1	0	0	0	0
2	NA	1	0	0	0	0
2	NB	1	0	0	0	0
2	NC	1	0	0	0	0
2	ND	1	0	0	0	0
2	OE	1	0	0	0	0
2	OF	1	0	0	0	0
2	OG	1	0	0	0	0
2	OH	1	0	0	0	0
2	OI	1	0	0	0	0
2	OJ	1	0	0	0	0
2	PC	1	0	0	0	0
2	PD	1	0	0	0	0
2	PE	1	0	0	0	0
2	PF	1	0	0	0	0
2	PG	1	0	0	0	0
2	PH	1	0	0	0	0
2	QG	1	0	0	0	0
2	QH	1	0	0	0	0
2	RA	1	0	0	0	0
2	RB	1	0	0	0	0
2	RC	1	0	0	0	0
2	RD	1	0	0	0	0
2	SE	1	0	0	0	0
2	SF	1	0	0	0	0
2	TA	1	0	0	0	0
2	TB	1	0	0	0	0
2	TI	1	0	0	0	0
2	TJ	1	0	0	0	0
2	WI	1	0	0	0	0
2	WJ	1	0	0	0	0
All	All	110208	0	109940	385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 2.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJ:7:PHE:O	1:JK:65:HIS:NE2	2.31	0.64
1:IH:7:PHE:O	1:II:65:HIS:NE2	2.28	0.64
1:BF:7:PHE:O	1:BG:65:HIS:NE2	2.31	0.63
1:KF:7:PHE:O	1:KG:65:HIS:NE2	2.35	0.59
1:QB:7:PHE:O	1:QC:65:HIS:NE2	2.34	0.59
1:KJ:7:PHE:O	1:KK:65:HIS:NE2	2.35	0.57
1:OH:7:PHE:O	1:OI:65:HIS:NE2	2.36	0.57
1:LA:65:HIS:NE2	1:LK:7:PHE:O	2.35	0.56
1:CF:7:PHE:O	1:CG:65:HIS:NE2	2.38	0.56
1:QF:7:PHE:O	1:QG:65:HIS:NE2	2.36	0.55
1:PI:7:PHE:O	1:PJ:65:HIS:NE2	2.38	0.55
1:AF:7:PHE:O	1:AG:65:HIS:NE2	2.37	0.54
1:GJ:7:PHE:O	1:GK:65:HIS:NE2	2.40	0.53
1:NH:7:PHE:O	1:NI:65:HIS:NE2	2.40	0.53
1:XH:7:PHE:O	1:XI:65:HIS:NE2	2.42	0.52
1:RC:40:GLU:HG2	1:RD:56:ARG:HG2	1.91	0.52
1:IE:7:PHE:O	1:IF:65:HIS:NE2	2.38	0.52
1:ND:39:GLY:O	1:NE:71:GLU:N	2.38	0.52
1:FI:7:PHE:O	1:FJ:65:HIS:NE2	2.44	0.51
1:BH:7:PHE:O	1:BI:65:HIS:NE2	2.43	0.50
1:OD:39:GLY:O	1:OE:71:GLU:N	2.40	0.50
1:KG:40:GLU:HG2	1:KH:56:ARG:HG2	1.93	0.50
1:FF:7:PHE:O	1:FG:65:HIS:NE2	2.44	0.50
1:HF:7:PHE:O	1:HG:65:HIS:NE2	2.42	0.50
1:GB:7:PHE:O	1:GC:65:HIS:NE2	2.43	0.50
1:JB:7:PHE:O	1:JC:65:HIS:NE2	2.41	0.50
1:TA:65:HIS:NE2	1:TK:7:PHE:O	2.41	0.49
1:UI:7:PHE:O	1:UJ:65:HIS:NE2	2.45	0.49
1:AH:7:PHE:O	1:AI:65:HIS:NE2	2.42	0.49
1:FB:7:PHE:O	1:FC:65:HIS:NE2	2.42	0.49
1:PD:7:PHE:O	1:PE:65:HIS:NE2	2.44	0.49
1:HA:65:HIS:NE2	1:HK:7:PHE:O	2.40	0.49
1:HH:7:PHE:O	1:HI:65:HIS:NE2	2.45	0.49
1:VA:7:PHE:O	1:VB:65:HIS:NE2	2.44	0.48
1:OD:7:PHE:O	1:OE:65:HIS:NE2	2.45	0.48
1:QH:7:PHE:O	1:QI:65:HIS:NE2	2.43	0.48
1:CB:7:PHE:O	1:CC:65:HIS:NE2	2.44	0.48
1:NB:7:PHE:O	1:NC:65:HIS:NE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UE:40:GLU:HG2	1:UF:56:ARG:HG2	1.95	0.48
1:BD:7:PHE:O	1:BE:65:HIS:NE2	2.40	0.48
1:MJ:7:PHE:O	1:MK:65:HIS:NE2	2.44	0.48
1:OA:65:HIS:NE2	1:OK:7:PHE:O	2.46	0.48
1:RA:7:PHE:O	1:RB:65:HIS:NE2	2.46	0.48
1:CH:40:GLU:HG2	1:CI:56:ARG:HG2	1.96	0.47
1:SB:7:PHE:O	1:SC:65:HIS:NE2	2.42	0.47
1:UF:7:PHE:O	1:UG:65:HIS:NE2	2.47	0.47
1:VH:7:PHE:O	1:VI:65:HIS:NE2	2.44	0.47
1:EH:7:PHE:O	1:EI:65:HIS:NE2	2.46	0.47
1:VC:40:GLU:HG2	1:VD:56:ARG:HG2	1.96	0.47
1:GA:7:PHE:O	1:GB:65:HIS:NE2	2.46	0.47
1:ED:7:PHE:O	1:EE:65:HIS:NE2	2.46	0.47
1:QA:65:HIS:NE2	1:QK:7:PHE:O	2.47	0.47
1:KD:7:PHE:O	1:KE:65:HIS:NE2	2.45	0.46
1:BE:40:GLU:HG2	1:BF:56:ARG:HG2	1.97	0.46
1:HD:7:PHE:O	1:HE:65:HIS:NE2	2.47	0.46
1:LF:7:PHE:O	1:LG:65:HIS:NE2	2.46	0.46
1:LI:7:PHE:O	1:LJ:65:HIS:NE2	2.48	0.45
1:WC:40:GLU:HG2	1:WD:56:ARG:HG2	1.97	0.45
1:PB:7:PHE:O	1:PC:65:HIS:NE2	2.45	0.45
1:TE:40:GLU:HG2	1:TF:56:ARG:HG2	1.97	0.45
1:TD:7:PHE:O	1:TE:65:HIS:NE2	2.46	0.45
1:SE:40:GLU:HG2	1:SF:56:ARG:HG2	1.98	0.45
1:VC:42:LEU:HD11	1:VD:52:ALA:HB1	1.98	0.45
1:MF:7:PHE:O	1:MG:65:HIS:NE2	2.46	0.44
1:NA:65:HIS:NE2	1:NK:7:PHE:O	2.47	0.44
1:MB:7:PHE:O	1:MC:65:HIS:NE2	2.45	0.44
1:XG:40:GLU:HG2	1:XH:56:ARG:HG2	1.99	0.44
1:RH:7:PHE:O	1:RI:65:HIS:NE2	2.46	0.44
1:EE:61:ILE:HB	1:EE:68:ILE:HG22	2.00	0.44
1:EG:61:ILE:HB	1:EG:68:ILE:HG22	2.00	0.44
1:FC:61:ILE:HB	1:FC:68:ILE:HG22	2.00	0.44
1:HF:61:ILE:HB	1:HF:68:ILE:HG22	2.00	0.44
1:JG:61:ILE:HB	1:JG:68:ILE:HG22	2.00	0.44
1:KB:61:ILE:HB	1:KB:68:ILE:HG22	2.00	0.44
1:MC:61:ILE:HB	1:MC:68:ILE:HG22	2.00	0.44
1:MJ:61:ILE:HB	1:MJ:68:ILE:HG22	2.00	0.44
1:PG:61:ILE:HB	1:PG:68:ILE:HG22	2.00	0.44
1:XF:61:ILE:HB	1:XF:68:ILE:HG22	2.00	0.44
1:XJ:61:ILE:HB	1:XJ:68:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:61:ILE:HB	1:BC:68:ILE:HG22	2.00	0.44
1:CC:61:ILE:HB	1:CC:68:ILE:HG22	2.00	0.44
1:DE:61:ILE:HB	1:DE:68:ILE:HG22	2.00	0.44
1:DF:7:PHE:O	1:DG:65:HIS:NE2	2.47	0.44
1:DJ:61:ILE:HB	1:DJ:68:ILE:HG22	2.00	0.44
1:FD:7:PHE:O	1:FE:65:HIS:NE2	2.50	0.44
1:FJ:61:ILE:HB	1:FJ:68:ILE:HG22	2.00	0.44
1:IE:40:GLU:HG2	1:IF:56:ARG:HG2	2.00	0.44
1:IF:61:ILE:HB	1:IF:68:ILE:HG22	2.00	0.44
1:JJ:61:ILE:HB	1:JJ:68:ILE:HG22	2.00	0.44
1:LJ:61:ILE:HB	1:LJ:68:ILE:HG22	2.00	0.44
1:NC:61:ILE:HB	1:NC:68:ILE:HG22	2.00	0.44
1:QE:61:ILE:HB	1:QE:68:ILE:HG22	2.00	0.44
1:QG:61:ILE:HB	1:QG:68:ILE:HG22	2.00	0.44
1:SB:61:ILE:HB	1:SB:68:ILE:HG22	2.00	0.44
1:TF:61:ILE:HB	1:TF:68:ILE:HG22	2.00	0.44
1:TJ:61:ILE:HB	1:TJ:68:ILE:HG22	2.00	0.44
1:UF:61:ILE:HB	1:UF:68:ILE:HG22	2.00	0.44
1:XH:61:ILE:HB	1:XH:68:ILE:HG22	2.00	0.44
1:IA:61:ILE:HB	1:IA:68:ILE:HG22	2.00	0.44
1:MK:61:ILE:HB	1:MK:68:ILE:HG22	2.00	0.44
1:PK:61:ILE:HB	1:PK:68:ILE:HG22	2.00	0.44
1:QH:61:ILE:HB	1:QH:68:ILE:HG22	2.00	0.44
1:RF:61:ILE:HB	1:RF:68:ILE:HG22	2.00	0.44
1:SK:61:ILE:HB	1:SK:68:ILE:HG22	2.00	0.44
1:TF:7:PHE:O	1:TG:65:HIS:NE2	2.48	0.44
1:TH:61:ILE:HB	1:TH:68:ILE:HG22	2.00	0.44
1:VH:61:ILE:HB	1:VH:68:ILE:HG22	2.00	0.44
1:CG:61:ILE:HB	1:CG:68:ILE:HG22	2.00	0.44
1:EH:61:ILE:HB	1:EH:68:ILE:HG22	2.00	0.44
1:JK:61:ILE:HB	1:JK:68:ILE:HG22	2.00	0.44
1:KK:61:ILE:HB	1:KK:68:ILE:HG22	2.00	0.44
1:LE:61:ILE:HB	1:LE:68:ILE:HG22	2.00	0.44
1:NF:61:ILE:HB	1:NF:68:ILE:HG22	2.00	0.44
1:OG:61:ILE:HB	1:OG:68:ILE:HG22	2.00	0.44
1:OH:61:ILE:HB	1:OH:68:ILE:HG22	2.00	0.44
1:OI:61:ILE:HB	1:OI:68:ILE:HG22	2.00	0.44
1:PJ:61:ILE:HB	1:PJ:68:ILE:HG22	2.00	0.44
1:QD:61:ILE:HB	1:QD:68:ILE:HG22	2.00	0.44
1:TA:61:ILE:HB	1:TA:68:ILE:HG22	2.00	0.44
1:UA:61:ILE:HB	1:UA:68:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:61:ILE:HB	1:AG:68:ILE:HG22	2.00	0.43
1:CB:61:ILE:HB	1:CB:68:ILE:HG22	2.00	0.43
1:ED:61:ILE:HB	1:ED:68:ILE:HG22	2.00	0.43
1:GB:61:ILE:HB	1:GB:68:ILE:HG22	2.00	0.43
1:GC:61:ILE:HB	1:GC:68:ILE:HG22	2.00	0.43
1:GG:61:ILE:HB	1:GG:68:ILE:HG22	2.00	0.43
1:HA:61:ILE:HB	1:HA:68:ILE:HG22	2.00	0.43
1:ID:61:ILE:HB	1:ID:68:ILE:HG22	2.00	0.43
1:IE:61:ILE:HB	1:IE:68:ILE:HG22	2.00	0.43
1:IH:61:ILE:HB	1:IH:68:ILE:HG22	2.00	0.43
1:JA:61:ILE:HB	1:JA:68:ILE:HG22	2.00	0.43
1:JB:61:ILE:HB	1:JB:68:ILE:HG22	2.00	0.43
1:OA:61:ILE:HB	1:OA:68:ILE:HG22	2.00	0.43
1:QC:61:ILE:HB	1:QC:68:ILE:HG22	2.00	0.43
1:RA:61:ILE:HB	1:RA:68:ILE:HG22	2.00	0.43
1:SC:61:ILE:HB	1:SC:68:ILE:HG22	2.00	0.43
1:TK:61:ILE:HB	1:TK:68:ILE:HG22	2.00	0.43
1:XA:61:ILE:HB	1:XA:68:ILE:HG22	2.00	0.43
1:XK:61:ILE:HB	1:XK:68:ILE:HG22	2.00	0.43
1:AA:61:ILE:HB	1:AA:68:ILE:HG22	2.00	0.43
1:AH:61:ILE:HB	1:AH:68:ILE:HG22	2.00	0.43
1:AI:61:ILE:HB	1:AI:68:ILE:HG22	2.00	0.43
1:BH:61:ILE:HB	1:BH:68:ILE:HG22	2.00	0.43
1:DB:61:ILE:HB	1:DB:68:ILE:HG22	2.00	0.43
1:EC:61:ILE:HB	1:EC:68:ILE:HG22	2.00	0.43
1:FG:61:ILE:HB	1:FG:68:ILE:HG22	2.00	0.43
1:GI:61:ILE:HB	1:GI:68:ILE:HG22	2.00	0.43
1:GJ:61:ILE:HB	1:GJ:68:ILE:HG22	2.00	0.43
1:HD:61:ILE:HB	1:HD:68:ILE:HG22	2.00	0.43
1:HI:61:ILE:HB	1:HI:68:ILE:HG22	2.00	0.43
1:HJ:61:ILE:HB	1:HJ:68:ILE:HG22	2.00	0.43
1:II:61:ILE:HB	1:II:68:ILE:HG22	2.00	0.43
1:IJ:61:ILE:HB	1:IJ:68:ILE:HG22	2.00	0.43
1:JF:61:ILE:HB	1:JF:68:ILE:HG22	2.00	0.43
1:KG:61:ILE:HB	1:KG:68:ILE:HG22	2.00	0.43
1:LB:61:ILE:HB	1:LB:68:ILE:HG22	2.00	0.43
1:LF:61:ILE:HB	1:LF:68:ILE:HG22	2.00	0.43
1:ND:61:ILE:HB	1:ND:68:ILE:HG22	2.00	0.43
1:PA:61:ILE:HB	1:PA:68:ILE:HG22	2.00	0.43
1:PB:61:ILE:HB	1:PB:68:ILE:HG22	2.00	0.43
1:RH:61:ILE:HB	1:RH:68:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RJ:61:ILE:HB	1:RJ:68:ILE:HG22	2.00	0.43
1:SG:61:ILE:HB	1:SG:68:ILE:HG22	2.00	0.43
1:TE:61:ILE:HB	1:TE:68:ILE:HG22	2.00	0.43
1:UH:61:ILE:HB	1:UH:68:ILE:HG22	2.00	0.43
1:WH:61:ILE:HB	1:WH:68:ILE:HG22	2.00	0.43
1:BD:61:ILE:HB	1:BD:68:ILE:HG22	2.00	0.43
1:BF:61:ILE:HB	1:BF:68:ILE:HG22	2.00	0.43
1:BG:61:ILE:HB	1:BG:68:ILE:HG22	2.00	0.43
1:BI:61:ILE:HB	1:BI:68:ILE:HG22	2.00	0.43
1:CI:61:ILE:HB	1:CI:68:ILE:HG22	2.00	0.43
1:CJ:61:ILE:HB	1:CJ:68:ILE:HG22	2.00	0.43
1:DF:61:ILE:HB	1:DF:68:ILE:HG22	2.00	0.43
1:EA:61:ILE:HB	1:EA:68:ILE:HG22	2.00	0.43
1:EG:7:PHE:O	1:EH:65:HIS:NE2	2.47	0.43
1:FK:61:ILE:HB	1:FK:68:ILE:HG22	2.00	0.43
1:HE:61:ILE:HB	1:HE:68:ILE:HG22	2.00	0.43
1:HH:61:ILE:HB	1:HH:68:ILE:HG22	2.00	0.43
1:KA:61:ILE:HB	1:KA:68:ILE:HG22	2.00	0.43
1:KC:61:ILE:HB	1:KC:68:ILE:HG22	2.00	0.43
1:KE:61:ILE:HB	1:KE:68:ILE:HG22	2.00	0.43
1:LC:61:ILE:HB	1:LC:68:ILE:HG22	2.00	0.43
1:MG:61:ILE:HB	1:MG:68:ILE:HG22	2.00	0.43
1:NG:61:ILE:HB	1:NG:68:ILE:HG22	2.00	0.43
1:NH:61:ILE:HB	1:NH:68:ILE:HG22	2.00	0.43
1:NI:61:ILE:HB	1:NI:68:ILE:HG22	2.00	0.43
1:UJ:61:ILE:HB	1:UJ:68:ILE:HG22	2.00	0.43
1:VK:61:ILE:HB	1:VK:68:ILE:HG22	2.00	0.43
1:WJ:61:ILE:HB	1:WJ:68:ILE:HG22	2.00	0.43
1:CA:61:ILE:HB	1:CA:68:ILE:HG22	2.00	0.43
1:CF:61:ILE:HB	1:CF:68:ILE:HG22	2.00	0.43
1:CH:61:ILE:HB	1:CH:68:ILE:HG22	2.00	0.43
1:DA:61:ILE:HB	1:DA:68:ILE:HG22	2.00	0.43
1:FE:61:ILE:HB	1:FE:68:ILE:HG22	2.00	0.43
1:GF:61:ILE:HB	1:GF:68:ILE:HG22	2.00	0.43
1:LA:61:ILE:HB	1:LA:68:ILE:HG22	2.00	0.43
1:MB:61:ILE:HB	1:MB:68:ILE:HG22	2.00	0.43
1:PD:61:ILE:HB	1:PD:68:ILE:HG22	2.00	0.43
1:VJ:61:ILE:HB	1:VJ:68:ILE:HG22	2.00	0.43
1:WD:61:ILE:HB	1:WD:68:ILE:HG22	2.00	0.43
1:BC:40:GLU:HG2	1:BD:56:ARG:HG2	2.01	0.43
1:DK:61:ILE:HB	1:DK:68:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:61:ILE:HB	1:FB:68:ILE:HG22	2.00	0.43
1:GH:61:ILE:HB	1:GH:68:ILE:HG22	2.00	0.43
1:HI:40:GLU:HG2	1:HJ:56:ARG:HG2	2.01	0.43
1:IC:61:ILE:HB	1:IC:68:ILE:HG22	2.00	0.43
1:JD:61:ILE:HB	1:JD:68:ILE:HG22	2.00	0.43
1:JF:7:PHE:O	1:JG:65:HIS:NE2	2.46	0.43
1:MD:61:ILE:HB	1:MD:68:ILE:HG22	2.00	0.43
1:ME:61:ILE:HB	1:ME:68:ILE:HG22	2.00	0.43
1:OE:61:ILE:HB	1:OE:68:ILE:HG22	2.00	0.43
1:PC:61:ILE:HB	1:PC:68:ILE:HG22	2.00	0.43
1:PF:61:ILE:HB	1:PF:68:ILE:HG22	2.00	0.43
1:PI:61:ILE:HB	1:PI:68:ILE:HG22	2.00	0.43
1:QF:61:ILE:HB	1:QF:68:ILE:HG22	2.00	0.43
1:SA:61:ILE:HB	1:SA:68:ILE:HG22	2.00	0.43
1:SE:61:ILE:HB	1:SE:68:ILE:HG22	2.00	0.43
1:SJ:61:ILE:HB	1:SJ:68:ILE:HG22	2.00	0.43
1:TI:61:ILE:HB	1:TI:68:ILE:HG22	2.00	0.43
1:UC:61:ILE:HB	1:UC:68:ILE:HG22	2.00	0.43
1:VB:61:ILE:HB	1:VB:68:ILE:HG22	2.00	0.43
1:XE:61:ILE:HB	1:XE:68:ILE:HG22	2.00	0.43
1:XI:61:ILE:HB	1:XI:68:ILE:HG22	2.00	0.43
1:DC:61:ILE:HB	1:DC:68:ILE:HG22	2.00	0.43
1:FI:61:ILE:HB	1:FI:68:ILE:HG22	2.00	0.43
1:GA:61:ILE:HB	1:GA:68:ILE:HG22	2.00	0.43
1:GK:61:ILE:HB	1:GK:68:ILE:HG22	2.00	0.43
1:HC:61:ILE:HB	1:HC:68:ILE:HG22	2.00	0.43
1:JC:61:ILE:HB	1:JC:68:ILE:HG22	2.00	0.43
1:JI:61:ILE:HB	1:JI:68:ILE:HG22	2.00	0.43
1:KH:61:ILE:HB	1:KH:68:ILE:HG22	2.00	0.43
1:KJ:61:ILE:HB	1:KJ:68:ILE:HG22	2.00	0.43
1:LG:61:ILE:HB	1:LG:68:ILE:HG22	2.00	0.43
1:MH:61:ILE:HB	1:MH:68:ILE:HG22	2.00	0.43
1:NJ:61:ILE:HB	1:NJ:68:ILE:HG22	2.00	0.43
1:QA:61:ILE:HB	1:QA:68:ILE:HG22	2.00	0.43
1:RC:61:ILE:HB	1:RC:68:ILE:HG22	2.00	0.43
1:RD:61:ILE:HB	1:RD:68:ILE:HG22	2.00	0.43
1:RK:61:ILE:HB	1:RK:68:ILE:HG22	2.00	0.43
1:SH:61:ILE:HB	1:SH:68:ILE:HG22	2.00	0.43
1:UD:61:ILE:HB	1:UD:68:ILE:HG22	2.00	0.43
1:VD:61:ILE:HB	1:VD:68:ILE:HG22	2.00	0.43
1:WB:61:ILE:HB	1:WB:68:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WF:61:ILE:HB	1:WF:68:ILE:HG22	2.00	0.43
1:XD:61:ILE:HB	1:XD:68:ILE:HG22	2.00	0.43
1:AB:61:ILE:HB	1:AB:68:ILE:HG22	2.00	0.43
1:BJ:61:ILE:HB	1:BJ:68:ILE:HG22	2.00	0.43
1:CK:61:ILE:HB	1:CK:68:ILE:HG22	2.00	0.43
1:DG:61:ILE:HB	1:DG:68:ILE:HG22	2.00	0.43
1:DI:61:ILE:HB	1:DI:68:ILE:HG22	2.00	0.43
1:DJ:7:PHE:O	1:DK:65:HIS:NE2	2.46	0.43
1:FA:61:ILE:HB	1:FA:68:ILE:HG22	2.00	0.43
1:FD:61:ILE:HB	1:FD:68:ILE:HG22	2.00	0.43
1:FH:61:ILE:HB	1:FH:68:ILE:HG22	2.00	0.43
1:LK:61:ILE:HB	1:LK:68:ILE:HG22	2.00	0.43
1:MA:61:ILE:HB	1:MA:68:ILE:HG22	2.00	0.43
1:PA:65:HIS:NE2	1:PK:7:PHE:O	2.47	0.43
1:UI:61:ILE:HB	1:UI:68:ILE:HG22	2.00	0.43
1:UK:61:ILE:HB	1:UK:68:ILE:HG22	2.00	0.43
1:VF:7:PHE:O	1:VG:65:HIS:NE2	2.47	0.43
1:WK:61:ILE:HB	1:WK:68:ILE:HG22	2.00	0.43
1:XG:61:ILE:HB	1:XG:68:ILE:HG22	2.00	0.43
1:AC:61:ILE:HB	1:AC:68:ILE:HG22	2.00	0.43
1:AJ:61:ILE:HB	1:AJ:68:ILE:HG22	2.00	0.43
1:AK:61:ILE:HB	1:AK:68:ILE:HG22	2.00	0.43
1:KD:61:ILE:HB	1:KD:68:ILE:HG22	2.00	0.43
1:LI:61:ILE:HB	1:LI:68:ILE:HG22	2.00	0.43
1:MI:61:ILE:HB	1:MI:68:ILE:HG22	2.00	0.43
1:NA:61:ILE:HB	1:NA:68:ILE:HG22	2.00	0.43
1:NC:7:PHE:O	1:ND:65:HIS:NE2	2.48	0.43
1:OB:61:ILE:HB	1:OB:68:ILE:HG22	2.00	0.43
1:OJ:61:ILE:HB	1:OJ:68:ILE:HG22	2.00	0.43
1:RI:61:ILE:HB	1:RI:68:ILE:HG22	2.00	0.43
1:TG:61:ILE:HB	1:TG:68:ILE:HG22	2.00	0.43
1:VF:61:ILE:HB	1:VF:68:ILE:HG22	2.00	0.43
1:WI:61:ILE:HB	1:WI:68:ILE:HG22	2.00	0.43
1:EF:61:ILE:HB	1:EF:68:ILE:HG22	2.00	0.43
1:IB:7:PHE:O	1:IC:65:HIS:NE2	2.48	0.43
1:JH:61:ILE:HB	1:JH:68:ILE:HG22	2.00	0.43
1:OC:61:ILE:HB	1:OC:68:ILE:HG22	2.00	0.43
1:OD:61:ILE:HB	1:OD:68:ILE:HG22	2.00	0.43
1:OK:61:ILE:HB	1:OK:68:ILE:HG22	2.00	0.43
1:PH:61:ILE:HB	1:PH:68:ILE:HG22	2.00	0.43
1:SD:61:ILE:HB	1:SD:68:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TC:61:ILE:HB	1:TC:68:ILE:HG22	2.00	0.43
1:VI:61:ILE:HB	1:VI:68:ILE:HG22	2.00	0.43
1:BA:61:ILE:HB	1:BA:68:ILE:HG22	2.00	0.43
1:LH:61:ILE:HB	1:LH:68:ILE:HG22	2.00	0.43
1:WE:61:ILE:HB	1:WE:68:ILE:HG22	2.00	0.43
1:AE:61:ILE:HB	1:AE:68:ILE:HG22	2.00	0.42
1:DH:61:ILE:HB	1:DH:68:ILE:HG22	2.00	0.42
1:KI:61:ILE:HB	1:KI:68:ILE:HG22	2.00	0.42
1:SI:61:ILE:HB	1:SI:68:ILE:HG22	2.00	0.42
1:TC:40:GLU:HG2	1:TD:56:ARG:HG2	2.00	0.42
1:AD:61:ILE:HB	1:AD:68:ILE:HG22	2.00	0.42
1:BK:61:ILE:HB	1:BK:68:ILE:HG22	2.00	0.42
1:GD:61:ILE:HB	1:GD:68:ILE:HG22	2.00	0.42
1:HB:61:ILE:HB	1:HB:68:ILE:HG22	2.00	0.42
1:IG:61:ILE:HB	1:IG:68:ILE:HG22	2.00	0.42
1:KF:61:ILE:HB	1:KF:68:ILE:HG22	2.00	0.42
1:MF:61:ILE:HB	1:MF:68:ILE:HG22	2.00	0.42
1:NK:61:ILE:HB	1:NK:68:ILE:HG22	2.00	0.42
1:QB:61:ILE:HB	1:QB:68:ILE:HG22	2.00	0.42
1:QI:61:ILE:HB	1:QI:68:ILE:HG22	2.00	0.42
1:TD:61:ILE:HB	1:TD:68:ILE:HG22	2.00	0.42
1:VA:61:ILE:HB	1:VA:68:ILE:HG22	2.00	0.42
1:VE:61:ILE:HB	1:VE:68:ILE:HG22	2.00	0.42
1:EK:61:ILE:HB	1:EK:68:ILE:HG22	2.00	0.42
1:HG:61:ILE:HB	1:HG:68:ILE:HG22	2.00	0.42
1:IB:61:ILE:HB	1:IB:68:ILE:HG22	2.00	0.42
1:LC:40:GLU:HG2	1:LD:56:ARG:HG2	2.01	0.42
1:QK:61:ILE:HB	1:QK:68:ILE:HG22	2.00	0.42
1:SF:61:ILE:HB	1:SF:68:ILE:HG22	2.00	0.42
1:WA:61:ILE:HB	1:WA:68:ILE:HG22	2.00	0.42
1:WI:7:PHE:O	1:WJ:65:HIS:NE2	2.51	0.42
1:CE:40:GLU:HG2	1:CF:56:ARG:HG2	2.01	0.42
1:EB:61:ILE:HB	1:EB:68:ILE:HG22	2.00	0.42
1:EI:61:ILE:HB	1:EI:68:ILE:HG22	2.00	0.42
1:RB:61:ILE:HB	1:RB:68:ILE:HG22	2.00	0.42
1:UB:61:ILE:HB	1:UB:68:ILE:HG22	2.00	0.42
1:XB:61:ILE:HB	1:XB:68:ILE:HG22	2.00	0.42
1:XC:61:ILE:HB	1:XC:68:ILE:HG22	2.00	0.42
1:XI:40:GLU:HG2	1:XJ:56:ARG:HG2	2.02	0.42
1:BB:61:ILE:HB	1:BB:68:ILE:HG22	2.00	0.42
1:CD:61:ILE:HB	1:CD:68:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FF:61:ILE:HB	1:FF:68:ILE:HG22	2.00	0.42
1:FJ:7:PHE:O	1:FK:65:HIS:NE2	2.50	0.42
1:IK:61:ILE:HB	1:IK:68:ILE:HG22	2.00	0.42
1:LD:61:ILE:HB	1:LD:68:ILE:HG22	2.00	0.42
1:OF:61:ILE:HB	1:OF:68:ILE:HG22	2.00	0.42
1:UG:61:ILE:HB	1:UG:68:ILE:HG22	2.00	0.42
1:VJ:7:PHE:O	1:VK:65:HIS:NE2	2.47	0.42
1:WE:40:GLU:HG2	1:WF:56:ARG:HG2	2.01	0.42
1:AF:61:ILE:HB	1:AF:68:ILE:HG22	2.00	0.42
1:RG:61:ILE:HB	1:RG:68:ILE:HG22	2.00	0.42
1:TB:61:ILE:HB	1:TB:68:ILE:HG22	2.00	0.42
1:VG:61:ILE:HB	1:VG:68:ILE:HG22	2.00	0.42
1:HK:61:ILE:HB	1:HK:68:ILE:HG22	2.00	0.42
1:NB:61:ILE:HB	1:NB:68:ILE:HG22	2.00	0.42
1:WG:61:ILE:HB	1:WG:68:ILE:HG22	2.00	0.42
1:AI:40:GLU:HG2	1:AJ:56:ARG:HG2	2.01	0.42
1:CE:61:ILE:HB	1:CE:68:ILE:HG22	2.00	0.42
1:DD:61:ILE:HB	1:DD:68:ILE:HG22	2.00	0.42
1:WC:61:ILE:HB	1:WC:68:ILE:HG22	2.00	0.42
1:XF:7:PHE:O	1:XG:65:HIS:NE2	2.47	0.42
1:BE:61:ILE:HB	1:BE:68:ILE:HG22	2.00	0.42
1:GE:61:ILE:HB	1:GE:68:ILE:HG22	2.00	0.42
1:MA:42:LEU:HD11	1:MB:52:ALA:HB1	2.02	0.42
1:MD:7:PHE:O	1:ME:65:HIS:NE2	2.47	0.42
1:NE:61:ILE:HB	1:NE:68:ILE:HG22	2.00	0.42
1:QJ:61:ILE:HB	1:QJ:68:ILE:HG22	2.00	0.42
1:EJ:61:ILE:HB	1:EJ:68:ILE:HG22	2.00	0.42
1:RE:61:ILE:HB	1:RE:68:ILE:HG22	2.00	0.42
1:QD:7:PHE:O	1:QE:65:HIS:NE2	2.50	0.41
1:UE:61:ILE:HB	1:UE:68:ILE:HG22	2.00	0.41
1:DE:40:GLU:HG2	1:DF:56:ARG:HG2	2.02	0.41
1:JE:61:ILE:HB	1:JE:68:ILE:HG22	2.00	0.41
1:SH:40:GLU:HG2	1:SI:56:ARG:HG2	2.02	0.41
1:VC:61:ILE:HB	1:VC:68:ILE:HG22	2.00	0.41
1:WA:40:GLU:HG2	1:WB:56:ARG:HG2	2.03	0.41
1:ME:7:PHE:O	1:MF:65:HIS:NE2	2.53	0.41
1:PE:61:ILE:HB	1:PE:68:ILE:HG22	2.00	0.41
1:WJ:39:GLY:O	1:WK:71:GLU:N	2.42	0.41
1:MH:40:GLU:HG2	1:MI:56:ARG:HG2	2.02	0.41
1:SJ:7:PHE:O	1:SK:65:HIS:NE2	2.47	0.41
1:TA:7:PHE:O	1:TB:65:HIS:NE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:7:PHE:O	1:EC:65:HIS:NE2	2.50	0.41
1:NA:40:GLU:HG2	1:NB:56:ARG:HG2	2.02	0.41
1:SD:7:PHE:O	1:SE:65:HIS:NE2	2.48	0.41
1:OB:7:PHE:O	1:OC:65:HIS:NE2	2.51	0.41
1:QB:40:GLU:HG2	1:QC:56:ARG:HG2	2.03	0.41
1:RF:7:PHE:O	1:RG:65:HIS:NE2	2.49	0.41
1:RC:42:LEU:HD11	1:RD:52:ALA:HB1	2.02	0.41
1:TB:7:PHE:O	1:TC:65:HIS:NE2	2.47	0.41
1:XA:40:GLU:HG2	1:XB:56:ARG:HG2	2.03	0.41
1:JE:40:GLU:HG2	1:JF:56:ARG:HG2	2.03	0.41
1:AB:7:PHE:O	1:AC:65:HIS:NE2	2.52	0.40
1:II:40:GLU:HG2	1:IJ:56:ARG:HG2	2.03	0.40
1:CG:40:GLU:HG2	1:CH:56:ARG:HG2	2.03	0.40
1:VE:40:GLU:HG2	1:VF:56:ARG:HG2	2.03	0.40
1:MA:40:GLU:HG2	1:MB:56:ARG:HG2	2.03	0.40
1:SG:7:PHE:O	1:SH:65:HIS:NE2	2.53	0.40
1:BB:7:PHE:O	1:BC:65:HIS:NE2	2.52	0.40
1:OC:7:PHE:O	1:OD:65:HIS:NE2	2.50	0.40
1:VA:40:GLU:HG2	1:VB:56:ARG:HG2	2.04	0.40

There are no symmetry-related clashes.

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	AA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	AK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	BK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	CK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	DK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	ED	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	EK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	FK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	GK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	HK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	ID	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	II	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	IJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	JK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	KK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	LK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	ME	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	MK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	ND	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	NK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	OK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	PK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	QK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	RK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	SK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	TK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	UK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	VK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	WK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	XA	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XB	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XC	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XD	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XE	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XF	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XG	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XH	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XI	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XJ	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
1	XK	51/74 (69%)	50 (98%)	1 (2%)	0	100	100
All	All	13464/19536 (69%)	13200 (98%)	264 (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	AA	46/62 (74%)	46 (100%)	0	100	100
1	AB	46/62 (74%)	46 (100%)	0	100	100
1	AC	46/62 (74%)	46 (100%)	0	100	100
1	AD	46/62 (74%)	46 (100%)	0	100	100
1	AE	46/62 (74%)	46 (100%)	0	100	100
1	AF	46/62 (74%)	46 (100%)	0	100	100
1	AG	46/62 (74%)	46 (100%)	0	100	100
1	AH	46/62 (74%)	46 (100%)	0	100	100
1	AI	46/62 (74%)	46 (100%)	0	100	100
1	AJ	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AK	46/62 (74%)	46 (100%)	0	100	100
1	BA	46/62 (74%)	46 (100%)	0	100	100
1	BB	46/62 (74%)	46 (100%)	0	100	100
1	BC	46/62 (74%)	46 (100%)	0	100	100
1	BD	46/62 (74%)	46 (100%)	0	100	100
1	BE	46/62 (74%)	46 (100%)	0	100	100
1	BF	46/62 (74%)	46 (100%)	0	100	100
1	BG	46/62 (74%)	46 (100%)	0	100	100
1	BH	46/62 (74%)	46 (100%)	0	100	100
1	BI	46/62 (74%)	46 (100%)	0	100	100
1	BJ	46/62 (74%)	46 (100%)	0	100	100
1	BK	46/62 (74%)	46 (100%)	0	100	100
1	CA	46/62 (74%)	46 (100%)	0	100	100
1	CB	46/62 (74%)	46 (100%)	0	100	100
1	CC	46/62 (74%)	46 (100%)	0	100	100
1	CD	46/62 (74%)	46 (100%)	0	100	100
1	CE	46/62 (74%)	46 (100%)	0	100	100
1	CF	46/62 (74%)	46 (100%)	0	100	100
1	CG	46/62 (74%)	46 (100%)	0	100	100
1	CH	46/62 (74%)	46 (100%)	0	100	100
1	CI	46/62 (74%)	46 (100%)	0	100	100
1	CJ	46/62 (74%)	46 (100%)	0	100	100
1	CK	46/62 (74%)	46 (100%)	0	100	100
1	DA	46/62 (74%)	46 (100%)	0	100	100
1	DB	46/62 (74%)	46 (100%)	0	100	100
1	DC	46/62 (74%)	46 (100%)	0	100	100
1	DD	46/62 (74%)	46 (100%)	0	100	100
1	DE	46/62 (74%)	46 (100%)	0	100	100
1	DF	46/62 (74%)	46 (100%)	0	100	100
1	DG	46/62 (74%)	46 (100%)	0	100	100
1	DH	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DI	46/62 (74%)	46 (100%)	0	100	100
1	DJ	46/62 (74%)	46 (100%)	0	100	100
1	DK	46/62 (74%)	46 (100%)	0	100	100
1	EA	46/62 (74%)	46 (100%)	0	100	100
1	EB	46/62 (74%)	46 (100%)	0	100	100
1	EC	46/62 (74%)	46 (100%)	0	100	100
1	ED	46/62 (74%)	46 (100%)	0	100	100
1	EE	46/62 (74%)	46 (100%)	0	100	100
1	EF	46/62 (74%)	46 (100%)	0	100	100
1	EG	46/62 (74%)	46 (100%)	0	100	100
1	EH	46/62 (74%)	46 (100%)	0	100	100
1	EI	46/62 (74%)	46 (100%)	0	100	100
1	EJ	46/62 (74%)	46 (100%)	0	100	100
1	EK	46/62 (74%)	46 (100%)	0	100	100
1	FA	46/62 (74%)	46 (100%)	0	100	100
1	FB	46/62 (74%)	46 (100%)	0	100	100
1	FC	46/62 (74%)	46 (100%)	0	100	100
1	FD	46/62 (74%)	46 (100%)	0	100	100
1	FE	46/62 (74%)	46 (100%)	0	100	100
1	FF	46/62 (74%)	46 (100%)	0	100	100
1	FG	46/62 (74%)	46 (100%)	0	100	100
1	FH	46/62 (74%)	46 (100%)	0	100	100
1	FI	46/62 (74%)	46 (100%)	0	100	100
1	FJ	46/62 (74%)	46 (100%)	0	100	100
1	FK	46/62 (74%)	46 (100%)	0	100	100
1	GA	46/62 (74%)	46 (100%)	0	100	100
1	GB	46/62 (74%)	46 (100%)	0	100	100
1	GC	46/62 (74%)	46 (100%)	0	100	100
1	GD	46/62 (74%)	46 (100%)	0	100	100
1	GE	46/62 (74%)	46 (100%)	0	100	100
1	GF	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GG	46/62 (74%)	46 (100%)	0	100	100
1	GH	46/62 (74%)	46 (100%)	0	100	100
1	GI	46/62 (74%)	46 (100%)	0	100	100
1	GJ	46/62 (74%)	46 (100%)	0	100	100
1	GK	46/62 (74%)	46 (100%)	0	100	100
1	HA	46/62 (74%)	46 (100%)	0	100	100
1	HB	46/62 (74%)	46 (100%)	0	100	100
1	HC	46/62 (74%)	46 (100%)	0	100	100
1	HD	46/62 (74%)	46 (100%)	0	100	100
1	HE	46/62 (74%)	46 (100%)	0	100	100
1	HF	46/62 (74%)	46 (100%)	0	100	100
1	HG	46/62 (74%)	46 (100%)	0	100	100
1	HH	46/62 (74%)	46 (100%)	0	100	100
1	HI	46/62 (74%)	46 (100%)	0	100	100
1	HJ	46/62 (74%)	46 (100%)	0	100	100
1	HK	46/62 (74%)	46 (100%)	0	100	100
1	IA	46/62 (74%)	46 (100%)	0	100	100
1	IB	46/62 (74%)	46 (100%)	0	100	100
1	IC	46/62 (74%)	46 (100%)	0	100	100
1	ID	46/62 (74%)	46 (100%)	0	100	100
1	IE	46/62 (74%)	46 (100%)	0	100	100
1	IF	46/62 (74%)	46 (100%)	0	100	100
1	IG	46/62 (74%)	46 (100%)	0	100	100
1	IH	46/62 (74%)	46 (100%)	0	100	100
1	II	46/62 (74%)	46 (100%)	0	100	100
1	IJ	46/62 (74%)	46 (100%)	0	100	100
1	IK	46/62 (74%)	46 (100%)	0	100	100
1	JA	46/62 (74%)	46 (100%)	0	100	100
1	JB	46/62 (74%)	46 (100%)	0	100	100
1	JC	46/62 (74%)	46 (100%)	0	100	100
1	JD	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JE	46/62 (74%)	46 (100%)	0	100	100
1	JF	46/62 (74%)	46 (100%)	0	100	100
1	JG	46/62 (74%)	46 (100%)	0	100	100
1	JH	46/62 (74%)	46 (100%)	0	100	100
1	JI	46/62 (74%)	46 (100%)	0	100	100
1	JJ	46/62 (74%)	46 (100%)	0	100	100
1	JK	46/62 (74%)	46 (100%)	0	100	100
1	KA	46/62 (74%)	46 (100%)	0	100	100
1	KB	46/62 (74%)	46 (100%)	0	100	100
1	KC	46/62 (74%)	46 (100%)	0	100	100
1	KD	46/62 (74%)	46 (100%)	0	100	100
1	KE	46/62 (74%)	46 (100%)	0	100	100
1	KF	46/62 (74%)	46 (100%)	0	100	100
1	KG	46/62 (74%)	46 (100%)	0	100	100
1	KH	46/62 (74%)	46 (100%)	0	100	100
1	KI	46/62 (74%)	46 (100%)	0	100	100
1	KJ	46/62 (74%)	46 (100%)	0	100	100
1	KK	46/62 (74%)	46 (100%)	0	100	100
1	LA	46/62 (74%)	46 (100%)	0	100	100
1	LB	46/62 (74%)	46 (100%)	0	100	100
1	LC	46/62 (74%)	46 (100%)	0	100	100
1	LD	46/62 (74%)	46 (100%)	0	100	100
1	LE	46/62 (74%)	46 (100%)	0	100	100
1	LF	46/62 (74%)	46 (100%)	0	100	100
1	LG	46/62 (74%)	46 (100%)	0	100	100
1	LH	46/62 (74%)	46 (100%)	0	100	100
1	LI	46/62 (74%)	46 (100%)	0	100	100
1	LJ	46/62 (74%)	46 (100%)	0	100	100
1	LK	46/62 (74%)	46 (100%)	0	100	100
1	MA	46/62 (74%)	46 (100%)	0	100	100
1	MB	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MC	46/62 (74%)	46 (100%)	0	100	100
1	MD	46/62 (74%)	46 (100%)	0	100	100
1	ME	46/62 (74%)	46 (100%)	0	100	100
1	MF	46/62 (74%)	46 (100%)	0	100	100
1	MG	46/62 (74%)	46 (100%)	0	100	100
1	MH	46/62 (74%)	46 (100%)	0	100	100
1	MI	46/62 (74%)	46 (100%)	0	100	100
1	MJ	46/62 (74%)	46 (100%)	0	100	100
1	MK	46/62 (74%)	46 (100%)	0	100	100
1	NA	46/62 (74%)	46 (100%)	0	100	100
1	NB	46/62 (74%)	46 (100%)	0	100	100
1	NC	46/62 (74%)	46 (100%)	0	100	100
1	ND	46/62 (74%)	46 (100%)	0	100	100
1	NE	46/62 (74%)	46 (100%)	0	100	100
1	NF	46/62 (74%)	46 (100%)	0	100	100
1	NG	46/62 (74%)	46 (100%)	0	100	100
1	NH	46/62 (74%)	46 (100%)	0	100	100
1	NI	46/62 (74%)	46 (100%)	0	100	100
1	NJ	46/62 (74%)	46 (100%)	0	100	100
1	NK	46/62 (74%)	46 (100%)	0	100	100
1	OA	46/62 (74%)	46 (100%)	0	100	100
1	OB	46/62 (74%)	46 (100%)	0	100	100
1	OC	46/62 (74%)	46 (100%)	0	100	100
1	OD	46/62 (74%)	46 (100%)	0	100	100
1	OE	46/62 (74%)	46 (100%)	0	100	100
1	OF	46/62 (74%)	46 (100%)	0	100	100
1	OG	46/62 (74%)	46 (100%)	0	100	100
1	OH	46/62 (74%)	46 (100%)	0	100	100
1	OI	46/62 (74%)	46 (100%)	0	100	100
1	OJ	46/62 (74%)	46 (100%)	0	100	100
1	OK	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PA	46/62 (74%)	46 (100%)	0	100	100
1	PB	46/62 (74%)	46 (100%)	0	100	100
1	PC	46/62 (74%)	46 (100%)	0	100	100
1	PD	46/62 (74%)	46 (100%)	0	100	100
1	PE	46/62 (74%)	46 (100%)	0	100	100
1	PF	46/62 (74%)	46 (100%)	0	100	100
1	PG	46/62 (74%)	46 (100%)	0	100	100
1	PH	46/62 (74%)	46 (100%)	0	100	100
1	PI	46/62 (74%)	46 (100%)	0	100	100
1	PJ	46/62 (74%)	46 (100%)	0	100	100
1	PK	46/62 (74%)	46 (100%)	0	100	100
1	QA	46/62 (74%)	46 (100%)	0	100	100
1	QB	46/62 (74%)	46 (100%)	0	100	100
1	QC	46/62 (74%)	46 (100%)	0	100	100
1	QD	46/62 (74%)	46 (100%)	0	100	100
1	QE	46/62 (74%)	46 (100%)	0	100	100
1	QF	46/62 (74%)	46 (100%)	0	100	100
1	QG	46/62 (74%)	46 (100%)	0	100	100
1	QH	46/62 (74%)	46 (100%)	0	100	100
1	QI	46/62 (74%)	46 (100%)	0	100	100
1	QJ	46/62 (74%)	46 (100%)	0	100	100
1	QK	46/62 (74%)	46 (100%)	0	100	100
1	RA	46/62 (74%)	46 (100%)	0	100	100
1	RB	46/62 (74%)	46 (100%)	0	100	100
1	RC	46/62 (74%)	46 (100%)	0	100	100
1	RD	46/62 (74%)	46 (100%)	0	100	100
1	RE	46/62 (74%)	46 (100%)	0	100	100
1	RF	46/62 (74%)	46 (100%)	0	100	100
1	RG	46/62 (74%)	46 (100%)	0	100	100
1	RH	46/62 (74%)	46 (100%)	0	100	100
1	RI	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RJ	46/62 (74%)	46 (100%)	0	100	100
1	RK	46/62 (74%)	46 (100%)	0	100	100
1	SA	46/62 (74%)	46 (100%)	0	100	100
1	SB	46/62 (74%)	46 (100%)	0	100	100
1	SC	46/62 (74%)	46 (100%)	0	100	100
1	SD	46/62 (74%)	46 (100%)	0	100	100
1	SE	46/62 (74%)	46 (100%)	0	100	100
1	SF	46/62 (74%)	46 (100%)	0	100	100
1	SG	46/62 (74%)	46 (100%)	0	100	100
1	SH	46/62 (74%)	46 (100%)	0	100	100
1	SI	46/62 (74%)	46 (100%)	0	100	100
1	SJ	46/62 (74%)	46 (100%)	0	100	100
1	SK	46/62 (74%)	46 (100%)	0	100	100
1	TA	46/62 (74%)	46 (100%)	0	100	100
1	TB	46/62 (74%)	46 (100%)	0	100	100
1	TC	46/62 (74%)	46 (100%)	0	100	100
1	TD	46/62 (74%)	46 (100%)	0	100	100
1	TE	46/62 (74%)	46 (100%)	0	100	100
1	TF	46/62 (74%)	46 (100%)	0	100	100
1	TG	46/62 (74%)	46 (100%)	0	100	100
1	TH	46/62 (74%)	46 (100%)	0	100	100
1	TI	46/62 (74%)	46 (100%)	0	100	100
1	TJ	46/62 (74%)	46 (100%)	0	100	100
1	TK	46/62 (74%)	46 (100%)	0	100	100
1	UA	46/62 (74%)	46 (100%)	0	100	100
1	UB	46/62 (74%)	46 (100%)	0	100	100
1	UC	46/62 (74%)	46 (100%)	0	100	100
1	UD	46/62 (74%)	46 (100%)	0	100	100
1	UE	46/62 (74%)	46 (100%)	0	100	100
1	UF	46/62 (74%)	46 (100%)	0	100	100
1	UG	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UH	46/62 (74%)	46 (100%)	0	100	100
1	UI	46/62 (74%)	46 (100%)	0	100	100
1	UJ	46/62 (74%)	46 (100%)	0	100	100
1	UK	46/62 (74%)	46 (100%)	0	100	100
1	VA	46/62 (74%)	46 (100%)	0	100	100
1	VB	46/62 (74%)	46 (100%)	0	100	100
1	VC	46/62 (74%)	46 (100%)	0	100	100
1	VD	46/62 (74%)	46 (100%)	0	100	100
1	VE	46/62 (74%)	46 (100%)	0	100	100
1	VF	46/62 (74%)	46 (100%)	0	100	100
1	VG	46/62 (74%)	46 (100%)	0	100	100
1	VH	46/62 (74%)	46 (100%)	0	100	100
1	VI	46/62 (74%)	46 (100%)	0	100	100
1	VJ	46/62 (74%)	46 (100%)	0	100	100
1	VK	46/62 (74%)	46 (100%)	0	100	100
1	WA	46/62 (74%)	46 (100%)	0	100	100
1	WB	46/62 (74%)	46 (100%)	0	100	100
1	WC	46/62 (74%)	46 (100%)	0	100	100
1	WD	46/62 (74%)	46 (100%)	0	100	100
1	WE	46/62 (74%)	46 (100%)	0	100	100
1	WF	46/62 (74%)	46 (100%)	0	100	100
1	WG	46/62 (74%)	46 (100%)	0	100	100
1	WH	46/62 (74%)	46 (100%)	0	100	100
1	WI	46/62 (74%)	46 (100%)	0	100	100
1	WJ	46/62 (74%)	46 (100%)	0	100	100
1	WK	46/62 (74%)	46 (100%)	0	100	100
1	XA	46/62 (74%)	46 (100%)	0	100	100
1	XB	46/62 (74%)	46 (100%)	0	100	100
1	XC	46/62 (74%)	46 (100%)	0	100	100
1	XD	46/62 (74%)	46 (100%)	0	100	100
1	XE	46/62 (74%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XF	46/62 (74%)	46 (100%)	0	100	100
1	XG	46/62 (74%)	46 (100%)	0	100	100
1	XH	46/62 (74%)	46 (100%)	0	100	100
1	XI	46/62 (74%)	46 (100%)	0	100	100
1	XJ	46/62 (74%)	46 (100%)	0	100	100
1	XK	46/62 (74%)	46 (100%)	0	100	100
All	All	12144/16368 (74%)	12144 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

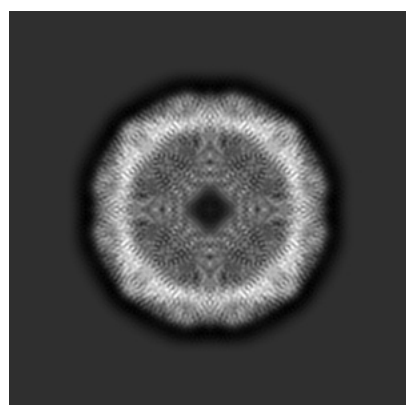
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4444. These allow visual inspection of the internal detail of the map and identification of artifacts.

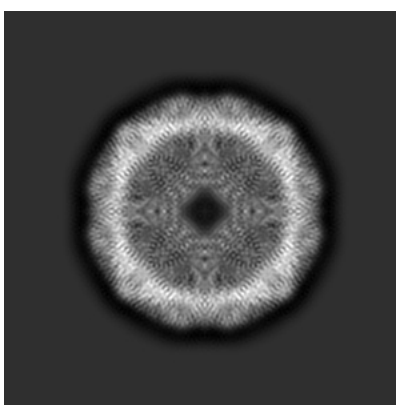
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

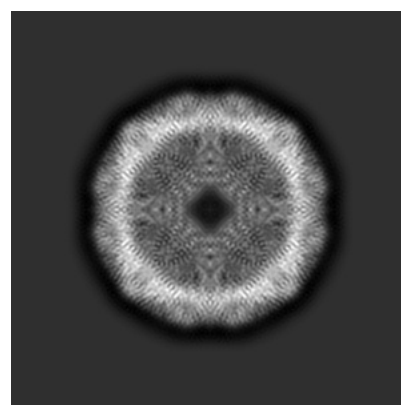
6.1.1 Primary map



X



Y

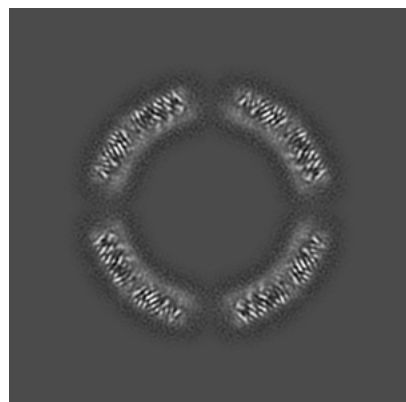


Z

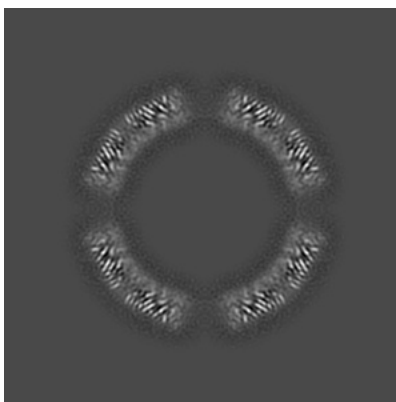
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

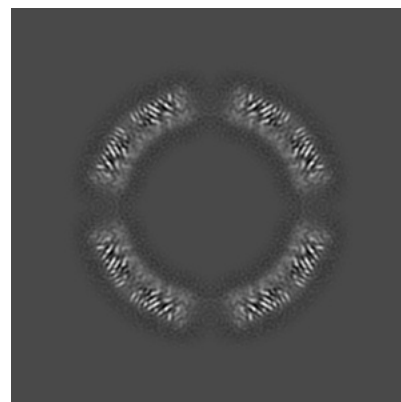
6.2.1 Primary map



X Index: 110



Y Index: 110

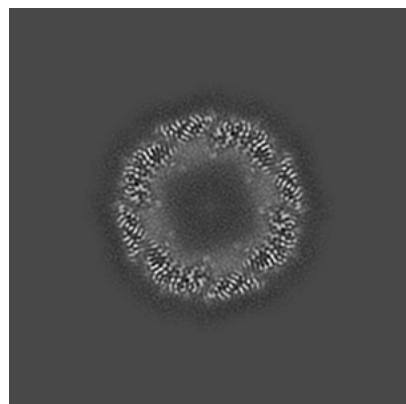


Z Index: 110

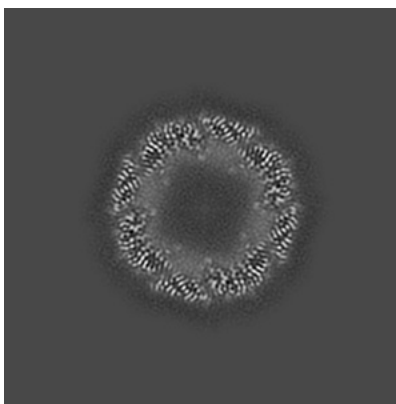
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

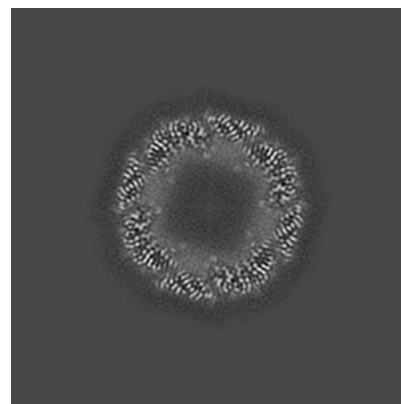
6.3.1 Primary map



X Index: 67



Y Index: 152

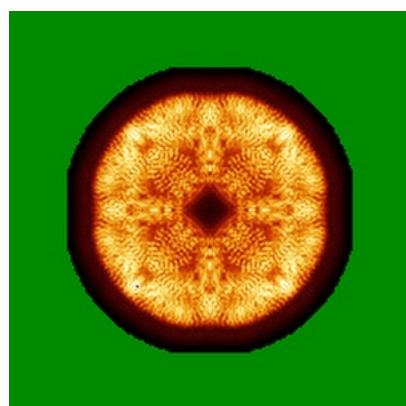


Z Index: 152

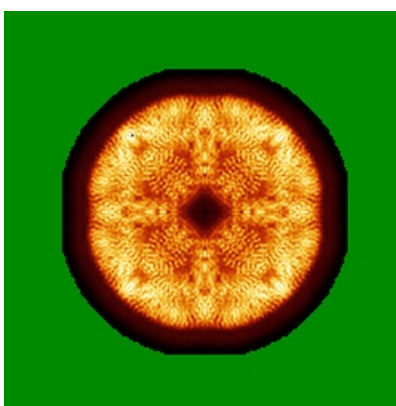
The images above show the largest variance slices of the map in three orthogonal directions.

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

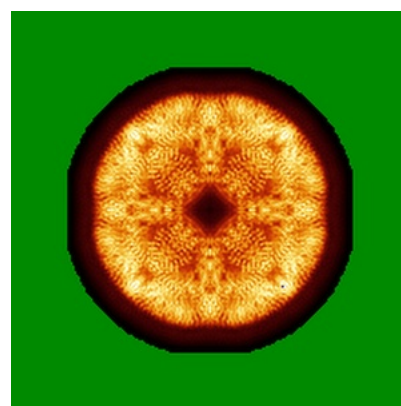
6.4.1 Primary map



X



Y

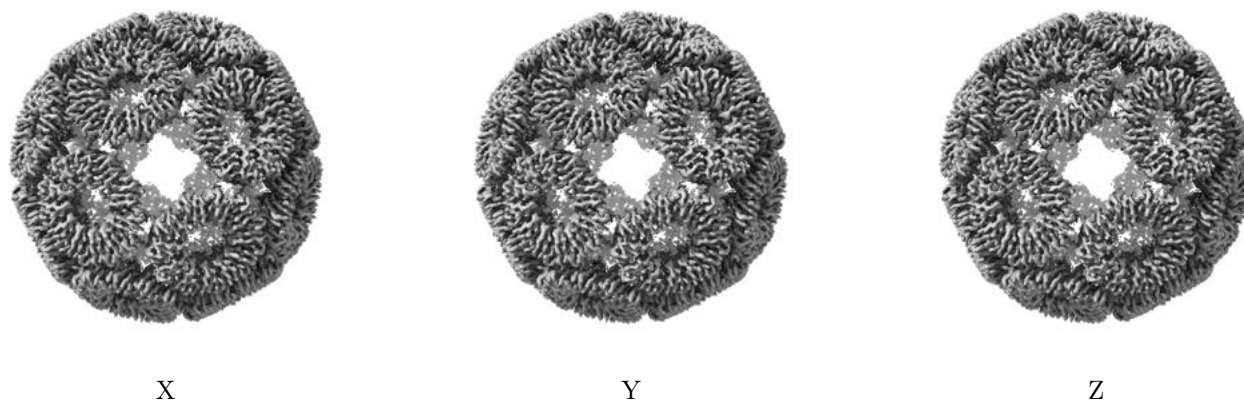


Z

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 0.115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

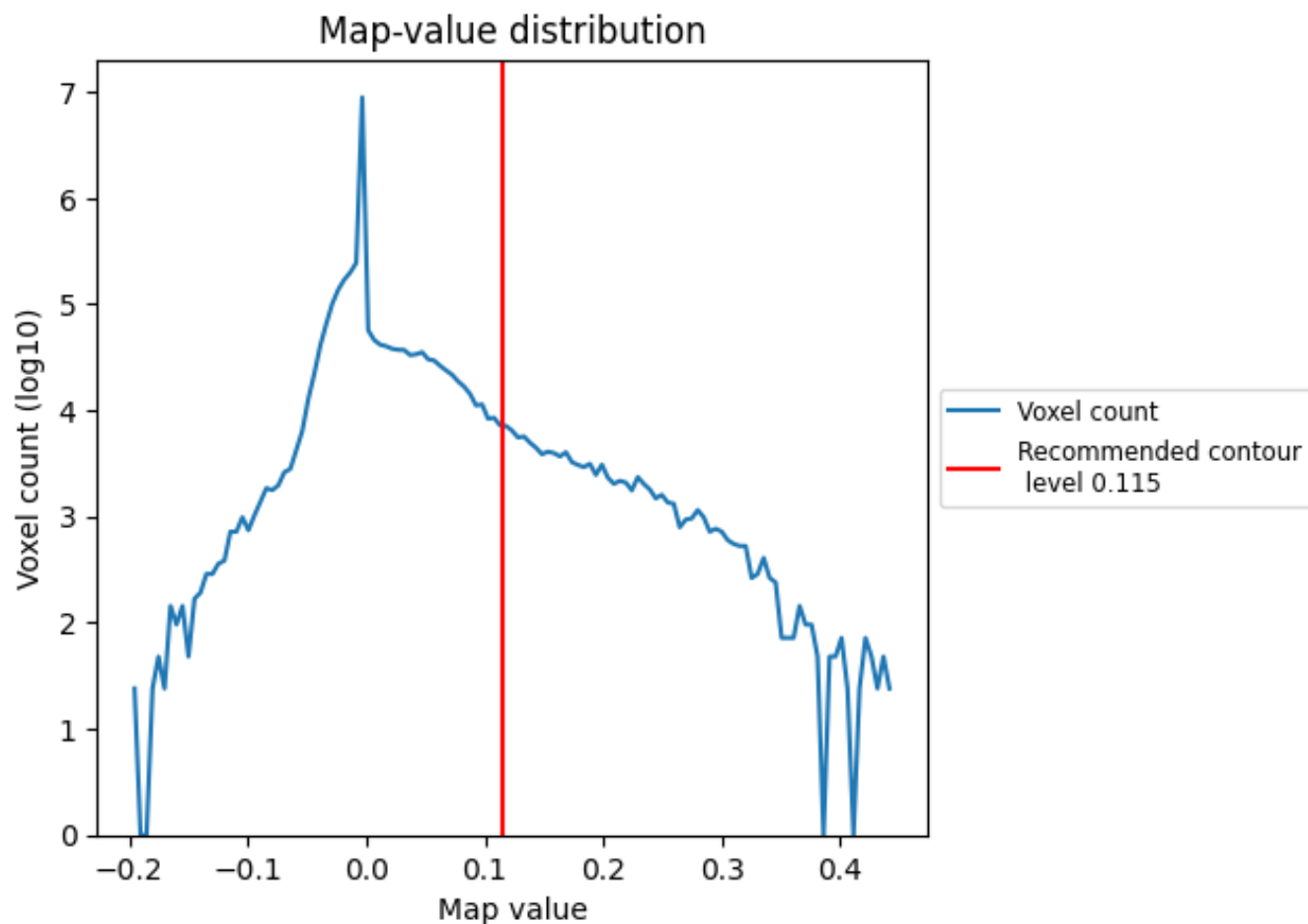
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

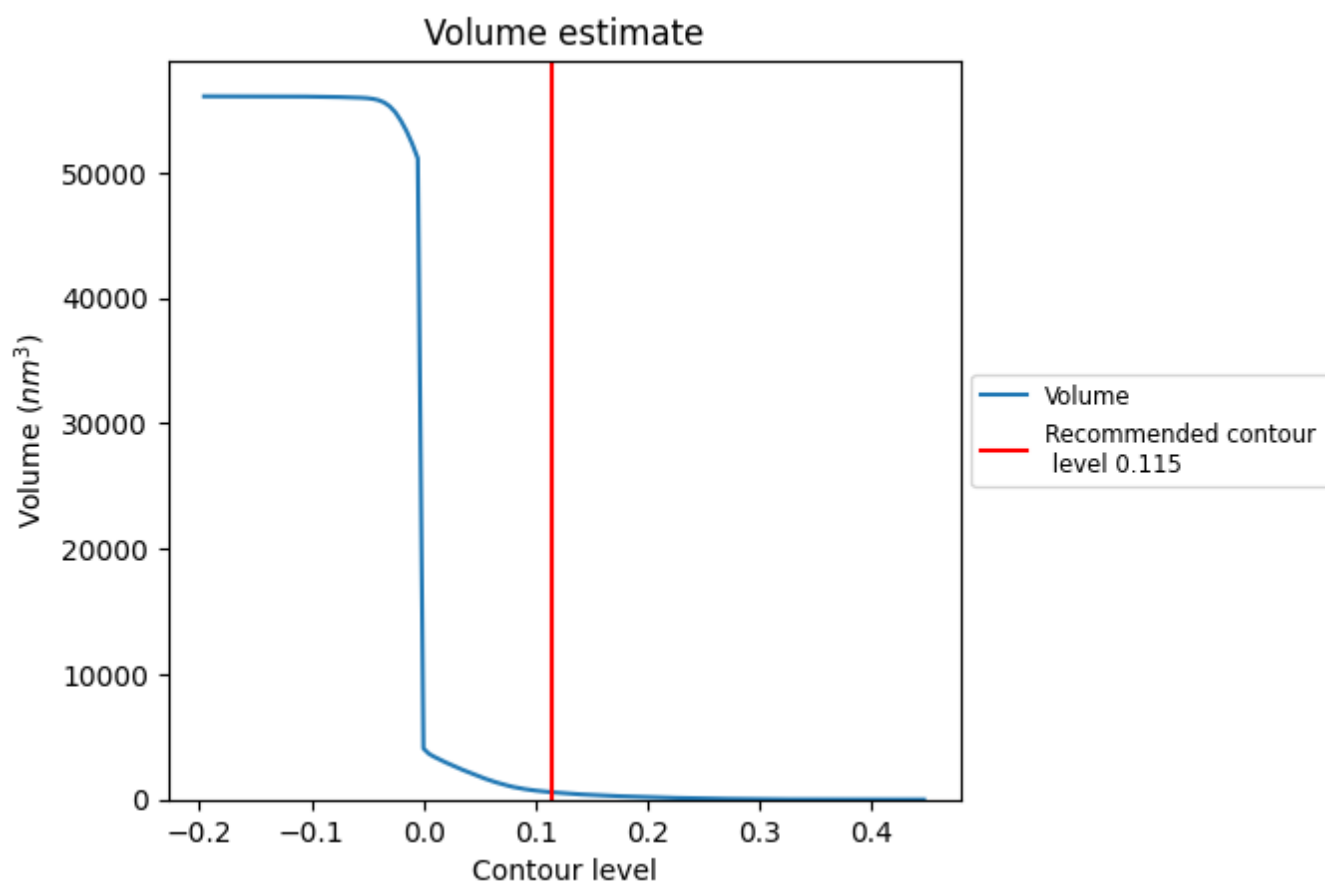
This section contains the results of statistical analysis of the map.

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.

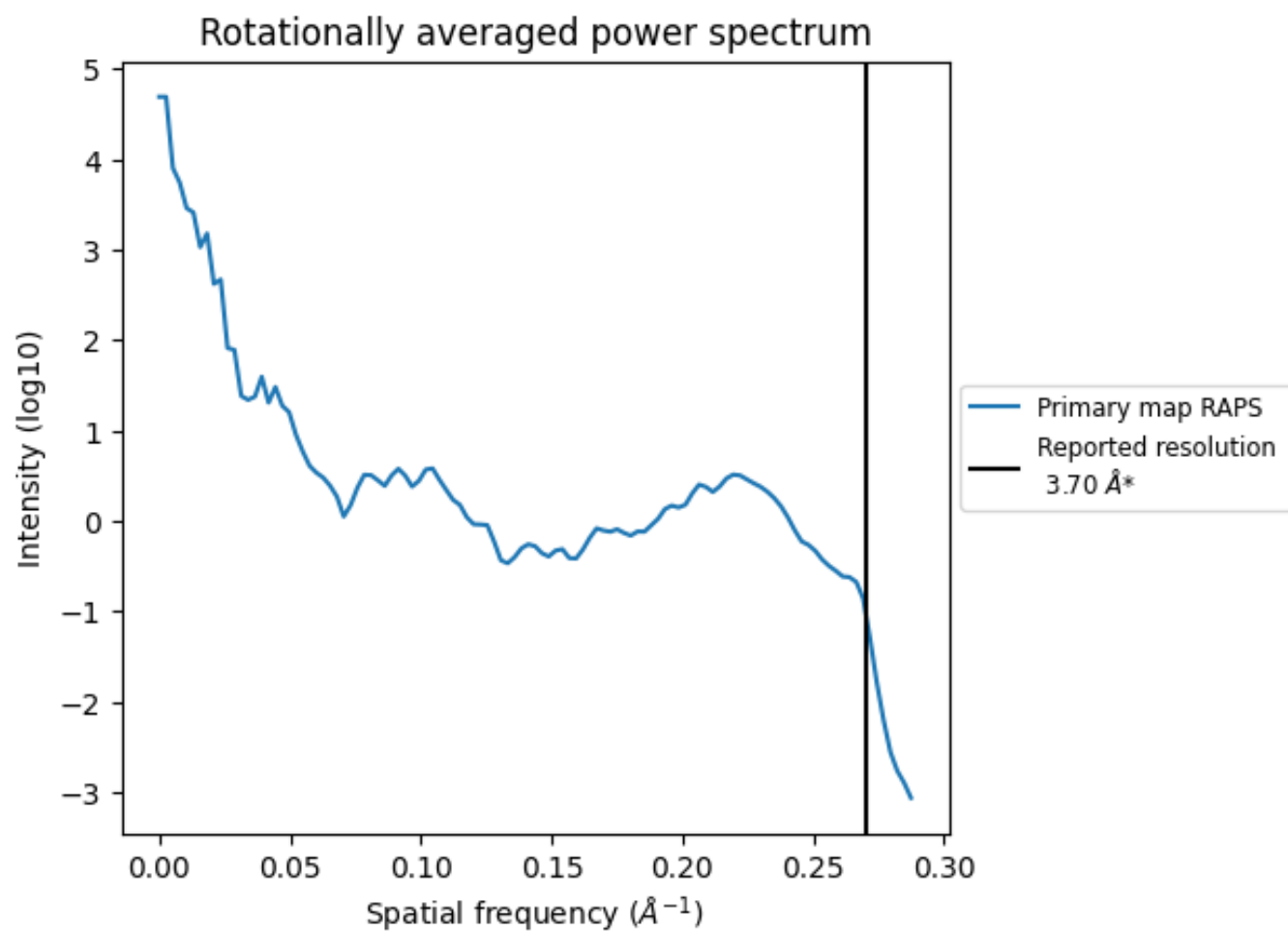
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 579 nm³; this corresponds to an approximate mass of 523 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 ⓘ

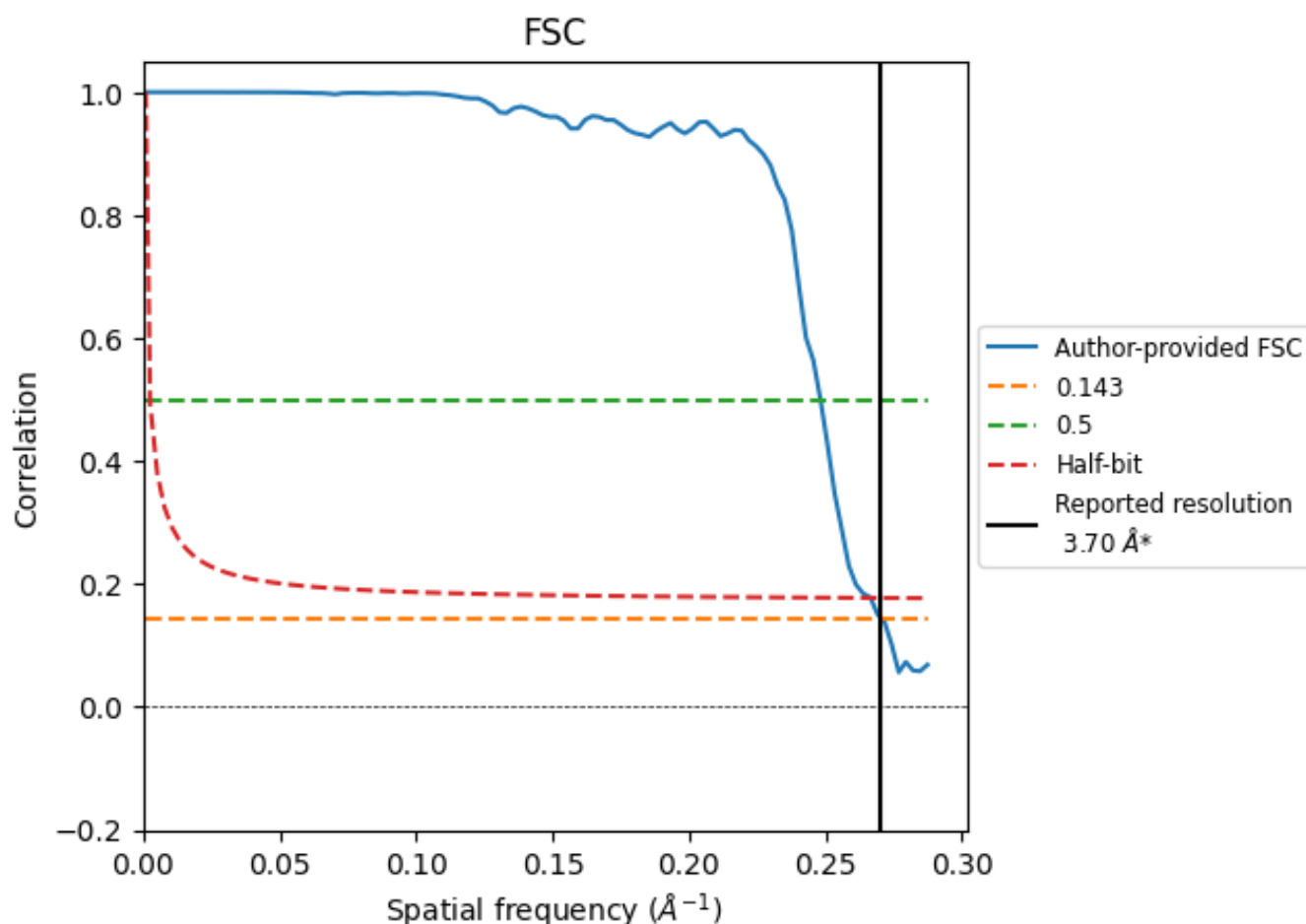


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.03	3.75
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

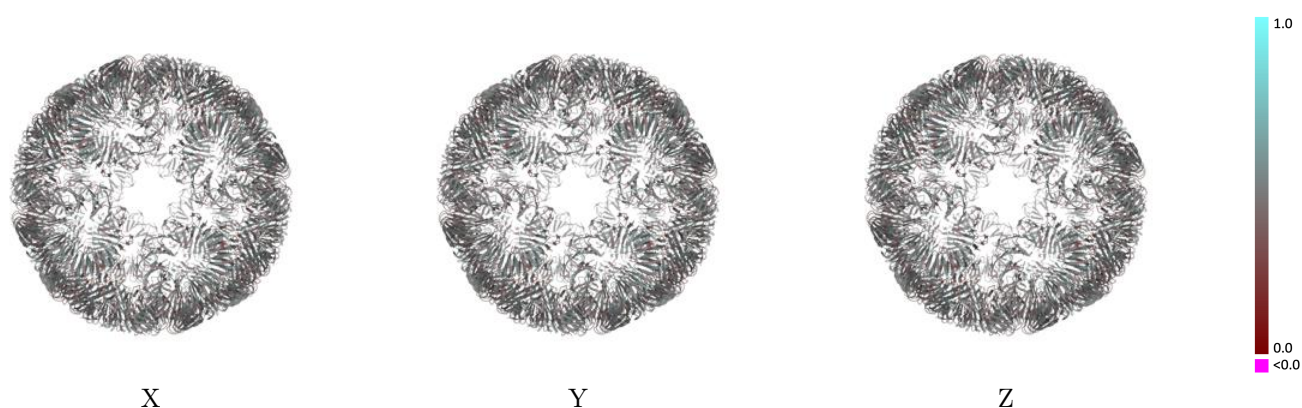
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4444 and PDB model 6RVW. Per-residue inclusion information can be found in section 3 on page 46.

9.1 Map-model overlay [i](#)

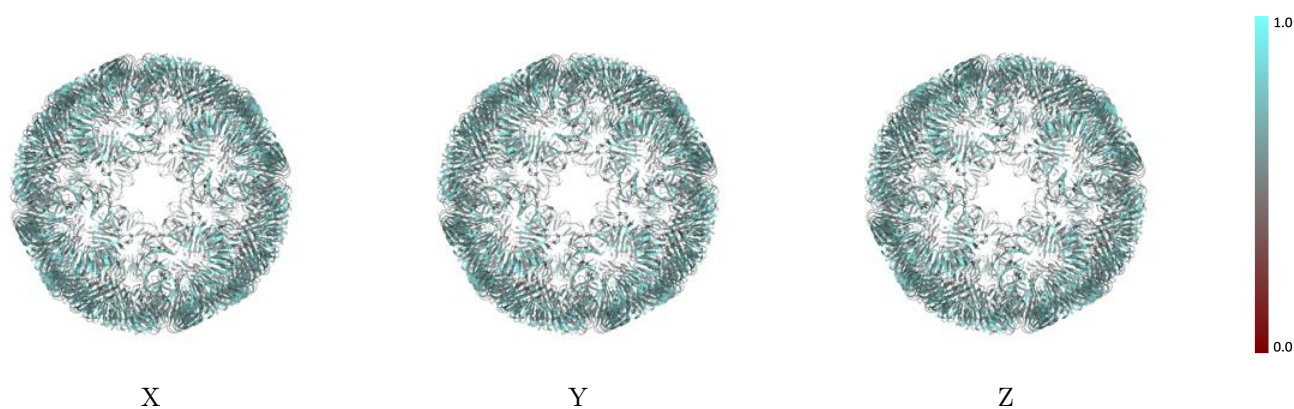
This section was not generated.

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



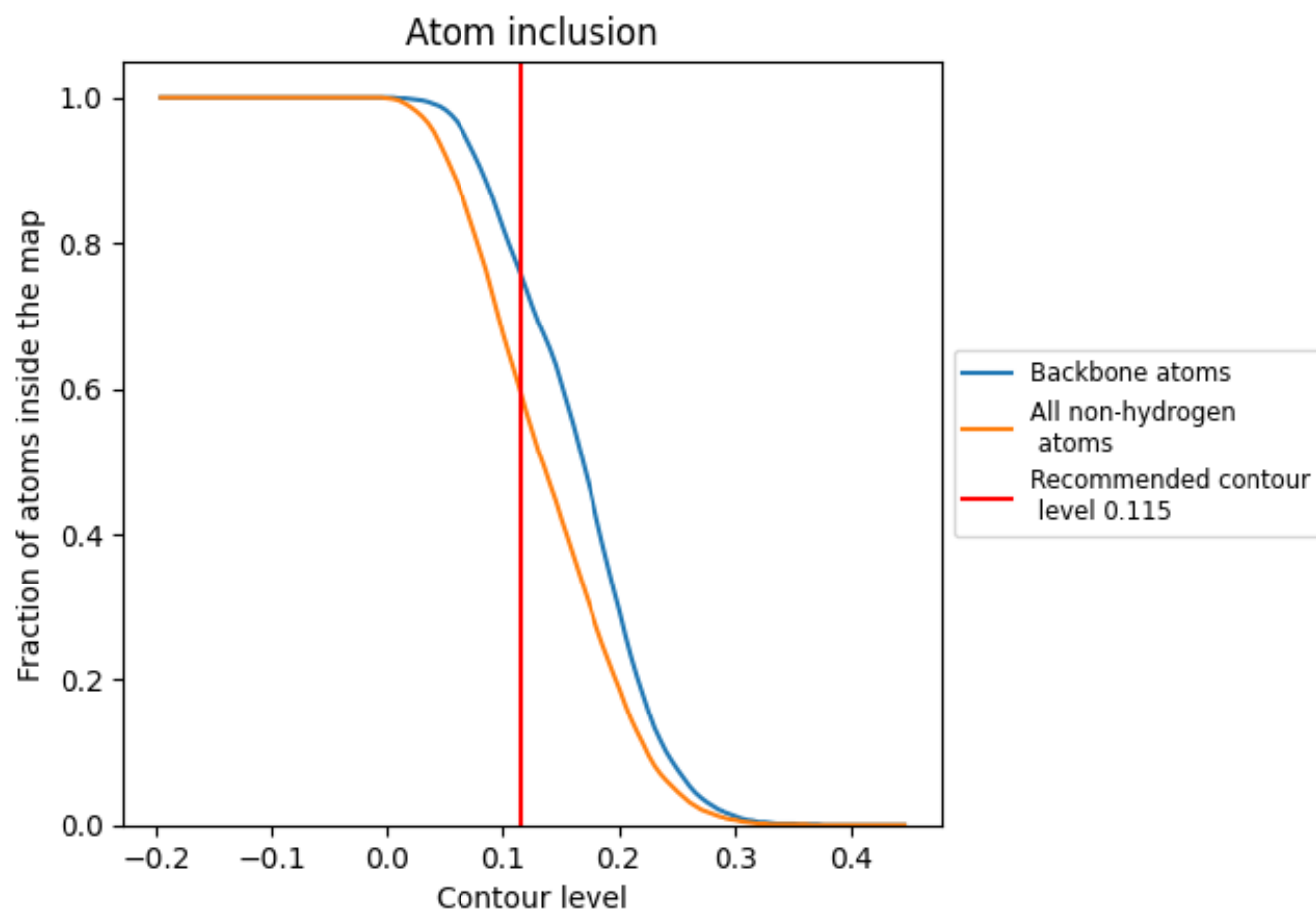
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% 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 (0.115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5970	 0.4490
AA	 0.5710	 0.4540
AB	 0.5980	 0.4480
AC	 0.5740	 0.4540
AD	 0.6170	 0.4440
AE	 0.6100	 0.4560
AF	 0.6050	 0.4600
AG	 0.6170	 0.4520
AH	 0.6120	 0.4430
AI	 0.5900	 0.4380
AJ	 0.5880	 0.4520
AK	 0.5650	 0.4520
BA	 0.5740	 0.4570
BB	 0.5950	 0.4530
BC	 0.5980	 0.4530
BD	 0.6120	 0.4450
BE	 0.6020	 0.4490
BF	 0.6020	 0.4630
BG	 0.6190	 0.4520
BH	 0.6150	 0.4380
BI	 0.5900	 0.4420
BJ	 0.5900	 0.4520
BK	 0.5600	 0.4480
CA	 0.5760	 0.4530
CB	 0.5950	 0.4520
CC	 0.5930	 0.4540
CD	 0.6170	 0.4410
CE	 0.6070	 0.4470
CF	 0.6050	 0.4580
CG	 0.6260	 0.4530
CH	 0.6060	 0.4440
CI	 0.5980	 0.4420
CJ	 0.5900	 0.4540
CK	 0.5700	 0.4490
DA	 0.5780	 0.4500



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Chain	Atom inclusion	Q-score
DB	 0.5980	 0.4520
DC	 0.5860	 0.4480
DD	 0.6100	 0.4430
DE	 0.6070	 0.4500
DF	 0.6050	 0.4560
DG	 0.6190	 0.4440
DH	 0.6100	 0.4360
DI	 0.6070	 0.4370
DJ	 0.5760	 0.4500
DK	 0.5650	 0.4480
EA	 0.5700	 0.4530
EB	 0.5990	 0.4490
EC	 0.5700	 0.4540
ED	 0.6160	 0.4430
EE	 0.6050	 0.4520
EF	 0.6100	 0.4520
EG	 0.6050	 0.4450
EH	 0.6100	 0.4400
EI	 0.6020	 0.4410
EJ	 0.5950	 0.4530
EK	 0.5650	 0.4550
FA	 0.5740	 0.4540
FB	 0.6000	 0.4490
FC	 0.5920	 0.4530
FD	 0.6160	 0.4480
FE	 0.6070	 0.4500
FF	 0.6070	 0.4630
FG	 0.6240	 0.4510
FH	 0.6070	 0.4440
FI	 0.6050	 0.4380
FJ	 0.5930	 0.4510
FK	 0.5630	 0.4460
GA	 0.5730	 0.4500
GB	 0.5940	 0.4460
GC	 0.5660	 0.4510
GD	 0.6100	 0.4410
GE	 0.6140	 0.4480
GF	 0.6110	 0.4580
GG	 0.6190	 0.4530
GH	 0.6050	 0.4460
GI	 0.6120	 0.4400
GJ	 0.5830	 0.4510

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Chain	Atom inclusion	Q-score
GK	 0.5650	 0.4500
HA	 0.5690	 0.4490
HB	 0.5980	 0.4480
HC	 0.5810	 0.4540
HD	 0.6190	 0.4480
HE	 0.6090	 0.4520
HF	 0.6040	 0.4630
HG	 0.6190	 0.4550
HH	 0.6120	 0.4400
HI	 0.5950	 0.4390
HJ	 0.5950	 0.4530
HK	 0.5680	 0.4490
IA	 0.5710	 0.4520
IB	 0.5930	 0.4490
IC	 0.5850	 0.4540
ID	 0.6140	 0.4450
IE	 0.6150	 0.4520
IF	 0.6150	 0.4500
IG	 0.6150	 0.4470
IH	 0.6070	 0.4360
II	 0.6050	 0.4380
IJ	 0.5810	 0.4490
IK	 0.5600	 0.4500
JA	 0.5700	 0.4460
JB	 0.5940	 0.4500
JC	 0.5740	 0.4540
JD	 0.6100	 0.4430
JE	 0.6050	 0.4470
JF	 0.6100	 0.4580
JG	 0.6160	 0.4530
JH	 0.6060	 0.4450
JI	 0.5990	 0.4440
JJ	 0.5940	 0.4520
JK	 0.5750	 0.4440
KA	 0.5730	 0.4570
KB	 0.5970	 0.4520
KC	 0.5830	 0.4580
KD	 0.6150	 0.4430
KE	 0.6020	 0.4520
KF	 0.6120	 0.4560
KG	 0.6210	 0.4490
KH	 0.6060	 0.4470

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Chain	Atom inclusion	Q-score
KI	 0.6060	 0.4440
KJ	 0.5940	 0.4510
KK	 0.5680	 0.4440
LA	 0.5740	 0.4470
LB	 0.5930	 0.4480
LC	 0.5930	 0.4530
LD	 0.6100	 0.4460
LE	 0.6010	 0.4530
LF	 0.5990	 0.4600
LG	 0.6230	 0.4450
LH	 0.6090	 0.4380
LI	 0.6050	 0.4400
LJ	 0.5880	 0.4480
LK	 0.5680	 0.4440
MA	 0.5750	 0.4520
MB	 0.5920	 0.4480
MC	 0.5850	 0.4570
MD	 0.6160	 0.4450
ME	 0.6050	 0.4500
MF	 0.6070	 0.4560
MG	 0.6210	 0.4500
MH	 0.6040	 0.4440
MI	 0.5940	 0.4410
MJ	 0.5970	 0.4530
MK	 0.5630	 0.4410
NA	 0.5760	 0.4510
NB	 0.6000	 0.4520
NC	 0.5810	 0.4560
ND	 0.6150	 0.4470
NE	 0.6060	 0.4500
NF	 0.6060	 0.4550
NG	 0.6160	 0.4480
NH	 0.6060	 0.4380
NI	 0.6060	 0.4410
NJ	 0.5970	 0.4530
NK	 0.5630	 0.4530
OA	 0.5680	 0.4530
OB	 0.5970	 0.4500
OC	 0.5800	 0.4540
OD	 0.6090	 0.4410
OE	 0.6050	 0.4530
OF	 0.6100	 0.4570

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Chain	Atom inclusion	Q-score
OG	 0.6260	 0.4460
OH	 0.6070	 0.4400
OI	 0.5980	 0.4410
OJ	 0.5980	 0.4520
OK	 0.5650	 0.4530
PA	 0.5770	 0.4490
PB	 0.5990	 0.4490
PC	 0.5930	 0.4480
PD	 0.6120	 0.4410
PE	 0.6050	 0.4490
PF	 0.6150	 0.4580
PG	 0.6170	 0.4560
PH	 0.6050	 0.4440
PI	 0.6060	 0.4400
PJ	 0.5850	 0.4510
PK	 0.5680	 0.4450
QA	 0.5700	 0.4480
QB	 0.5920	 0.4500
QC	 0.5680	 0.4510
QD	 0.6210	 0.4460
QE	 0.6140	 0.4550
QF	 0.6060	 0.4600
QG	 0.6290	 0.4480
QH	 0.6100	 0.4460
QI	 0.5970	 0.4440
QJ	 0.5990	 0.4540
QK	 0.5580	 0.4530
RA	 0.5810	 0.4510
RB	 0.5980	 0.4470
RC	 0.5810	 0.4530
RD	 0.6120	 0.4400
RE	 0.6060	 0.4530
RF	 0.6010	 0.4580
RG	 0.6280	 0.4440
RH	 0.6060	 0.4390
RI	 0.6110	 0.4330
RJ	 0.5800	 0.4450
RK	 0.5650	 0.4440
SA	 0.5750	 0.4500
SB	 0.5940	 0.4450
SC	 0.5770	 0.4530
SD	 0.6060	 0.4370

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Chain	Atom inclusion	Q-score
SE	 0.6020	 0.4460
SF	 0.6070	 0.4540
SG	 0.6260	 0.4510
SH	 0.6040	 0.4420
SI	 0.5920	 0.4410
SJ	 0.5750	 0.4500
SK	 0.5800	 0.4470
TA	 0.5780	 0.4460
TB	 0.5980	 0.4480
TC	 0.5770	 0.4540
TD	 0.6160	 0.4450
TE	 0.6090	 0.4530
TF	 0.6110	 0.4570
TG	 0.6210	 0.4460
TH	 0.6060	 0.4430
TI	 0.6070	 0.4390
TJ	 0.6000	 0.4490
TK	 0.5730	 0.4470
UA	 0.5800	 0.4500
UB	 0.5940	 0.4500
UC	 0.5770	 0.4530
UD	 0.5970	 0.4460
UE	 0.6090	 0.4540
UF	 0.6160	 0.4530
UG	 0.6180	 0.4450
UH	 0.5920	 0.4380
UI	 0.6040	 0.4390
UJ	 0.5920	 0.4470
UK	 0.5700	 0.4470
VA	 0.5800	 0.4520
VB	 0.5990	 0.4500
VC	 0.5870	 0.4540
VD	 0.6040	 0.4400
VE	 0.6090	 0.4520
VF	 0.6180	 0.4580
VG	 0.6260	 0.4470
VH	 0.6110	 0.4400
VI	 0.6090	 0.4320
VJ	 0.5800	 0.4480
VK	 0.5630	 0.4450
WA	 0.5700	 0.4520
WB	 0.5920	 0.4490

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Chain	Atom inclusion	Q-score
WC	 0.5820	 0.4540
WD	 0.6110	 0.4460
WE	 0.6060	 0.4510
WF	 0.6040	 0.4540
WG	 0.6160	 0.4460
WH	 0.6060	 0.4390
WI	 0.5950	 0.4390
WJ	 0.5950	 0.4490
WK	 0.5630	 0.4460
XA	 0.5750	 0.4530
XB	 0.5920	 0.4520
XC	 0.5850	 0.4490
XD	 0.5990	 0.4420
XE	 0.5970	 0.4490
XF	 0.6010	 0.4560
XG	 0.6180	 0.4460
XH	 0.5990	 0.4390
XI	 0.6110	 0.4400
XJ	 0.5850	 0.4480
XK	 0.5580	 0.4450