



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:26 AM UTC

PDB ID : 6RVV / pdb_00006rvv
EMDB ID : EMD-4443
Title : Structure of left-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:

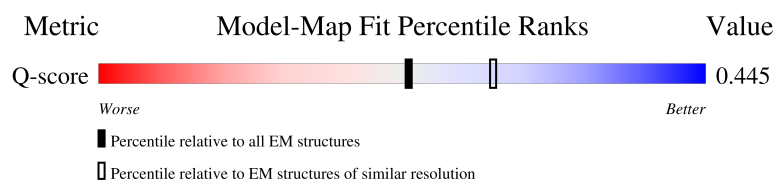
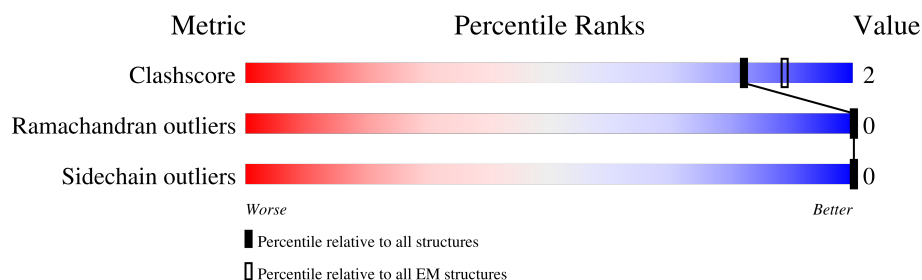
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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.



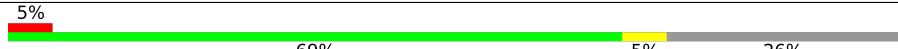
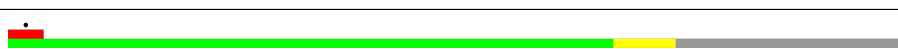
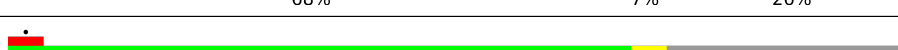
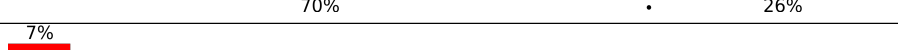
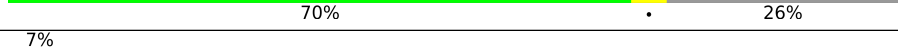
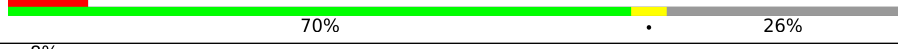
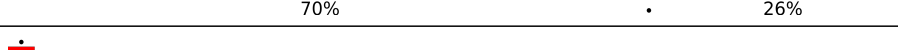
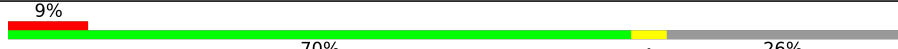
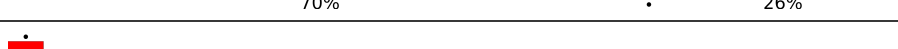
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	9% 69% 5% 26%
1	AB	74	9% 66% 8% 26%
1	AC	74	9% 69% 5% 26%
1	AD	74	• 64% 11% 26%

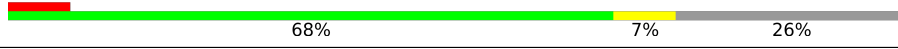
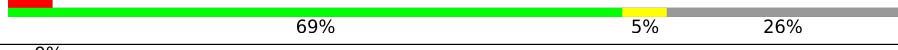
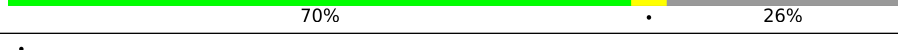
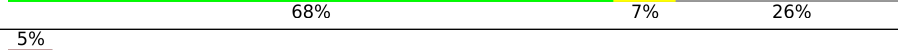
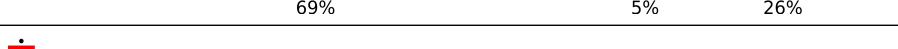
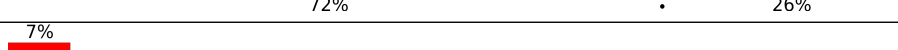
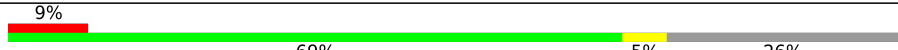
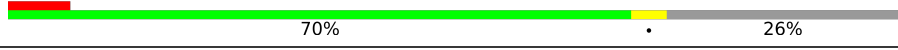
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Mol	Chain	Length	Quality of chain
1	AE	74	
1	AF	74	
1	AG	74	
1	AH	74	
1	AI	74	
1	AJ	74	
1	AK	74	
1	BA	74	
1	BB	74	
1	BC	74	
1	BD	74	
1	BE	74	
1	BF	74	
1	BG	74	
1	BH	74	
1	BI	74	
1	BJ	74	
1	BK	74	
1	CA	74	
1	CB	74	
1	CC	74	
1	CD	74	
1	CE	74	
1	CF	74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

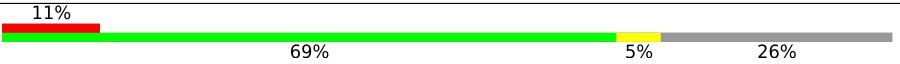
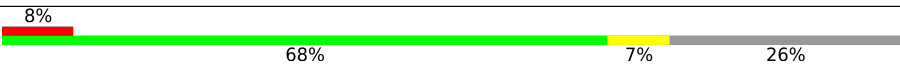
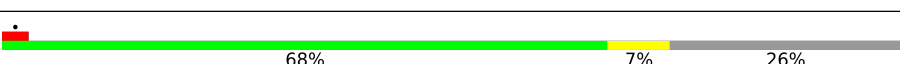
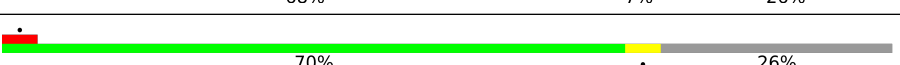
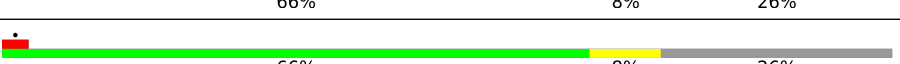
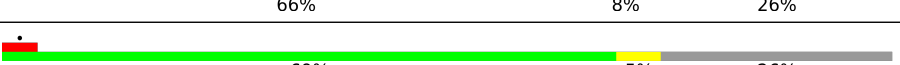
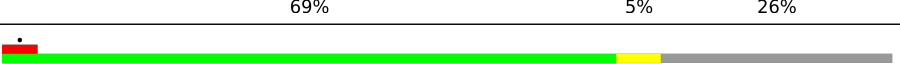
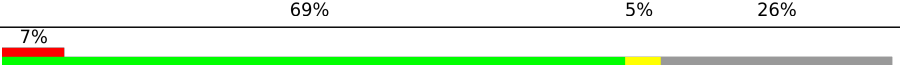
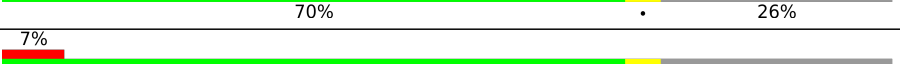
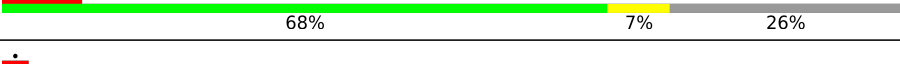
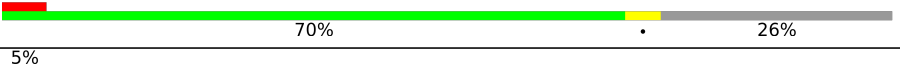
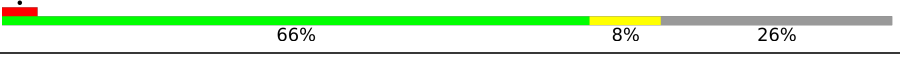
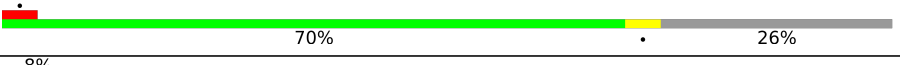
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Mol	Chain	Length	Quality of chain
1	JF	74	
1	JG	74	
1	JH	74	
1	JI	74	
1	JJ	74	
1	JK	74	
1	KA	74	
1	KB	74	
1	KC	74	
1	KD	74	
1	KE	74	
1	KF	74	
1	KG	74	
1	KH	74	
1	KI	74	
1	KJ	74	
1	KK	74	
1	LA	74	
1	LB	74	
1	LC	74	
1	LD	74	
1	LE	74	
1	LF	74	
1	LG	74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

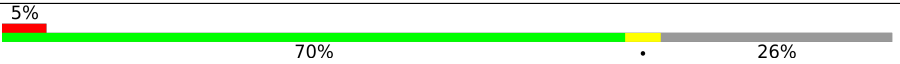
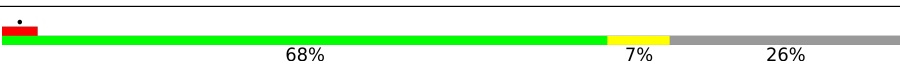
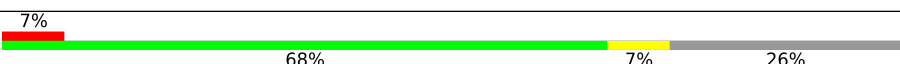
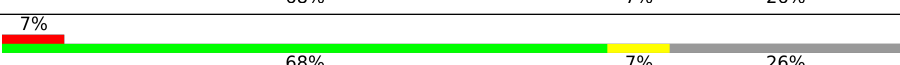
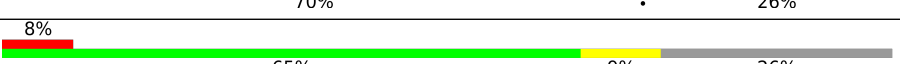
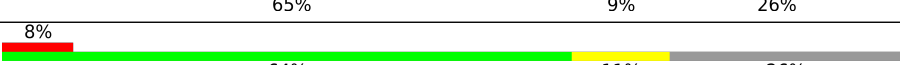
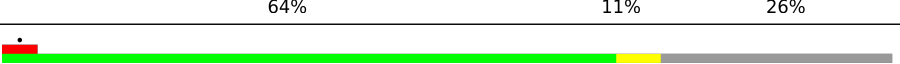
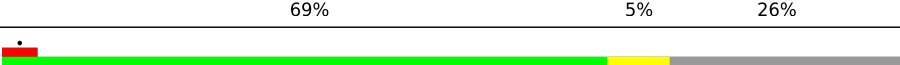
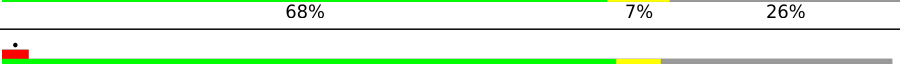
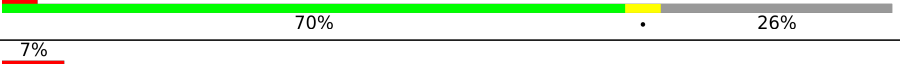
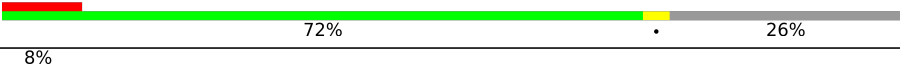
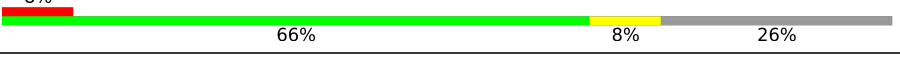
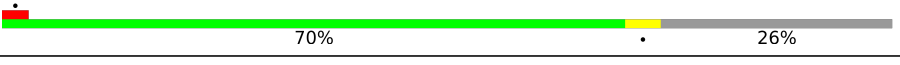
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Mol	Chain	Length	Quality of chain
1	OA	74	
1	OB	74	
1	OC	74	
1	OD	74	
1	OE	74	
1	OF	74	
1	OG	74	
1	OH	74	
1	OI	74	
1	OJ	74	
1	OK	74	
1	PA	74	
1	PB	74	
1	PC	74	
1	PD	74	
1	PE	74	
1	PF	74	
1	PG	74	
1	PH	74	
1	PI	74	
1	PJ	74	
1	PK	74	
1	QA	74	
1	QB	74	
1	QC	74	

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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 [i](#)

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	FC	1	Total 1	Au 1	0
2	FD	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

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Mol	Chain	Residues	Atoms		AltConf
2	FI	1	Total 1	Au 1	0
2	FJ	1	Total 1	Au 1	0
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

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Mol	Chain	Residues	Atoms		AltConf
2	IH	1	Total 1	Au 1	0
2	II	1	Total 1	Au 1	0
2	IJ	1	Total 1	Au 1	0
2	JA	1	Total 1	Au 1	0
2	JB	1	Total 1	Au 1	0
2	JG	1	Total 1	Au 1	0
2	JH	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	LE	1	Total 1	Au 1	0
2	LF	1	Total 1	Au 1	0
2	LG	1	Total 1	Au 1	0
2	LH	1	Total 1	Au 1	0
2	LI	1	Total 1	Au 1	0
2	LJ	1	Total 1	Au 1	0
2	MA	1	Total 1	Au 1	0
2	MB	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	NE	1	Total 1	Au 1	0
2	NF	1	Total 1	Au 1	0
2	OA	1	Total 1	Au 1	0
2	OB	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	PA	1	Total 1	Au 1	0
2	PB	1	Total 1	Au 1	0
2	PC	1	Total 1	Au 1	0
2	PD	1	Total 1	Au 1	0
2	QG	1	Total 1	Au 1	0
2	QH	1	Total 1	Au 1	0
2	RC	1	Total 1	Au 1	0
2	RD	1	Total 1	Au 1	0
2	RE	1	Total 1	Au 1	0
2	RF	1	Total 1	Au 1	0
2	SE	1	Total 1	Au 1	0
2	SF	1	Total 1	Au 1	0
2	TE	1	Total 1	Au 1	0

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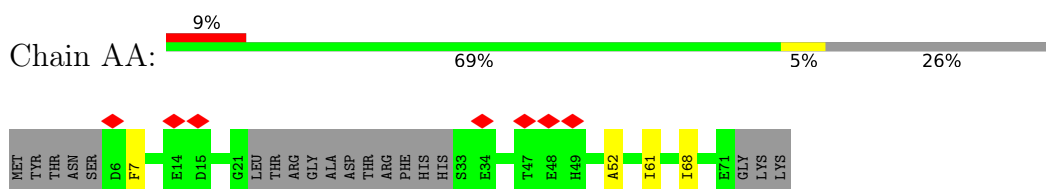
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Mol	Chain	Residues	Atoms		AltConf
2	TF	1	Total 1	Au 1	0
2	TI	1	Total 1	Au 1	0
2	TJ	1	Total 1	Au 1	0
2	WA	1	Total 1	Au 1	0
2	WB	1	Total 1	Au 1	0

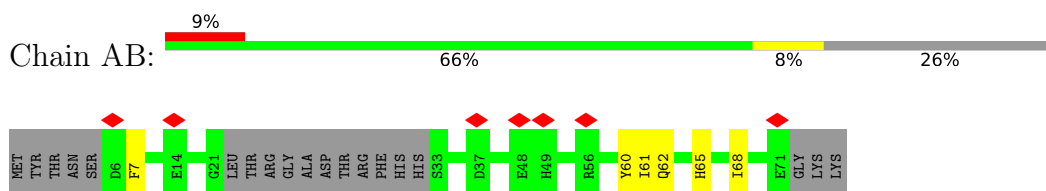
3 Residue-property plots [i](#)

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.

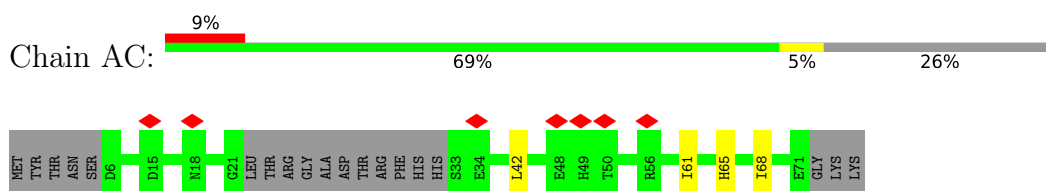
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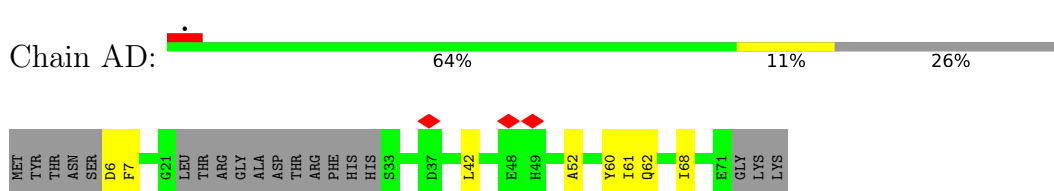
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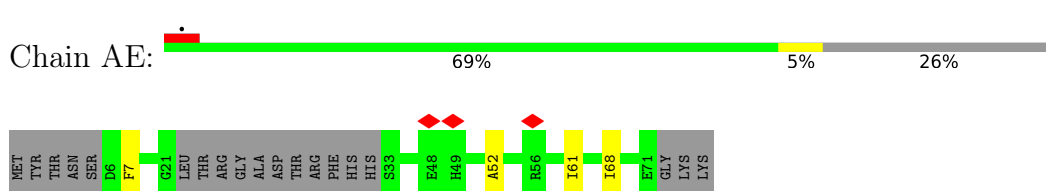
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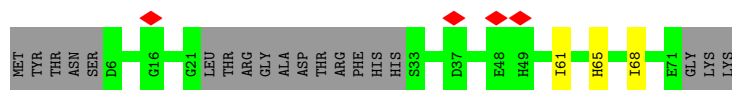
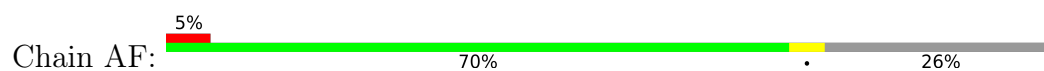
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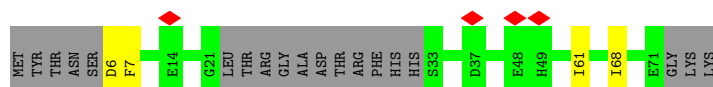
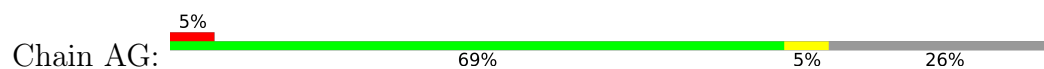
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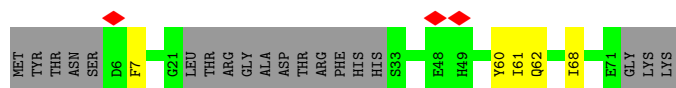
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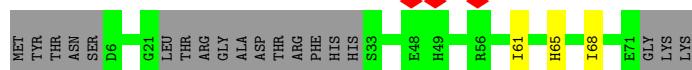
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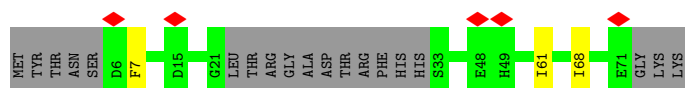
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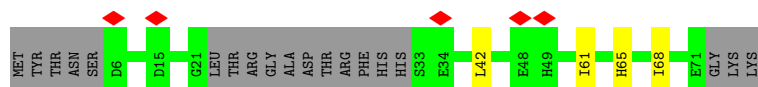
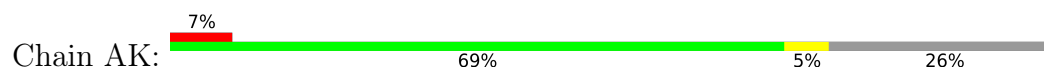
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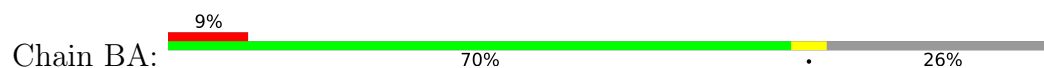
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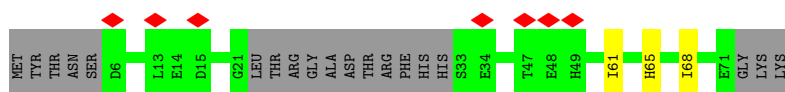


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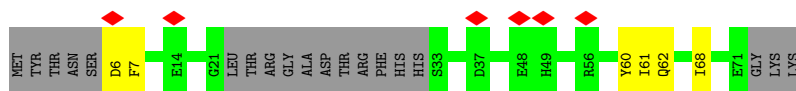


● Molecule 1: Transcription attenuation protein MtrB

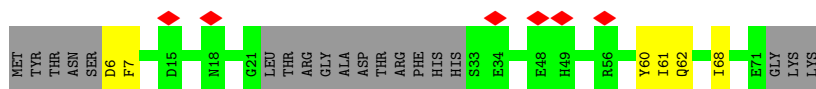




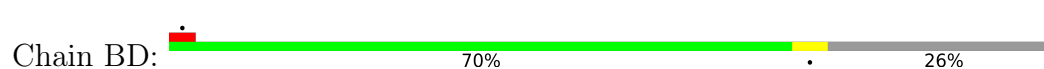
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



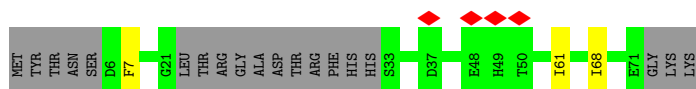
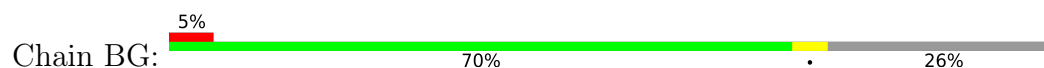
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

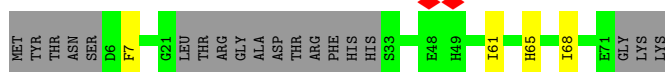


- Molecule 1: Transcription attenuation protein MtrB



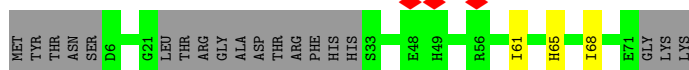
- Molecule 1: Transcription attenuation protein MtrB

Chain BH:  69% 5% 26%



- Molecule 1: Transcription attenuation protein MtrB

Chain BI:  70% 0% 26%



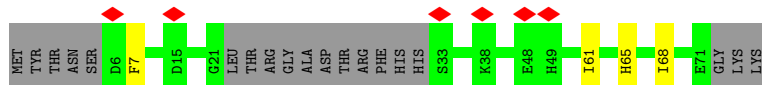
- Molecule 1: Transcription attenuation protein MtrB

Chain BJ:  7% 69% 5% 26%



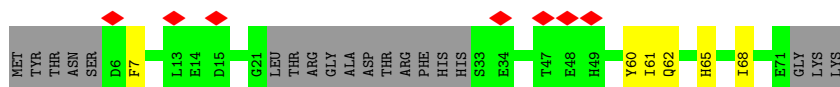
- Molecule 1: Transcription attenuation protein MtrB

Chain BK:  8% 69% 5% 26%



- Molecule 1: Transcription attenuation protein MtrB

Chain CA:  9% 66% 8% 26%



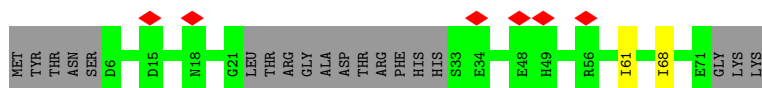
- Molecule 1: Transcription attenuation protein MtrB

Chain CB:  9% 70% 0% 26%



- Molecule 1: Transcription attenuation protein MtrB

Chain CC:  8% 72% 0% 26%



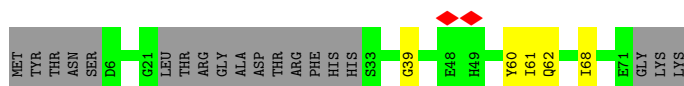
● Molecule 1: Transcription attenuation protein MtrB

Chain CD:  70% 26%

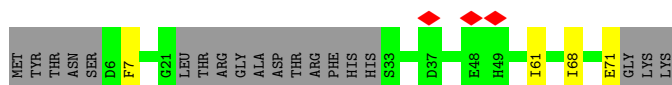
● Molecule 1: Transcription attenuation protein MtrB

Chain CE:  70% 26%

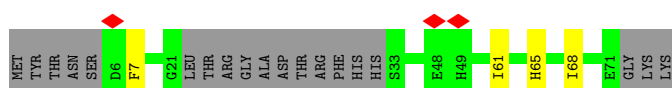
● Molecule 1: Transcription attenuation protein MtrB

Chain CF:  68% 7% 26%

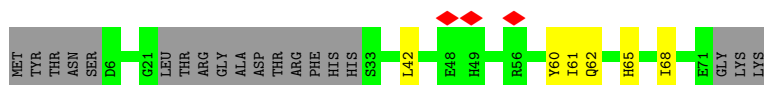
● Molecule 1: Transcription attenuation protein MtrB

Chain CG:  69% 5% 26%

● Molecule 1: Transcription attenuation protein MtrB

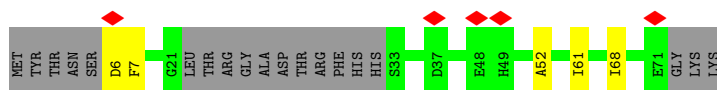
Chain CH:  69% 5% 26%

● Molecule 1: Transcription attenuation protein MtrB

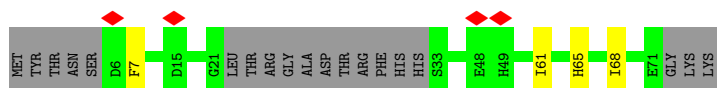
Chain CI:  66% 8% 26%

● Molecule 1: Transcription attenuation protein MtrB

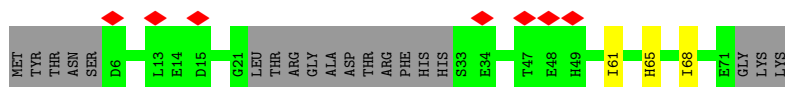
Chain CJ:  7% 68% 7% 26%



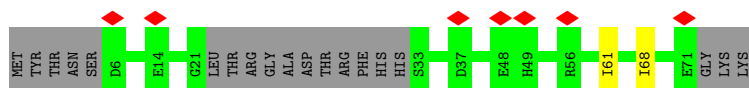
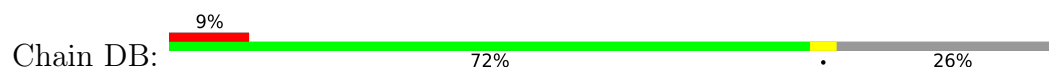
- Molecule 1: Transcription attenuation protein MtrB



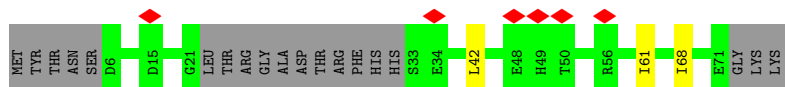
- Molecule 1: Transcription attenuation protein MtrB



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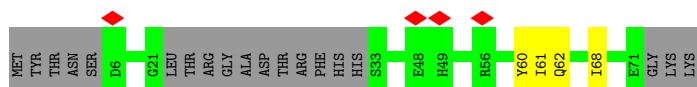
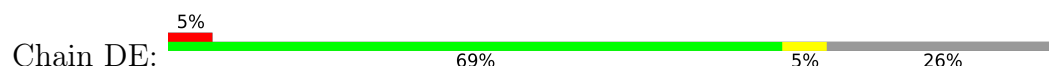
- Molecule 1: Transcription attenuation protein MtrB



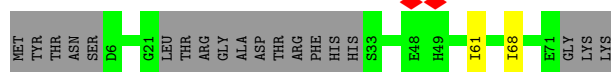
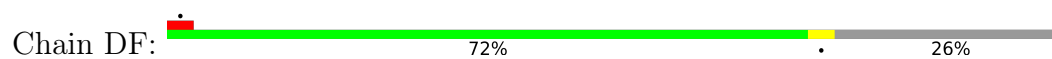
- Molecule 1: Transcription attenuation protein MtrB



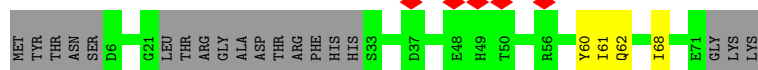
- Molecule 1: Transcription attenuation protein MtrB



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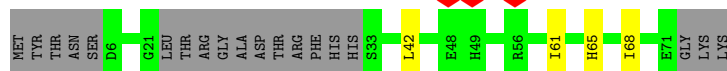
- Molecule 1: Transcription attenuation protein MtrB



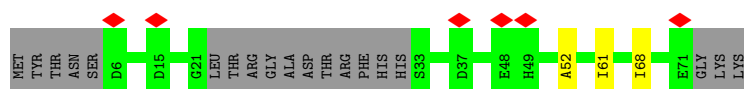
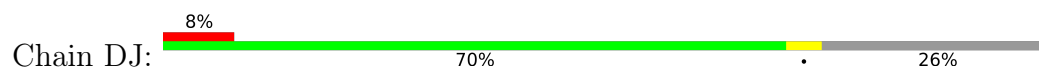
- Molecule 1: Transcription attenuation protein MtrB



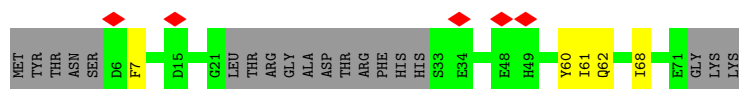
- Molecule 1: Transcription attenuation protein MtrB



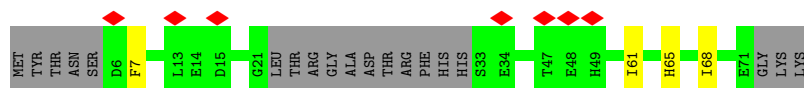
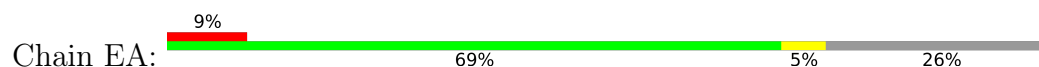
- Molecule 1: Transcription attenuation protein MtrB



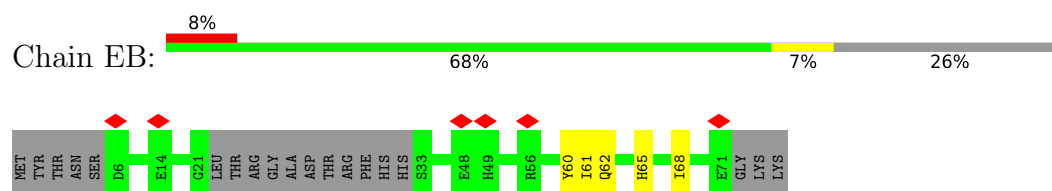
- Molecule 1: Transcription attenuation protein MtrB



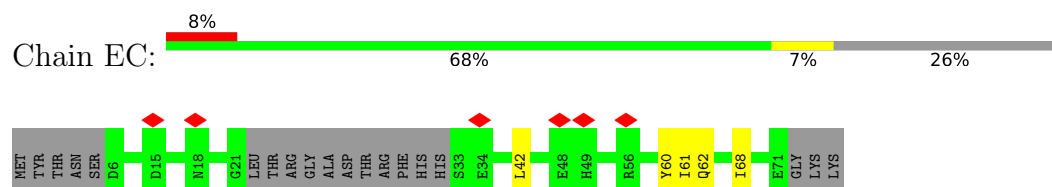
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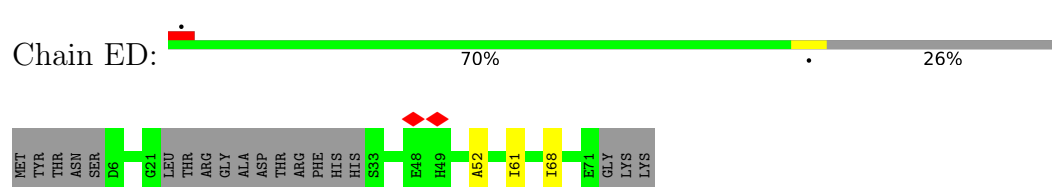
● Molecule 1: Transcription attenuation protein MtrB



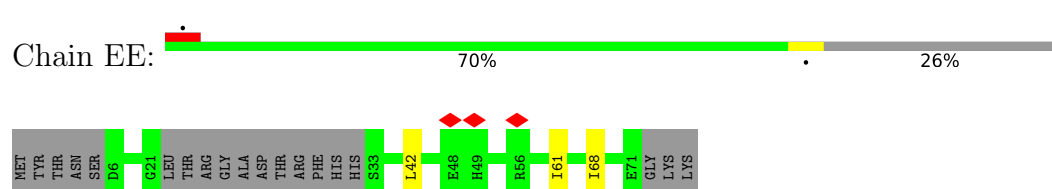
● Molecule 1: Transcription attenuation protein MtrB



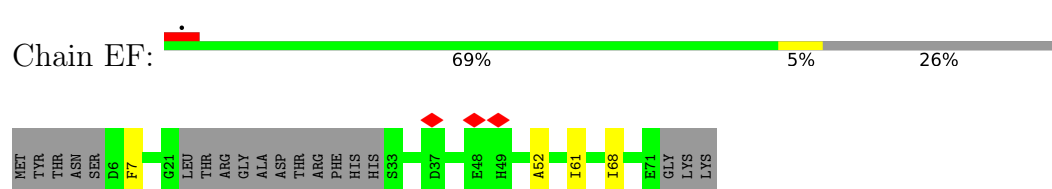
● Molecule 1: Transcription attenuation protein MtrB



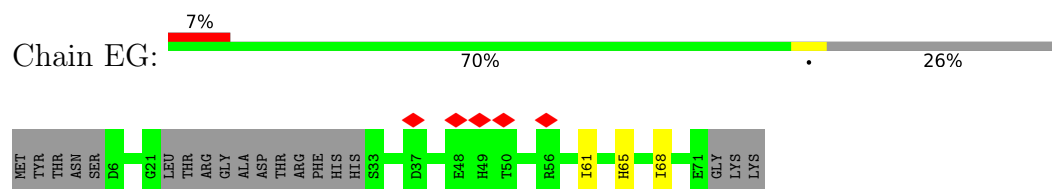
● Molecule 1: Transcription attenuation protein MtrB



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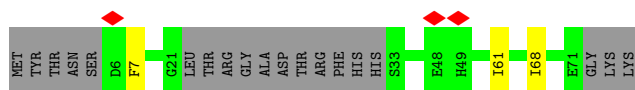


● Molecule 1: Transcription attenuation protein MtrB



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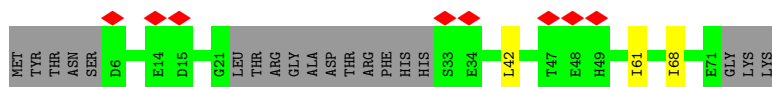
- Molecule 1: Transcription attenuation protein MtrB



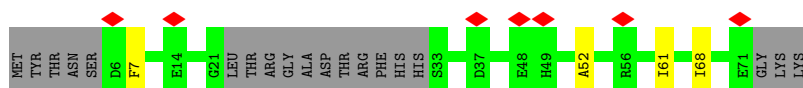
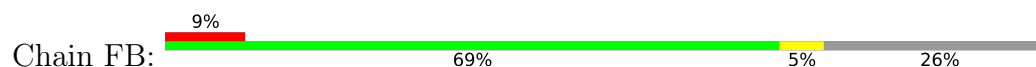
- Molecule 1: Transcription attenuation protein MtrB



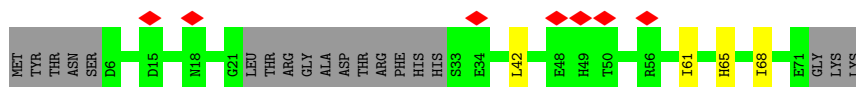
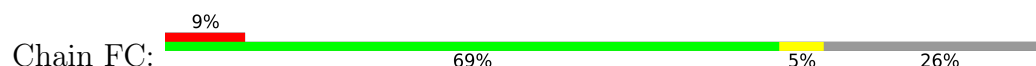
- Molecule 1: Transcription attenuation protein MtrB



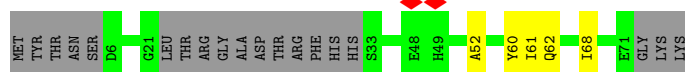
- Molecule 1: Transcription attenuation protein MtrB



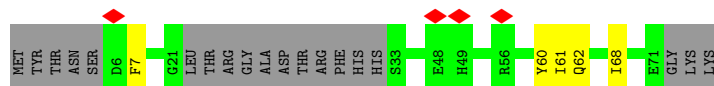
- Molecule 1: Transcription attenuation protein MtrB



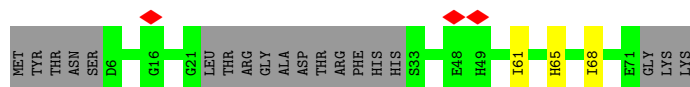
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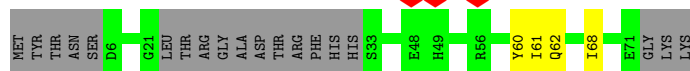
- Molecule 1: Transcription attenuation protein MtrB



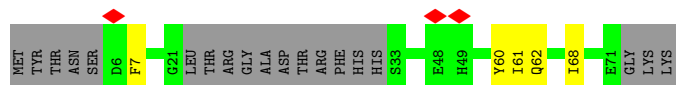
- Molecule 1: Transcription attenuation protein MtrB



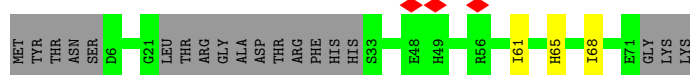
- Molecule 1: Transcription attenuation protein MtrB



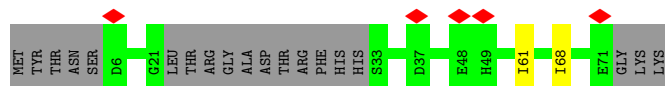
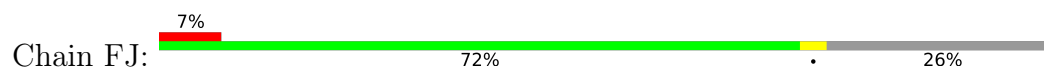
- Molecule 1: Transcription attenuation protein MtrB



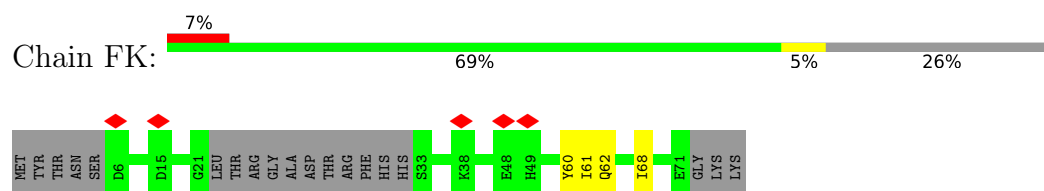
- Molecule 1: Transcription attenuation protein MtrB



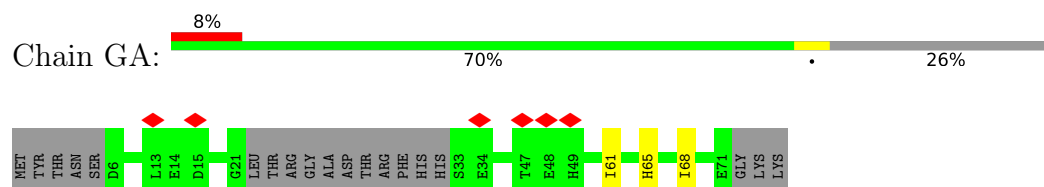
- Molecule 1: Transcription attenuation protein MtrB



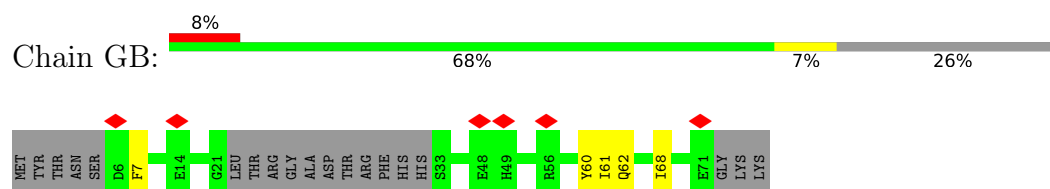
• Molecule 1: Transcription attenuation protein MtrB



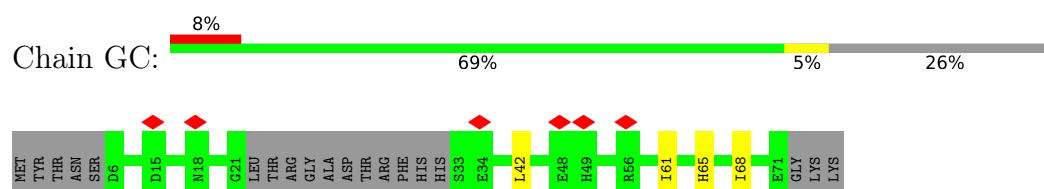
• Molecule 1: Transcription attenuation protein MtrB



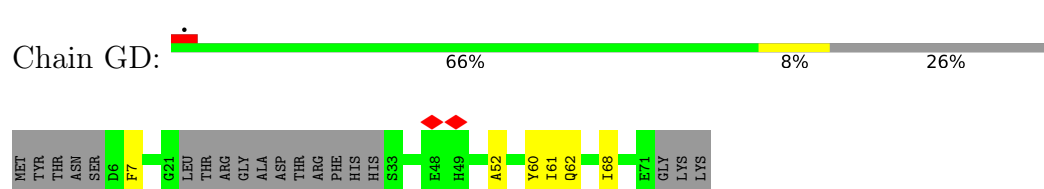
• Molecule 1: Transcription attenuation protein MtrB



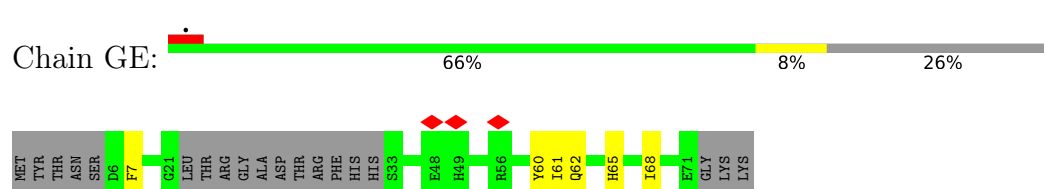
• Molecule 1: Transcription attenuation protein MtrB



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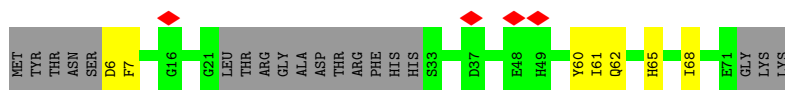


• Molecule 1: Transcription attenuation protein MtrB



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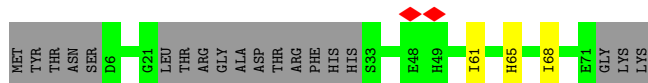




- Molecule 1: Transcription attenuation protein MtrB



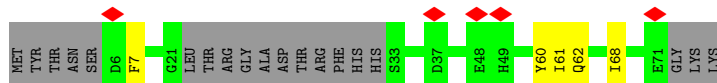
- Molecule 1: Transcription attenuation protein MtrB



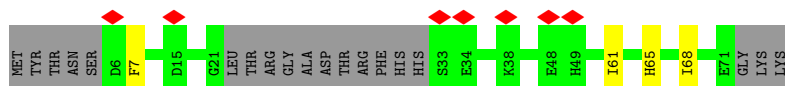
- Molecule 1: Transcription attenuation protein MtrB



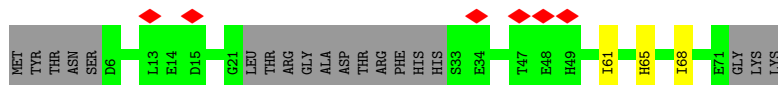
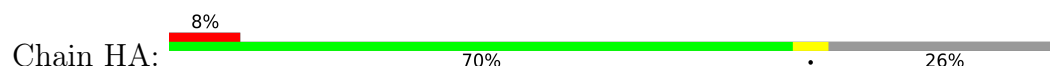
- Molecule 1: Transcription attenuation protein MtrB



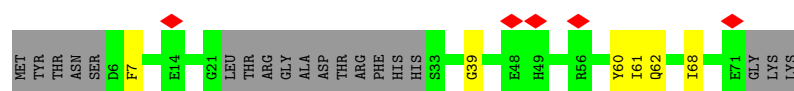
- Molecule 1: Transcription attenuation protein MtrB



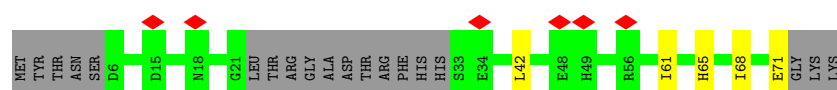
- Molecule 1: Transcription attenuation protein MtrB



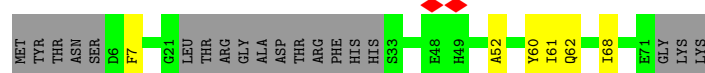
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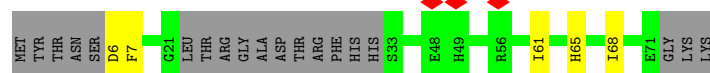
- Molecule 1: Transcription attenuation protein MtrB



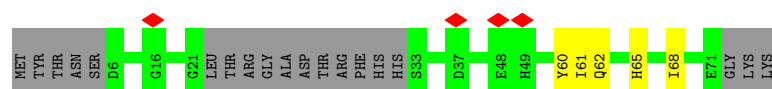
- Molecule 1: Transcription attenuation protein MtrB



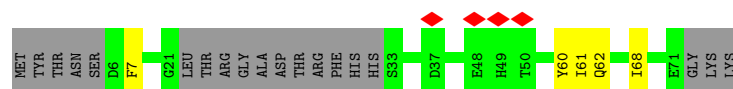
- Molecule 1: Transcription attenuation protein MtrB



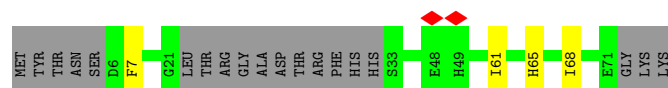
- Molecule 1: Transcription attenuation protein MtrB



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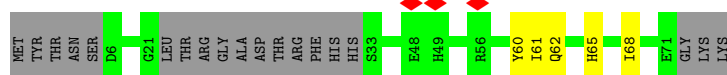


- Molecule 1: Transcription attenuation protein MtrB



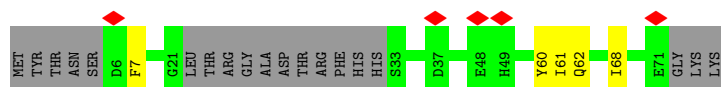
• Molecule 1: Transcription attenuation protein MtrB

Chain HI:  68% 7% 26%



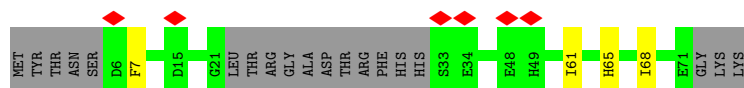
• Molecule 1: Transcription attenuation protein MtrB

Chain HJ:  68% 7% 26%



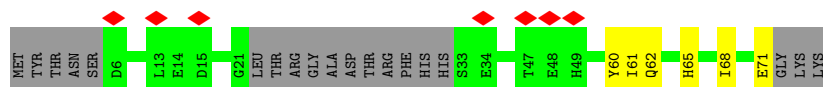
• Molecule 1: Transcription attenuation protein MtrB

Chain HK:  69% 8% 26%



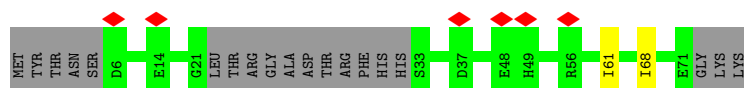
• Molecule 1: Transcription attenuation protein MtrB

Chain IA:  66% 9% 26%



• Molecule 1: Transcription attenuation protein MtrB

Chain IB:  72% 8% 26%



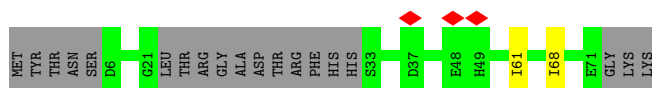
• Molecule 1: Transcription attenuation protein MtrB

Chain IC:  72% 8% 26%

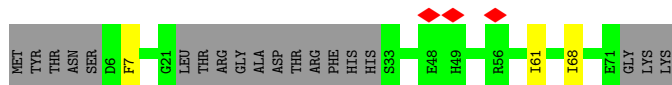


• Molecule 1: Transcription attenuation protein MtrB

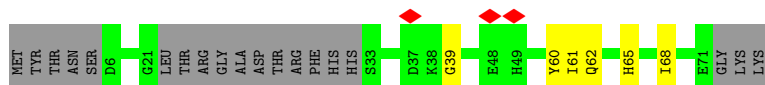
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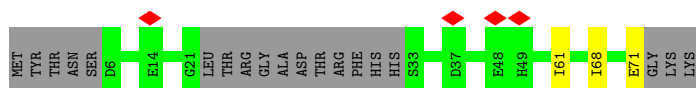
- Molecule 1: Transcription attenuation protein MtrB



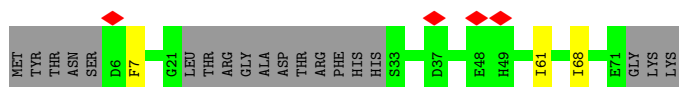
- Molecule 1: Transcription attenuation protein MtrB



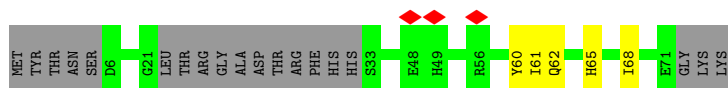
- Molecule 1: Transcription attenuation protein MtrB



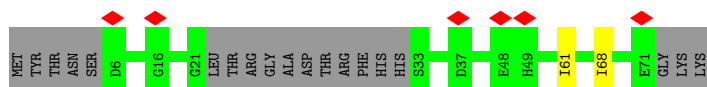
- Molecule 1: Transcription attenuation protein MtrB



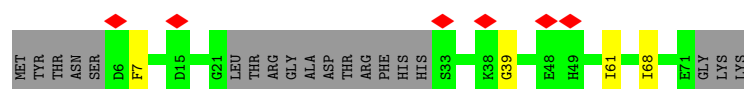
- Molecule 1: Transcription attenuation protein MtrB



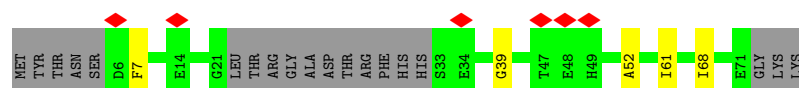
- Molecule 1: Transcription attenuation protein MtrB



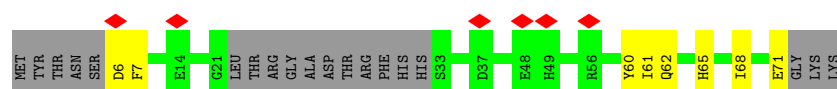
- Molecule 1: Transcription attenuation protein MtrB



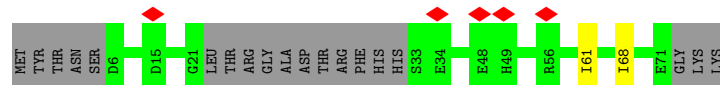
- Molecule 1: Transcription attenuation protein MtrB



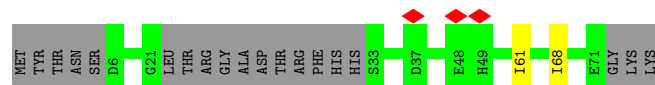
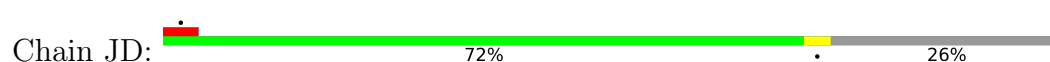
- Molecule 1: Transcription attenuation protein MtrB



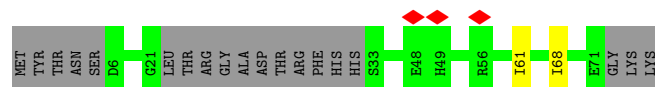
- Molecule 1: Transcription attenuation protein MtrB



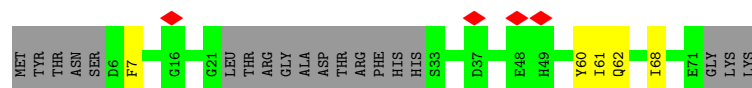
- Molecule 1: Transcription attenuation protein MtrB



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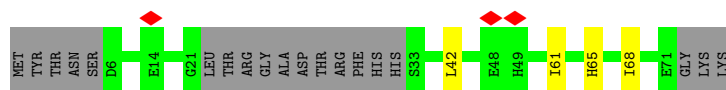


- Molecule 1: Transcription attenuation protein MtrB



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Chain JG:  69% 5% 26%



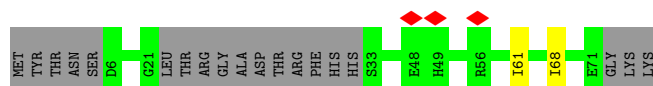
- Molecule 1: Transcription attenuation protein MtrB

Chain JH:  70% 0% 26%



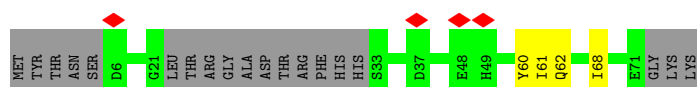
- Molecule 1: Transcription attenuation protein MtrB

Chain JI:  72% 0% 26%



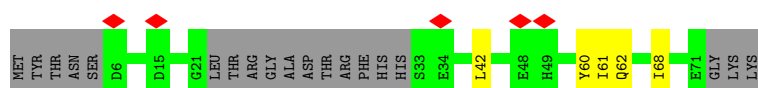
- Molecule 1: Transcription attenuation protein MtrB

Chain JJ:  5% 69% 5% 26%



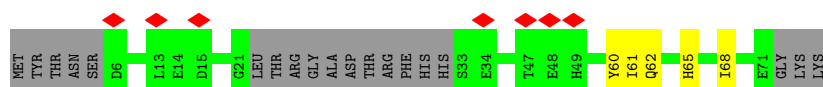
- Molecule 1: Transcription attenuation protein MtrB

Chain JK:  7% 68% 7% 26%



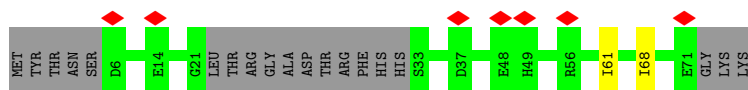
- Molecule 1: Transcription attenuation protein MtrB

Chain KA:  9% 68% 7% 26%

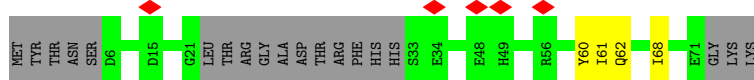


- Molecule 1: Transcription attenuation protein MtrB

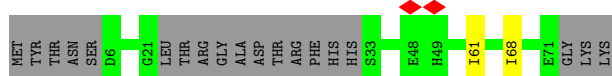
Chain KB:  9% 72% 0% 26%



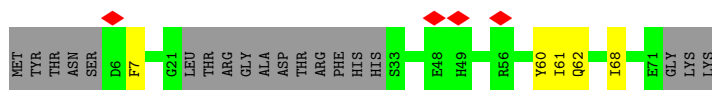
- Molecule 1: Transcription attenuation protein MtrB



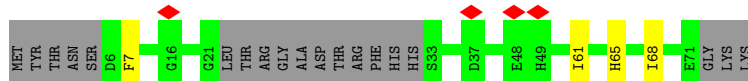
- Molecule 1: Transcription attenuation protein MtrB



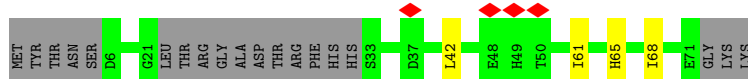
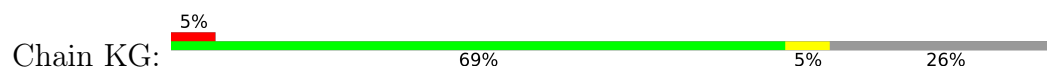
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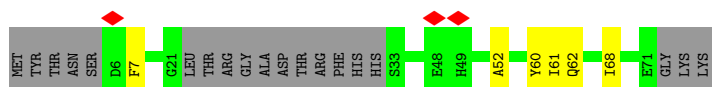
- Molecule 1: Transcription attenuation protein MtrB



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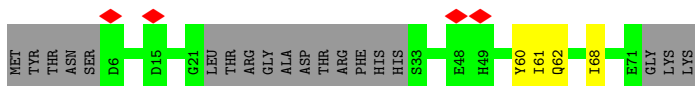
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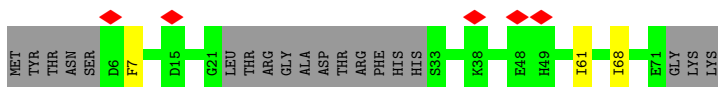
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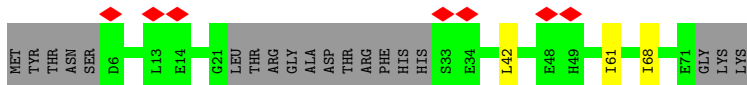
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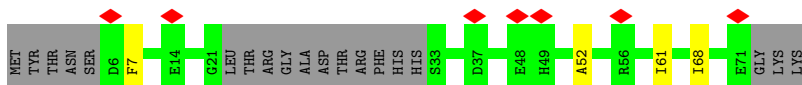
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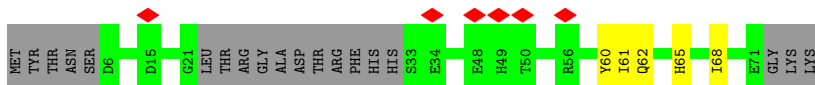
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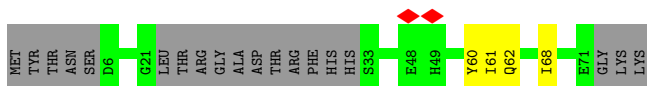
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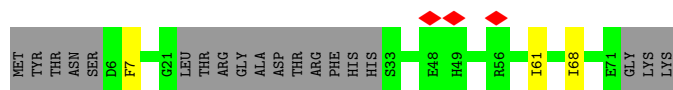


- Molecule 1: Transcription attenuation protein MtrB



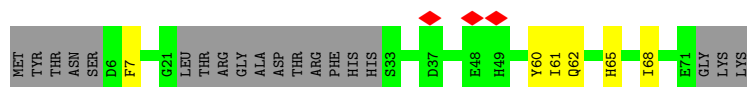
● Molecule 1: Transcription attenuation protein MtrB

Chain LE:  70% 26%



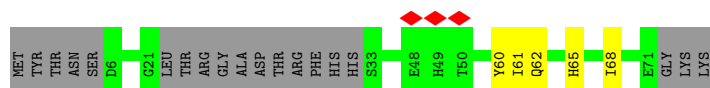
● Molecule 1: Transcription attenuation protein MtrB

Chain LF:  66% 8% 26%



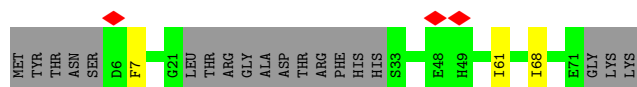
● Molecule 1: Transcription attenuation protein MtrB

Chain LG:  68% 7% 26%



● Molecule 1: Transcription attenuation protein MtrB

Chain LH:  70% 26%



● Molecule 1: Transcription attenuation protein MtrB

Chain LI:  70% 26%



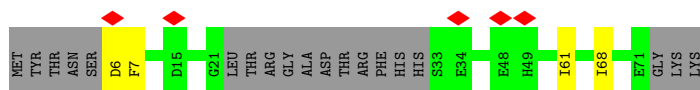
● Molecule 1: Transcription attenuation protein MtrB

Chain LJ:  7% 72% 26%

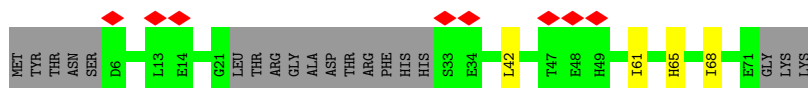
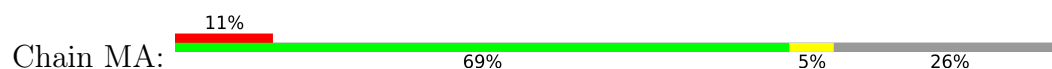


● Molecule 1: Transcription attenuation protein MtrB

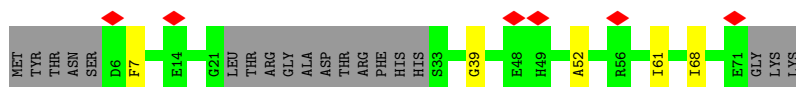
Chain LK:  7% 69% 5% 26%



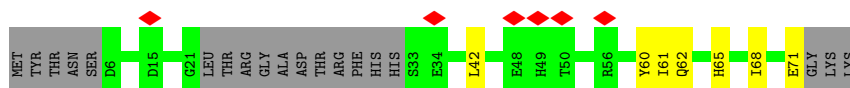
- Molecule 1: Transcription attenuation protein MtrB



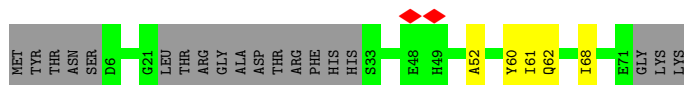
- Molecule 1: Transcription attenuation protein MtrB



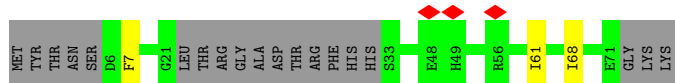
- Molecule 1: Transcription attenuation protein MtrB



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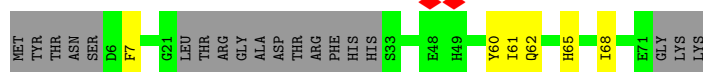
- Molecule 1: Transcription attenuation protein MtrB



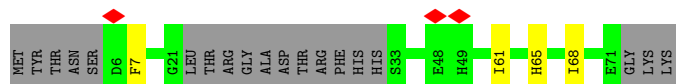
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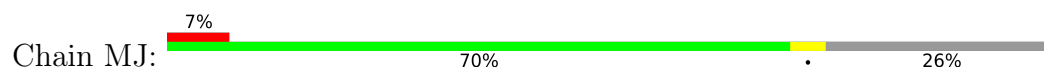
- Molecule 1: Transcription attenuation protein MtrB



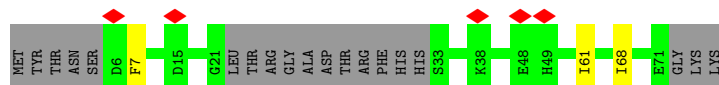
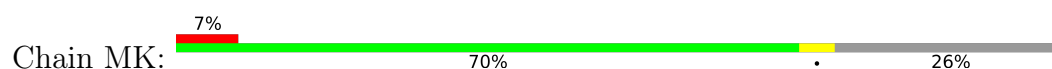
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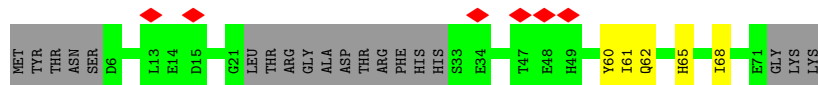
- Molecule 1: Transcription attenuation protein MtrB



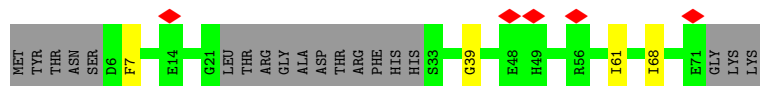
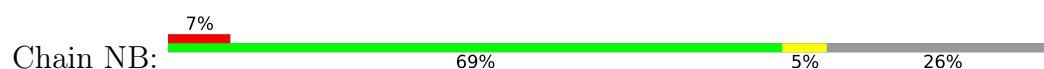
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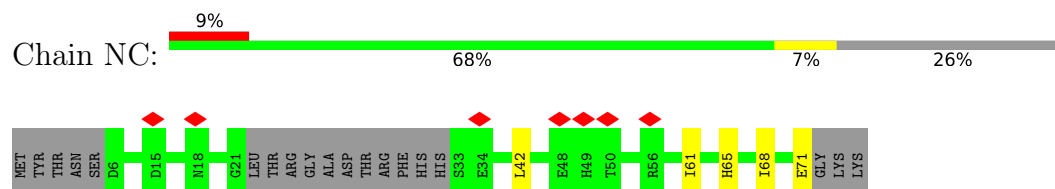
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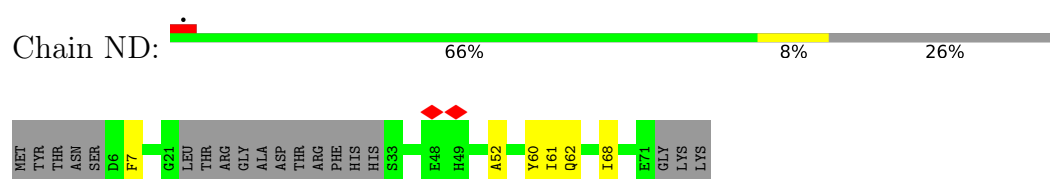
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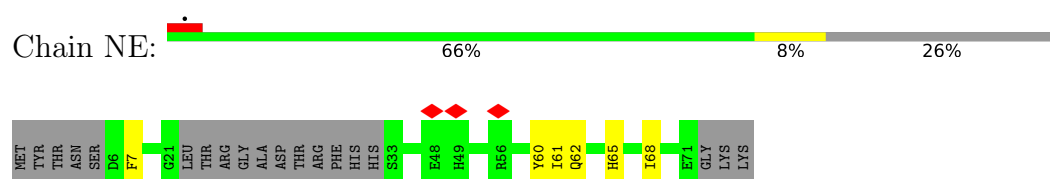
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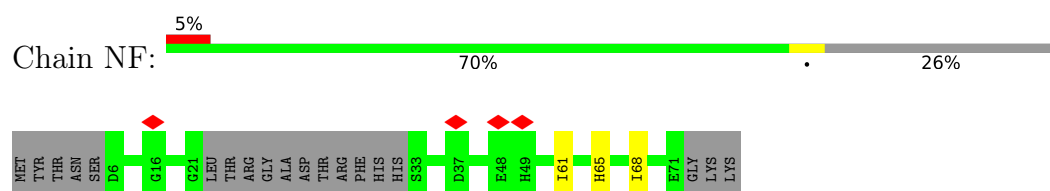
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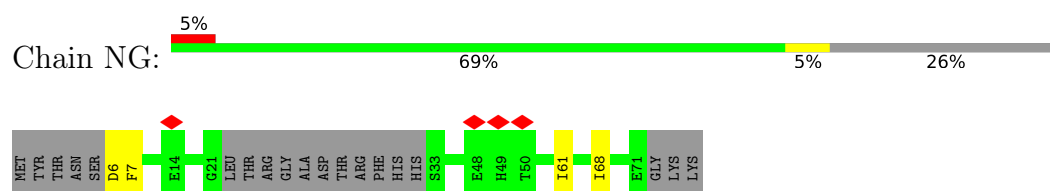
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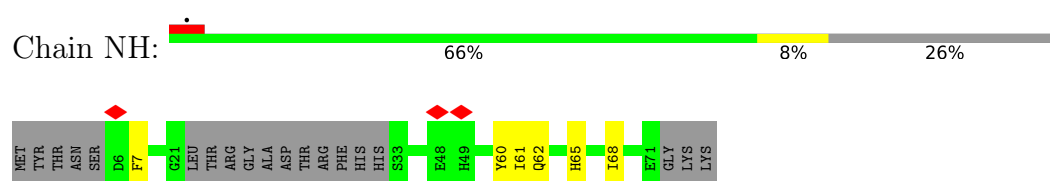
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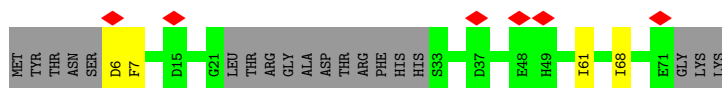


- Molecule 1: Transcription attenuation protein MtrB

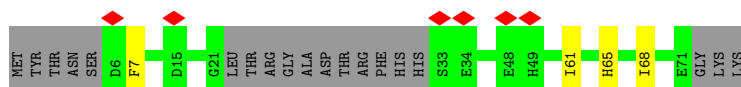




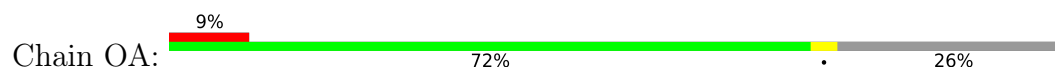
- Molecule 1: Transcription attenuation protein MtrB



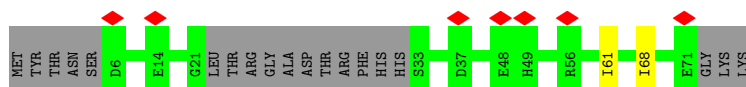
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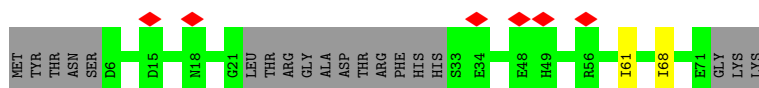
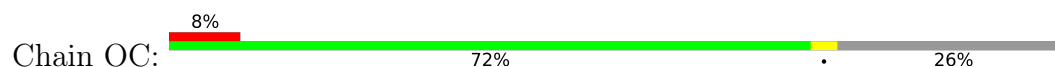
- Molecule 1: Transcription attenuation protein MtrB



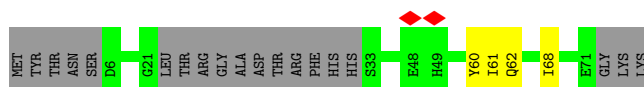
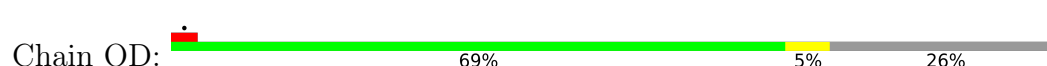
- Molecule 1: Transcription attenuation protein MtrB



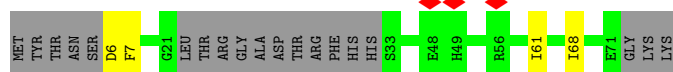
- Molecule 1: Transcription attenuation protein MtrB



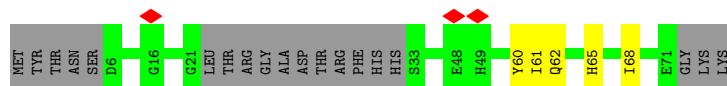
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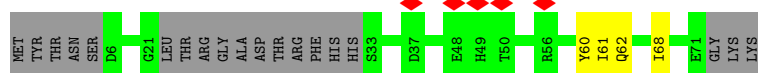
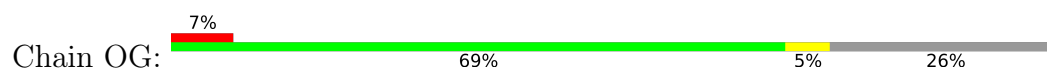
- Molecule 1: Transcription attenuation protein MtrB



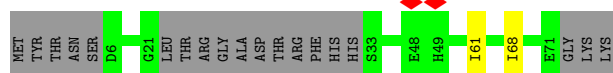
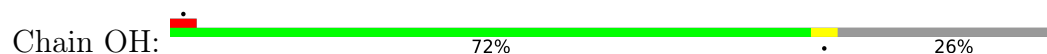
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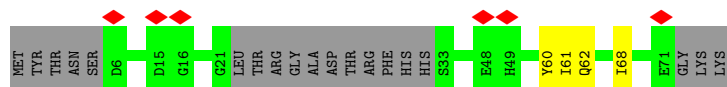
- Molecule 1: Transcription attenuation protein MtrB



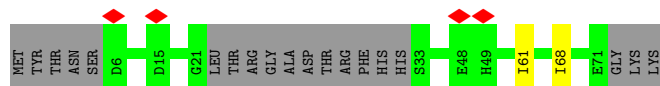
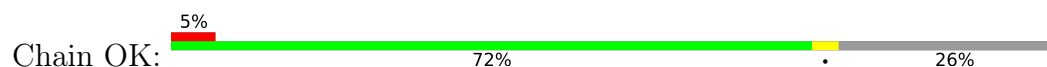
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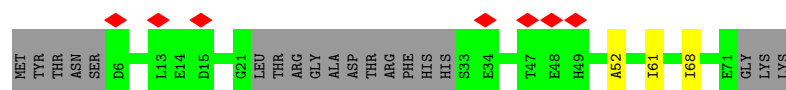
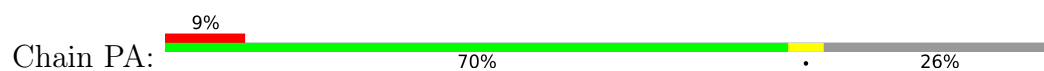
- Molecule 1: Transcription attenuation protein MtrB



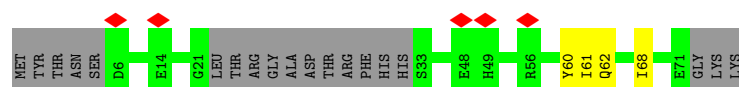
- Molecule 1: Transcription attenuation protein MtrB



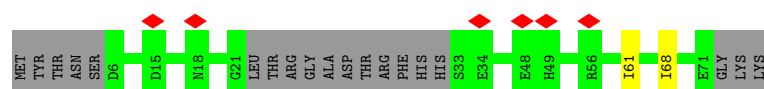
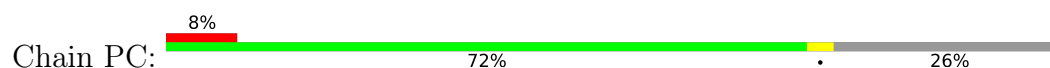
● Molecule 1: Transcription attenuation protein MtrB



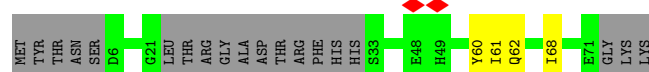
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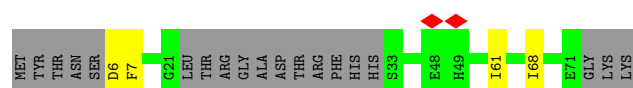
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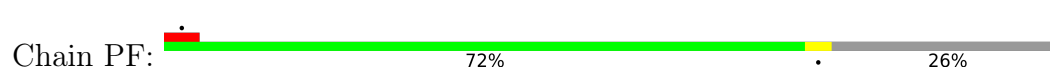
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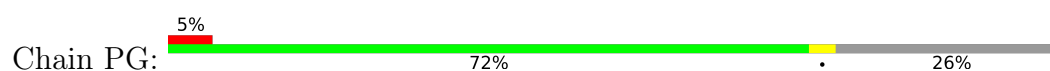
● Molecule 1: Transcription attenuation protein MtrB

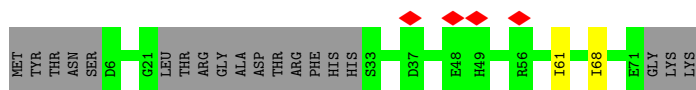


● Molecule 1: Transcription attenuation protein MtrB

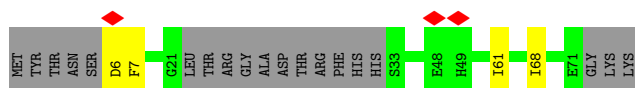


● Molecule 1: Transcription attenuation protein MtrB

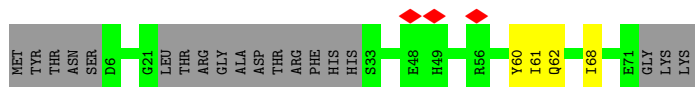




- Molecule 1: Transcription attenuation protein MtrB



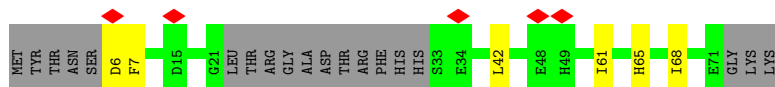
- Molecule 1: Transcription attenuation protein MtrB



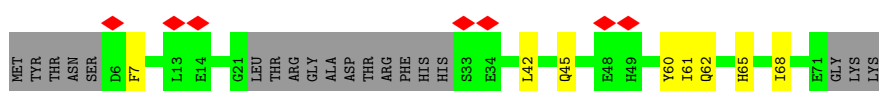
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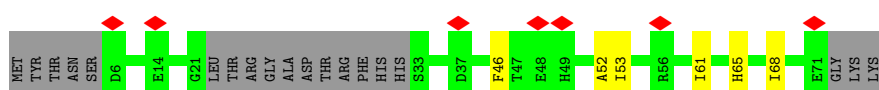
- Molecule 1: Transcription attenuation protein MtrB



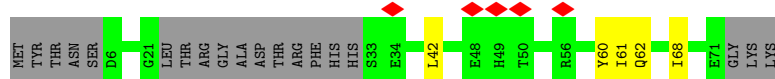
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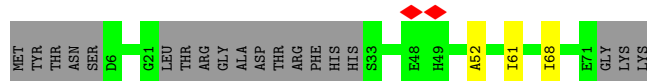
- Molecule 1: Transcription attenuation protein MtrB



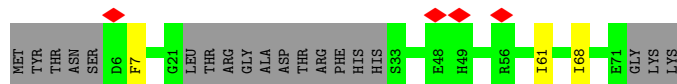
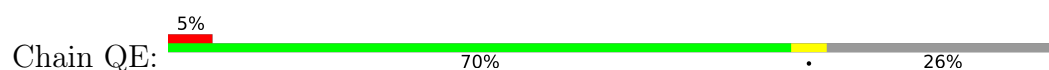
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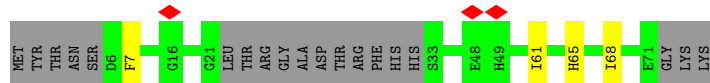
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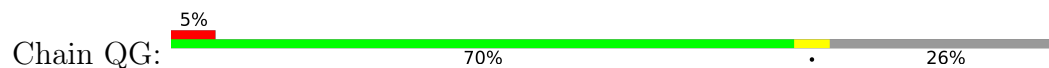
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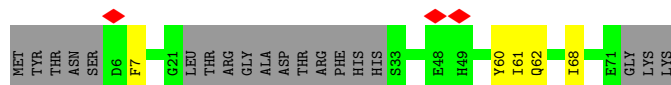
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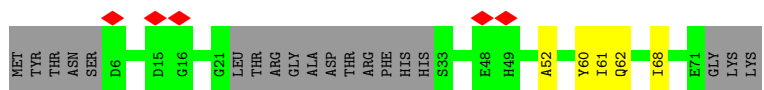


- Molecule 1: Transcription attenuation protein MtrB

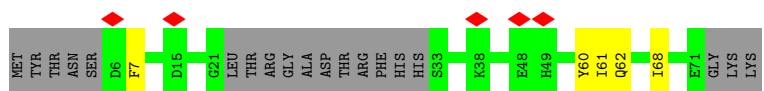




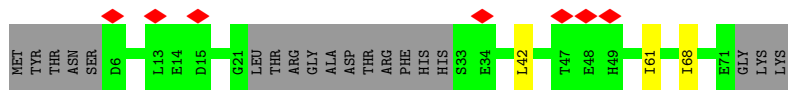
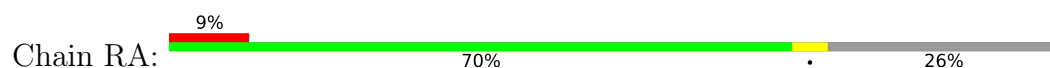
- Molecule 1: Transcription attenuation protein MtrB



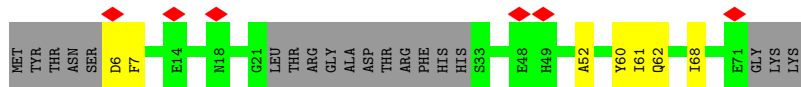
- Molecule 1: Transcription attenuation protein MtrB



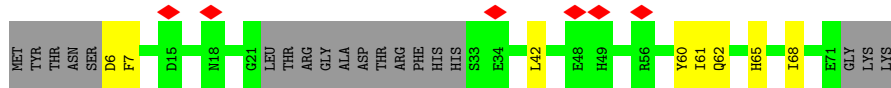
- Molecule 1: Transcription attenuation protein MtrB



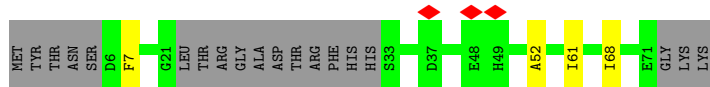
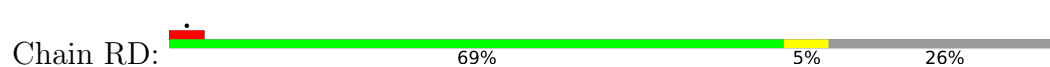
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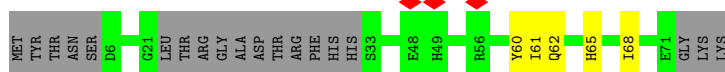
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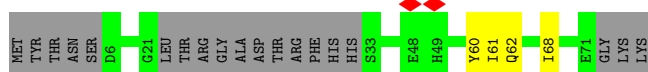
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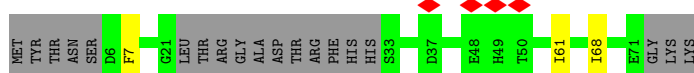
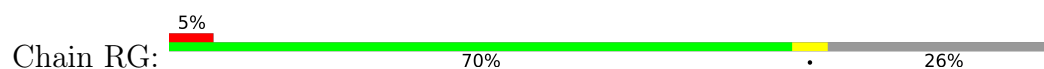
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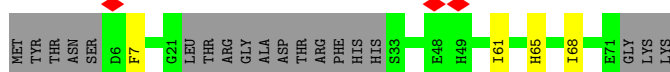
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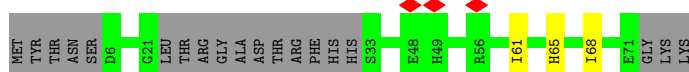
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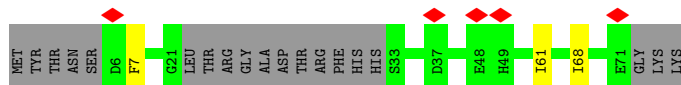
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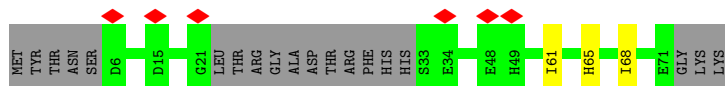
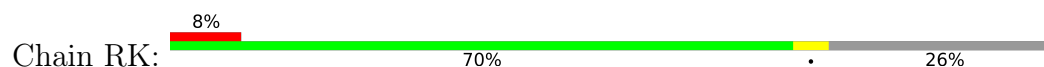
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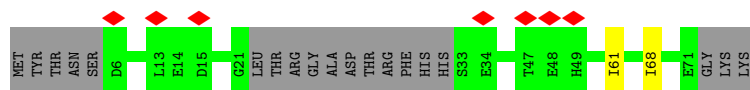
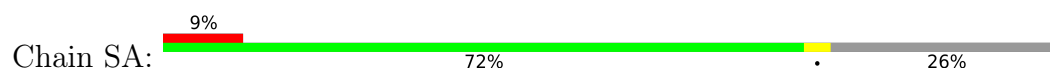
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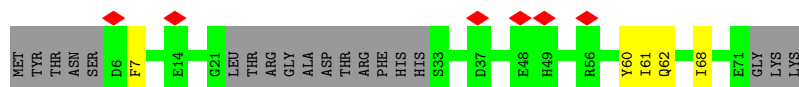
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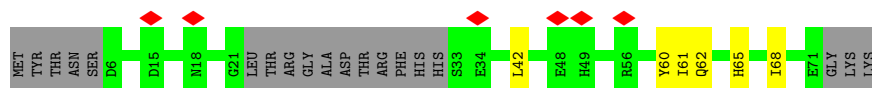
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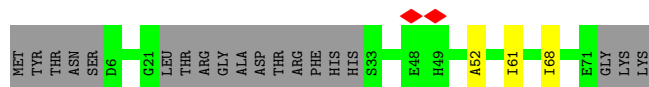
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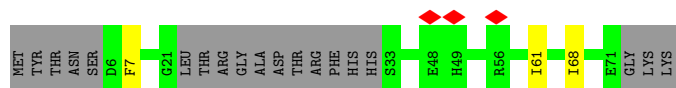
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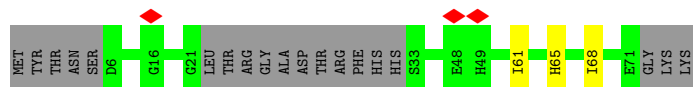
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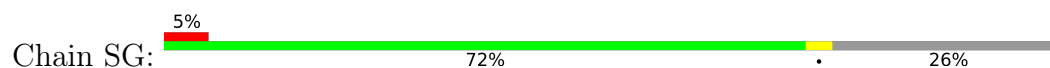
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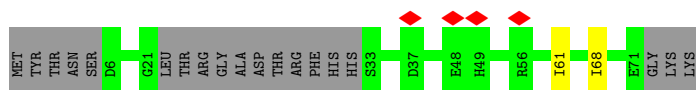


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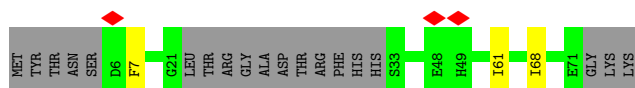


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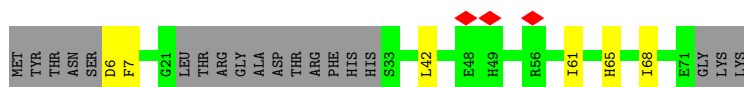




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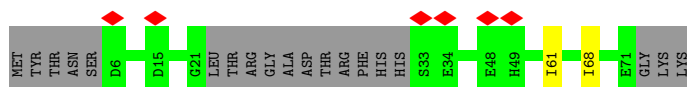
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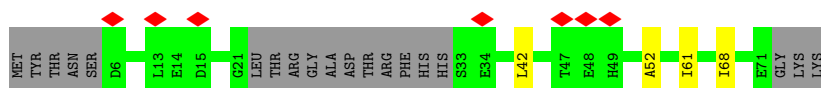
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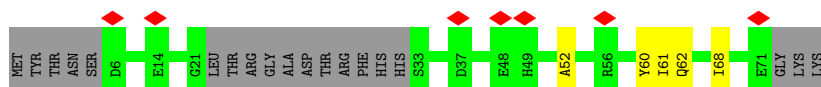
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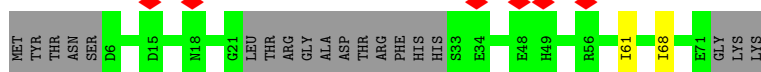
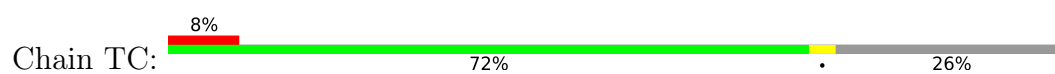
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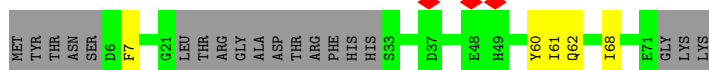
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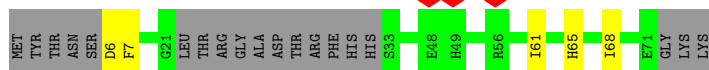
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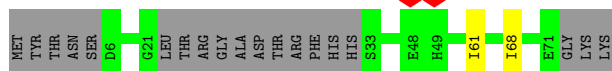
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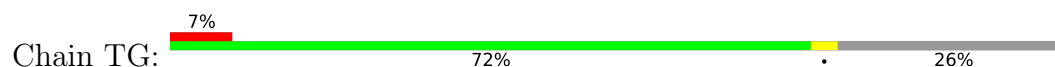
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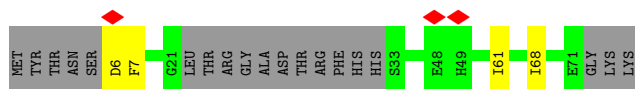
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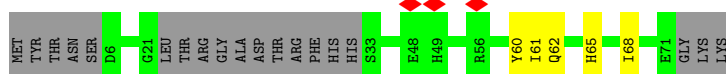
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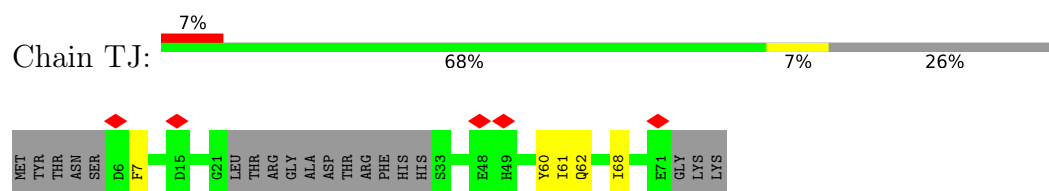
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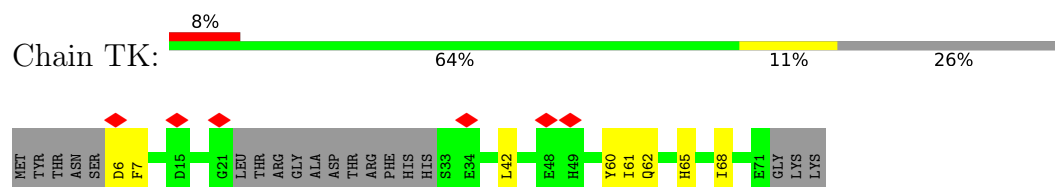
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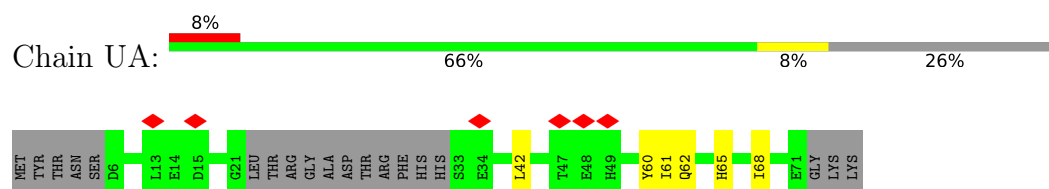
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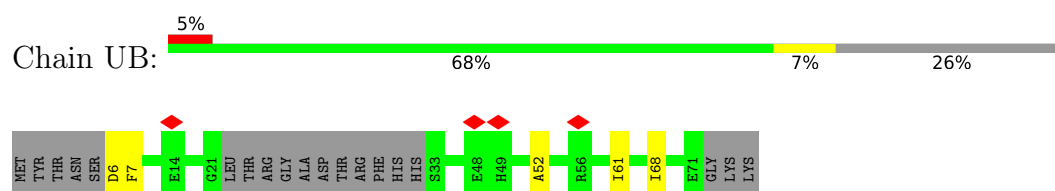
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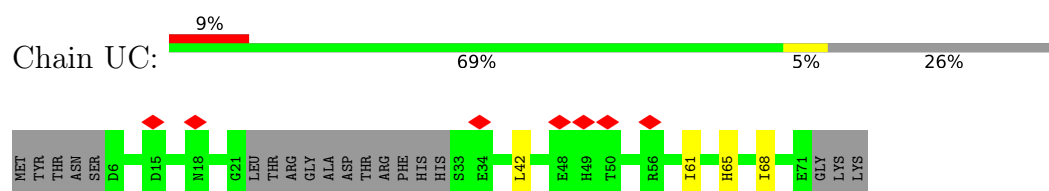
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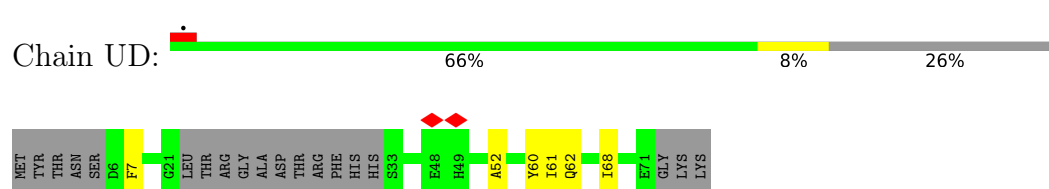
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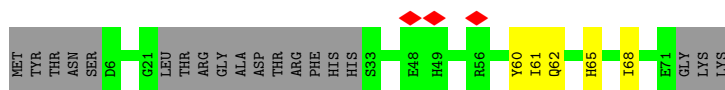


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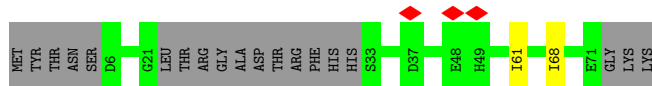
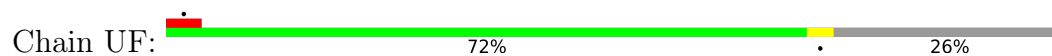


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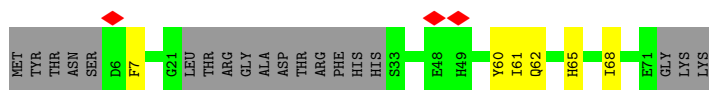
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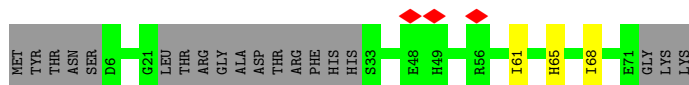
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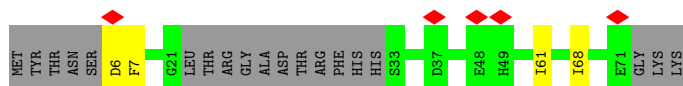
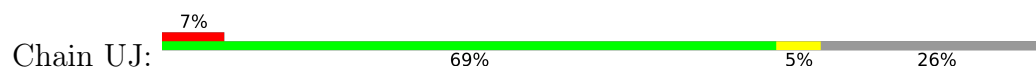
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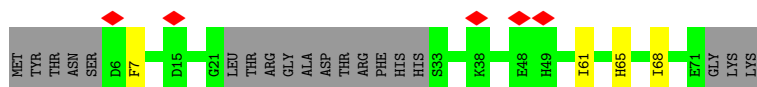
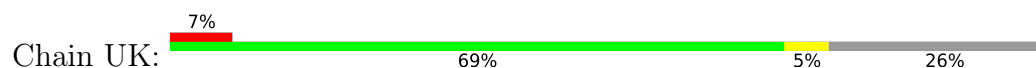
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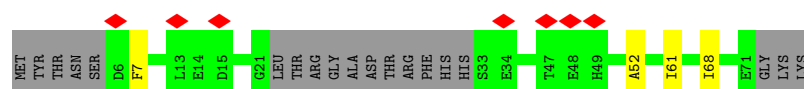
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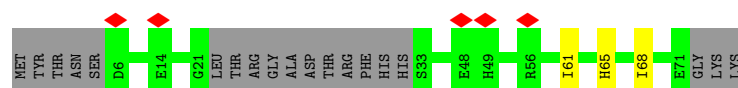
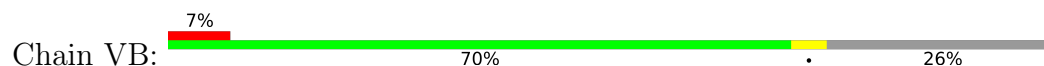
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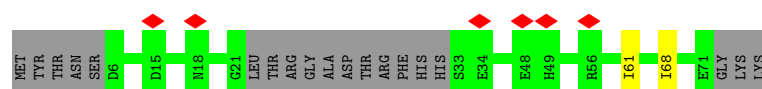
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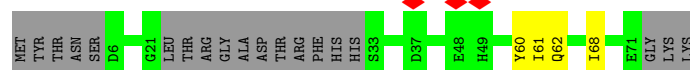
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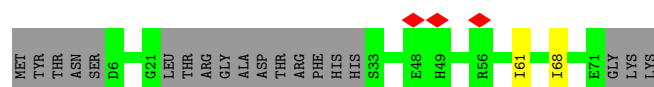
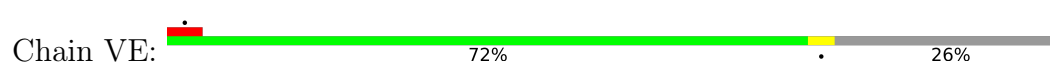
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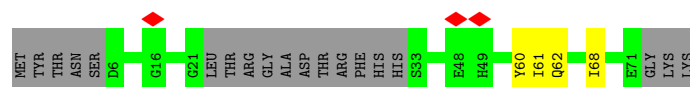
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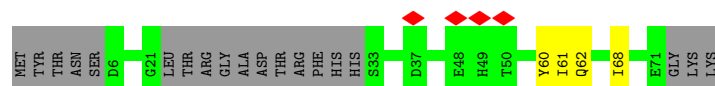
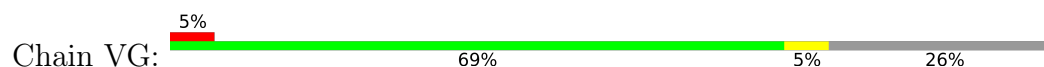
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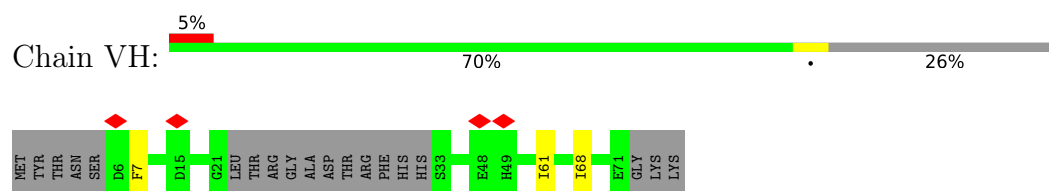
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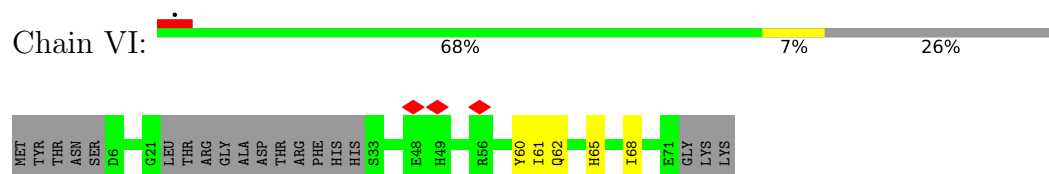
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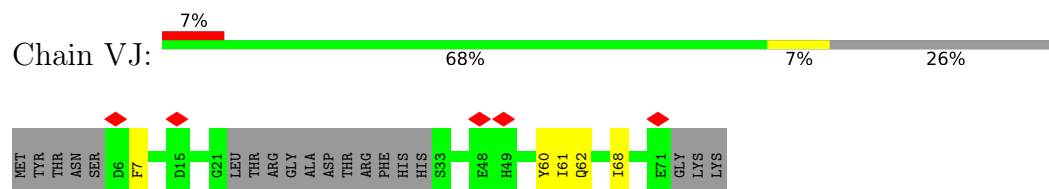
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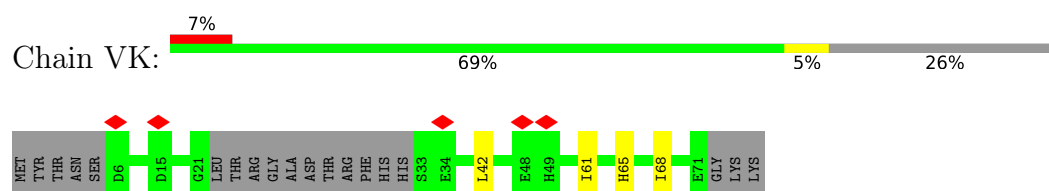
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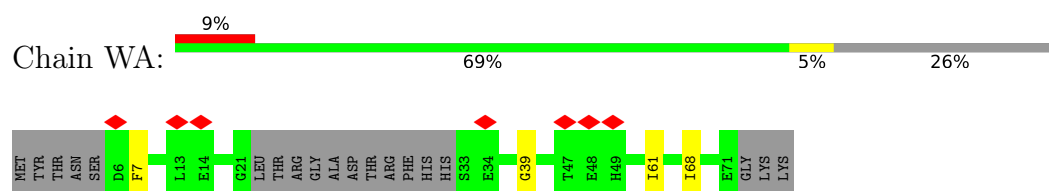
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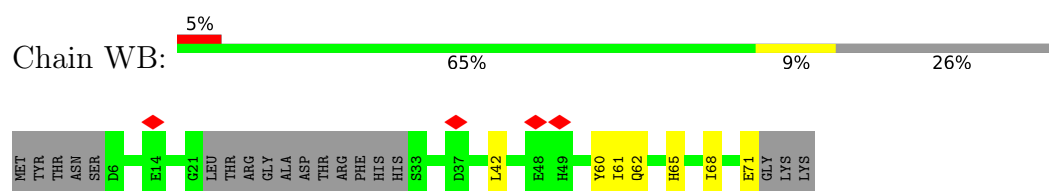
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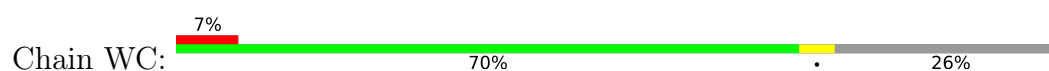
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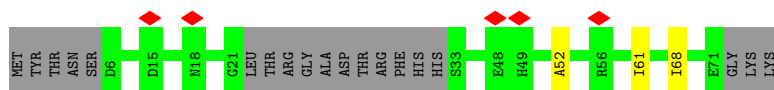


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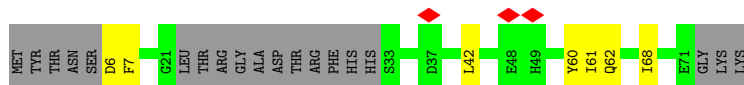


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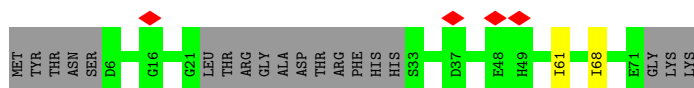
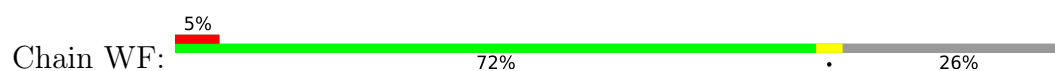
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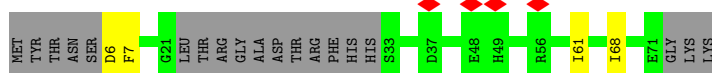
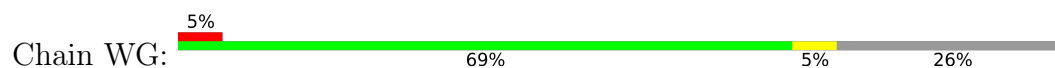
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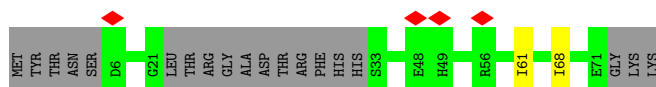
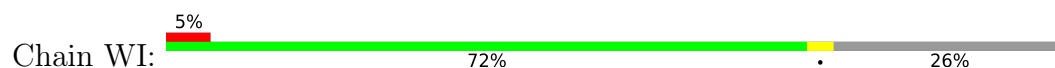
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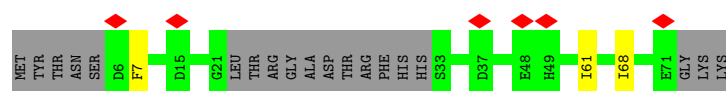
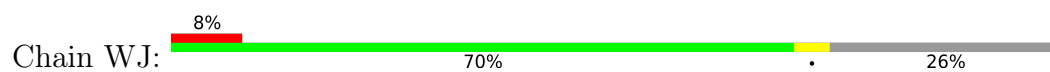
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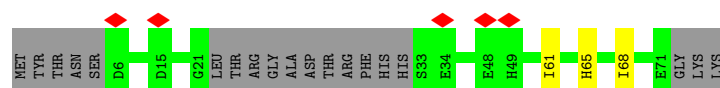
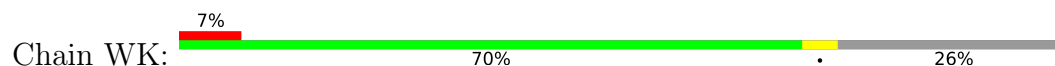
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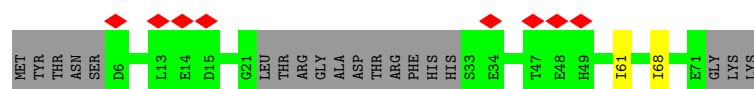
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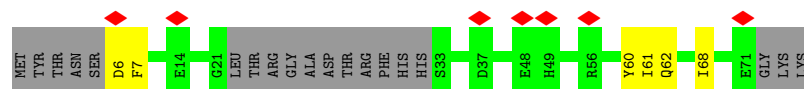
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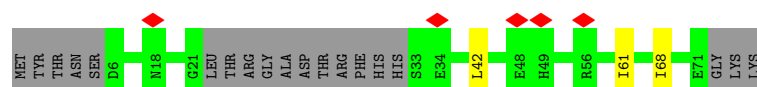
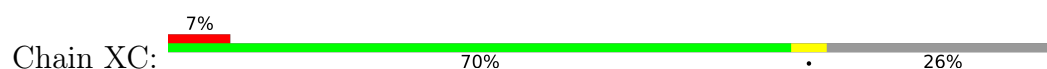
- Molecule 1: Transcription attenuation protein MtrB



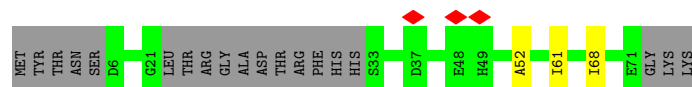
- Molecule 1: Transcription attenuation protein MtrB



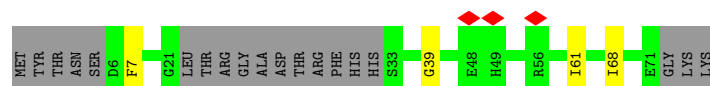
- Molecule 1: Transcription attenuation protein MtrB



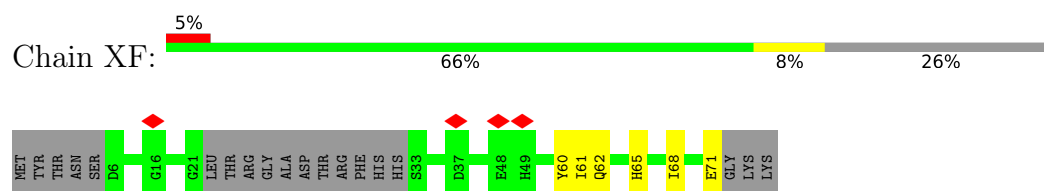
- Molecule 1: Transcription attenuation protein MtrB



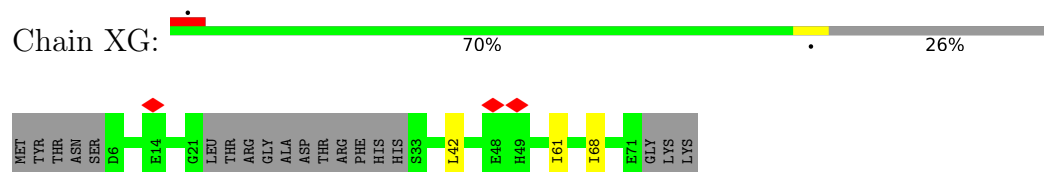
- Molecule 1: Transcription attenuation protein MtrB



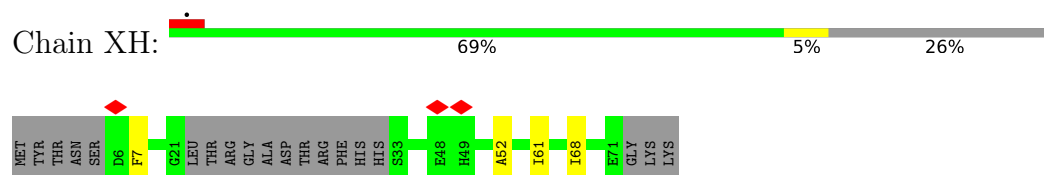
● Molecule 1: Transcription attenuation protein MtrB



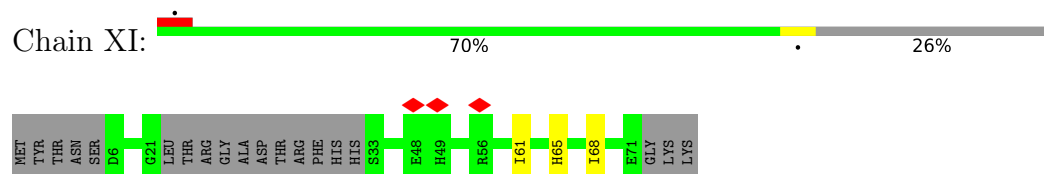
● Molecule 1: Transcription attenuation protein MtrB



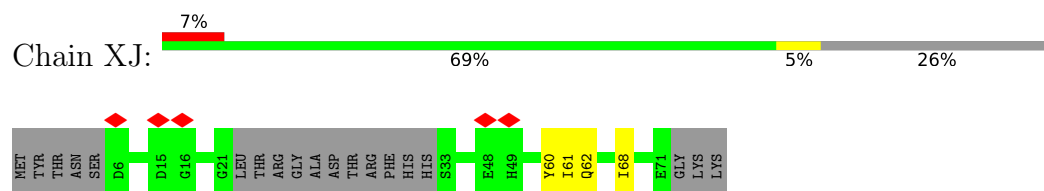
● Molecule 1: Transcription attenuation protein MtrB



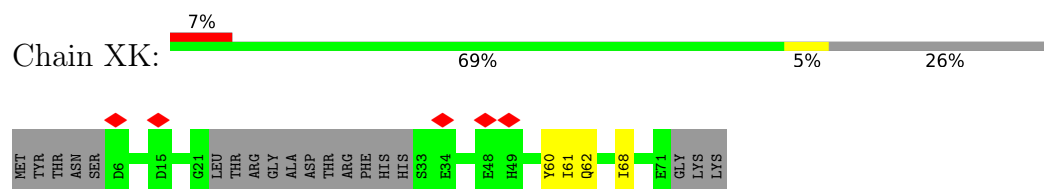
● Molecule 1: Transcription attenuation protein MtrB



● Molecule 1: Transcription attenuation protein MtrB



● Molecule 1: Transcription attenuation protein MtrB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82125	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	0.458	Depositor
Minimum map value	-0.207	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.115	Depositor
Map size ($\text{\AA}$)	382.8, 382.8, 382.8	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.30	0/420	0.40	0/564
1	AB	0.30	0/420	0.40	0/564
1	AC	0.30	0/420	0.40	0/564
1	AD	0.30	0/420	0.40	0/564
1	AE	0.30	0/420	0.40	0/564
1	AF	0.30	0/420	0.40	0/564
1	AG	0.30	0/420	0.39	0/564
1	AH	0.30	0/420	0.40	0/564
1	AI	0.30	0/420	0.39	0/564
1	AJ	0.30	0/420	0.40	0/564
1	AK	0.30	0/420	0.40	0/564
1	BA	0.30	0/420	0.40	0/564
1	BB	0.30	0/420	0.40	0/564
1	BC	0.30	0/420	0.40	0/564
1	BD	0.30	0/420	0.39	0/564
1	BE	0.30	0/420	0.40	0/564
1	BF	0.30	0/420	0.40	0/564
1	BG	0.30	0/420	0.40	0/564
1	BH	0.30	0/420	0.40	0/564
1	BI	0.30	0/420	0.40	0/564
1	BJ	0.30	0/420	0.40	0/564
1	BK	0.30	0/420	0.40	0/564
1	CA	0.30	0/420	0.40	0/564
1	CB	0.30	0/420	0.40	0/564
1	CC	0.30	0/420	0.40	0/564
1	CD	0.30	0/420	0.40	0/564
1	CE	0.30	0/420	0.40	0/564
1	CF	0.30	0/420	0.40	0/564
1	CG	0.30	0/420	0.40	0/564
1	CH	0.30	0/420	0.40	0/564
1	CI	0.30	0/420	0.40	0/564
1	CJ	0.30	0/420	0.40	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CK	0.30	0/420	0.40	0/564
1	DA	0.29	0/420	0.40	0/564
1	DB	0.29	0/420	0.40	0/564
1	DC	0.30	0/420	0.40	0/564
1	DD	0.30	0/420	0.40	0/564
1	DE	0.30	0/420	0.40	0/564
1	DF	0.30	0/420	0.40	0/564
1	DG	0.30	0/420	0.40	0/564
1	DH	0.30	0/420	0.40	0/564
1	DI	0.30	0/420	0.39	0/564
1	DJ	0.30	0/420	0.40	0/564
1	DK	0.30	0/420	0.40	0/564
1	EA	0.30	0/420	0.40	0/564
1	EB	0.30	0/420	0.40	0/564
1	EC	0.30	0/420	0.40	0/564
1	ED	0.30	0/420	0.40	0/564
1	EE	0.30	0/420	0.40	0/564
1	EF	0.30	0/420	0.39	0/564
1	EG	0.30	0/420	0.40	0/564
1	EH	0.30	0/420	0.40	0/564
1	EI	0.30	0/420	0.40	0/564
1	EJ	0.30	0/420	0.40	0/564
1	EK	0.30	0/420	0.40	0/564
1	FA	0.30	0/420	0.40	0/564
1	FB	0.30	0/420	0.40	0/564
1	FC	0.29	0/420	0.39	0/564
1	FD	0.30	0/420	0.40	0/564
1	FE	0.30	0/420	0.39	0/564
1	FF	0.30	0/420	0.40	0/564
1	FG	0.30	0/420	0.40	0/564
1	FH	0.30	0/420	0.40	0/564
1	FI	0.30	0/420	0.40	0/564
1	FJ	0.30	0/420	0.40	0/564
1	FK	0.30	0/420	0.40	0/564
1	GA	0.30	0/420	0.40	0/564
1	GB	0.30	0/420	0.40	0/564
1	GC	0.30	0/420	0.40	0/564
1	GD	0.30	0/420	0.40	0/564
1	GE	0.30	0/420	0.39	0/564
1	GF	0.30	0/420	0.40	0/564
1	GG	0.30	0/420	0.40	0/564
1	GH	0.30	0/420	0.40	0/564
1	GI	0.30	0/420	0.40	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GJ	0.30	0/420	0.40	0/564
1	GK	0.30	0/420	0.40	0/564
1	HA	0.30	0/420	0.40	0/564
1	HB	0.30	0/420	0.40	0/564
1	HC	0.30	0/420	0.40	0/564
1	HD	0.30	0/420	0.40	0/564
1	HE	0.30	0/420	0.40	0/564
1	HF	0.30	0/420	0.40	0/564
1	HG	0.30	0/420	0.39	0/564
1	HH	0.30	0/420	0.40	0/564
1	HI	0.30	0/420	0.40	0/564
1	HJ	0.30	0/420	0.40	0/564
1	HK	0.30	0/420	0.40	0/564
1	IA	0.30	0/420	0.40	0/564
1	IB	0.30	0/420	0.40	0/564
1	IC	0.30	0/420	0.40	0/564
1	ID	0.30	0/420	0.40	0/564
1	IE	0.30	0/420	0.40	0/564
1	IF	0.30	0/420	0.40	0/564
1	IG	0.30	0/420	0.40	0/564
1	IH	0.30	0/420	0.40	0/564
1	II	0.30	0/420	0.40	0/564
1	IJ	0.30	0/420	0.40	0/564
1	IK	0.30	0/420	0.40	0/564
1	JA	0.30	0/420	0.40	0/564
1	JB	0.30	0/420	0.40	0/564
1	JC	0.30	0/420	0.40	0/564
1	JD	0.30	0/420	0.40	0/564
1	JE	0.30	0/420	0.40	0/564
1	JF	0.30	0/420	0.40	0/564
1	JG	0.30	0/420	0.40	0/564
1	JH	0.30	0/420	0.40	0/564
1	JI	0.30	0/420	0.40	0/564
1	JJ	0.30	0/420	0.40	0/564
1	JK	0.30	0/420	0.40	0/564
1	KA	0.30	0/420	0.40	0/564
1	KB	0.30	0/420	0.40	0/564
1	KC	0.30	0/420	0.40	0/564
1	KD	0.30	0/420	0.40	0/564
1	KE	0.30	0/420	0.40	0/564
1	KF	0.30	0/420	0.40	0/564
1	KG	0.30	0/420	0.40	0/564
1	KH	0.30	0/420	0.40	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	KI	0.30	0/420	0.40	0/564
1	KJ	0.30	0/420	0.40	0/564
1	KK	0.30	0/420	0.40	0/564
1	LA	0.30	0/420	0.40	0/564
1	LB	0.30	0/420	0.40	0/564
1	LC	0.30	0/420	0.40	0/564
1	LD	0.30	0/420	0.40	0/564
1	LE	0.30	0/420	0.40	0/564
1	LF	0.30	0/420	0.40	0/564
1	LG	0.30	0/420	0.40	0/564
1	LH	0.30	0/420	0.39	0/564
1	LI	0.30	0/420	0.40	0/564
1	LJ	0.30	0/420	0.40	0/564
1	LK	0.30	0/420	0.40	0/564
1	MA	0.30	0/420	0.40	0/564
1	MB	0.30	0/420	0.40	0/564
1	MC	0.30	0/420	0.40	0/564
1	MD	0.30	0/420	0.40	0/564
1	ME	0.30	0/420	0.40	0/564
1	MF	0.30	0/420	0.40	0/564
1	MG	0.30	0/420	0.40	0/564
1	MH	0.30	0/420	0.40	0/564
1	MI	0.30	0/420	0.40	0/564
1	MJ	0.30	0/420	0.40	0/564
1	MK	0.30	0/420	0.40	0/564
1	NA	0.30	0/420	0.40	0/564
1	NB	0.30	0/420	0.40	0/564
1	NC	0.30	0/420	0.40	0/564
1	ND	0.30	0/420	0.40	0/564
1	NE	0.30	0/420	0.40	0/564
1	NF	0.30	0/420	0.40	0/564
1	NG	0.30	0/420	0.40	0/564
1	NH	0.30	0/420	0.40	0/564
1	NI	0.30	0/420	0.40	0/564
1	NJ	0.30	0/420	0.40	0/564
1	NK	0.30	0/420	0.40	0/564
1	OA	0.30	0/420	0.40	0/564
1	OB	0.30	0/420	0.40	0/564
1	OC	0.30	0/420	0.40	0/564
1	OD	0.30	0/420	0.40	0/564
1	OE	0.30	0/420	0.40	0/564
1	OF	0.30	0/420	0.40	0/564
1	OG	0.30	0/420	0.40	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	OH	0.30	0/420	0.40	0/564
1	OI	0.30	0/420	0.40	0/564
1	OJ	0.30	0/420	0.40	0/564
1	OK	0.30	0/420	0.40	0/564
1	PA	0.30	0/420	0.40	0/564
1	PB	0.30	0/420	0.40	0/564
1	PC	0.30	0/420	0.40	0/564
1	PD	0.30	0/420	0.40	0/564
1	PE	0.30	0/420	0.40	0/564
1	PF	0.30	0/420	0.39	0/564
1	PG	0.30	0/420	0.40	0/564
1	PH	0.30	0/420	0.40	0/564
1	PI	0.30	0/420	0.40	0/564
1	PJ	0.30	0/420	0.40	0/564
1	PK	0.30	0/420	0.40	0/564
1	QA	0.29	0/420	0.40	0/564
1	QB	0.30	0/420	0.40	0/564
1	QC	0.30	0/420	0.40	0/564
1	QD	0.30	0/420	0.40	0/564
1	QE	0.30	0/420	0.40	0/564
1	QF	0.30	0/420	0.40	0/564
1	QG	0.30	0/420	0.40	0/564
1	QH	0.30	0/420	0.40	0/564
1	QI	0.30	0/420	0.40	0/564
1	QJ	0.30	0/420	0.40	0/564
1	QK	0.30	0/420	0.40	0/564
1	RA	0.30	0/420	0.40	0/564
1	RB	0.30	0/420	0.40	0/564
1	RC	0.30	0/420	0.40	0/564
1	RD	0.30	0/420	0.40	0/564
1	RE	0.30	0/420	0.40	0/564
1	RF	0.30	0/420	0.40	0/564
1	RG	0.30	0/420	0.40	0/564
1	RH	0.30	0/420	0.39	0/564
1	RI	0.30	0/420	0.40	0/564
1	RJ	0.30	0/420	0.40	0/564
1	RK	0.30	0/420	0.40	0/564
1	SA	0.30	0/420	0.40	0/564
1	SB	0.30	0/420	0.40	0/564
1	SC	0.30	0/420	0.40	0/564
1	SD	0.30	0/420	0.40	0/564
1	SE	0.30	0/420	0.40	0/564
1	SF	0.30	0/420	0.40	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	SG	0.30	0/420	0.40	0/564
1	SH	0.30	0/420	0.40	0/564
1	SI	0.30	0/420	0.40	0/564
1	SJ	0.30	0/420	0.40	0/564
1	SK	0.30	0/420	0.40	0/564
1	TA	0.30	0/420	0.40	0/564
1	TB	0.30	0/420	0.40	0/564
1	TC	0.30	0/420	0.40	0/564
1	TD	0.30	0/420	0.40	0/564
1	TE	0.30	0/420	0.40	0/564
1	TF	0.30	0/420	0.40	0/564
1	TG	0.30	0/420	0.40	0/564
1	TH	0.30	0/420	0.40	0/564
1	TI	0.30	0/420	0.40	0/564
1	TJ	0.30	0/420	0.40	0/564
1	TK	0.30	0/420	0.40	0/564
1	UA	0.30	0/420	0.40	0/564
1	UB	0.30	0/420	0.40	0/564
1	UC	0.30	0/420	0.40	0/564
1	UD	0.30	0/420	0.40	0/564
1	UE	0.30	0/420	0.40	0/564
1	UF	0.30	0/420	0.40	0/564
1	UG	0.30	0/420	0.40	0/564
1	UH	0.30	0/420	0.40	0/564
1	UI	0.30	0/420	0.40	0/564
1	UJ	0.30	0/420	0.40	0/564
1	UK	0.30	0/420	0.40	0/564
1	VA	0.30	0/420	0.40	0/564
1	VB	0.30	0/420	0.40	0/564
1	VC	0.30	0/420	0.40	0/564
1	VD	0.30	0/420	0.40	0/564
1	VE	0.30	0/420	0.40	0/564
1	VF	0.30	0/420	0.40	0/564
1	VG	0.30	0/420	0.40	0/564
1	VH	0.30	0/420	0.40	0/564
1	VI	0.30	0/420	0.40	0/564
1	VJ	0.30	0/420	0.40	0/564
1	VK	0.30	0/420	0.40	0/564
1	WA	0.30	0/420	0.40	0/564
1	WB	0.30	0/420	0.40	0/564
1	WC	0.30	0/420	0.40	0/564
1	WD	0.30	0/420	0.40	0/564
1	WE	0.30	0/420	0.39	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	WF	0.30	0/420	0.39	0/564
1	WG	0.30	0/420	0.40	0/564
1	WH	0.30	0/420	0.39	0/564
1	WI	0.30	0/420	0.40	0/564
1	WJ	0.30	0/420	0.40	0/564
1	WK	0.30	0/420	0.40	0/564
1	XA	0.30	0/420	0.39	0/564
1	XB	0.30	0/420	0.40	0/564
1	XC	0.30	0/420	0.40	0/564
1	XD	0.30	0/420	0.40	0/564
1	XE	0.30	0/420	0.40	0/564
1	XF	0.30	0/420	0.40	0/564
1	XG	0.30	0/420	0.40	0/564
1	XH	0.30	0/420	0.40	0/564
1	XI	0.30	0/420	0.40	0/564
1	XJ	0.30	0/420	0.40	0/564
1	XK	0.30	0/420	0.40	0/564
All	All	0.30	0/110880	0.40	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	3	0
1	AB	417	0	416	4	0
1	AC	417	0	416	3	0
1	AD	417	0	416	5	0
1	AE	417	0	416	3	0
1	AF	417	0	416	2	0
1	AG	417	0	417	2	0
1	AH	417	0	416	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	417	0	417	2	0
1	AJ	417	0	416	2	0
1	AK	417	0	417	3	0
1	BA	417	0	416	2	0
1	BB	417	0	417	3	0
1	BC	417	0	416	3	0
1	BD	417	0	416	2	0
1	BE	417	0	417	4	0
1	BF	417	0	416	3	0
1	BG	417	0	416	2	0
1	BH	417	0	416	3	0
1	BI	417	0	416	2	0
1	BJ	417	0	416	3	0
1	BK	417	0	417	3	0
1	CA	417	0	417	4	0
1	CB	417	0	416	2	0
1	CC	417	0	416	1	0
1	CD	417	0	416	2	0
1	CE	417	0	417	2	0
1	CF	417	0	416	3	0
1	CG	417	0	416	3	0
1	CH	417	0	416	3	0
1	CI	417	0	416	4	0
1	CJ	417	0	416	4	0
1	CK	417	0	417	3	0
1	DA	417	0	416	2	0
1	DB	417	0	416	1	0
1	DC	417	0	416	2	0
1	DD	417	0	417	3	0
1	DE	417	0	416	2	0
1	DF	417	0	417	1	0
1	DG	417	0	416	2	0
1	DH	417	0	417	2	0
1	DI	417	0	416	3	0
1	DJ	417	0	416	2	0
1	DK	417	0	417	3	0
1	EA	417	0	416	3	0
1	EB	417	0	416	3	0
1	EC	417	0	416	3	0
1	ED	417	0	417	2	0
1	EE	417	0	416	2	0
1	EF	417	0	416	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EG	417	0	417	2	0
1	EH	417	0	417	2	0
1	EI	417	0	416	3	0
1	EJ	417	0	416	2	0
1	EK	417	0	417	2	0
1	FA	417	0	416	2	0
1	FB	417	0	416	3	0
1	FC	417	0	416	3	0
1	FD	417	0	417	3	0
1	FE	417	0	416	3	0
1	FF	417	0	417	2	0
1	FG	417	0	417	2	0
1	FH	417	0	417	3	0
1	FI	417	0	416	2	0
1	FJ	417	0	416	1	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	3	0
1	GD	417	0	416	4	0
1	GE	417	0	417	4	0
1	GF	417	0	416	4	0
1	GG	417	0	416	3	0
1	GH	417	0	416	2	0
1	GI	417	0	416	2	0
1	GJ	417	0	416	3	0
1	GK	417	0	417	3	0
1	HA	417	0	416	2	0
1	HB	417	0	416	4	0
1	HC	417	0	416	4	0
1	HD	417	0	417	4	0
1	HE	417	0	417	4	0
1	HF	417	0	416	3	0
1	HG	417	0	416	3	0
1	HH	417	0	416	3	0
1	HI	417	0	416	3	0
1	HJ	417	0	416	3	0
1	HK	417	0	417	3	0
1	IA	417	0	417	4	0
1	IB	417	0	416	1	0
1	IC	417	0	417	1	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	2	0
1	IF	417	0	416	4	0
1	IG	417	0	416	2	0
1	IH	417	0	416	2	0
1	II	417	0	416	3	0
1	IJ	417	0	416	1	0
1	IK	417	0	417	3	0
1	JA	417	0	416	4	0
1	JB	417	0	416	5	0
1	JC	417	0	416	1	0
1	JD	417	0	416	1	0
1	JE	417	0	416	1	0
1	JF	417	0	416	3	0
1	JG	417	0	417	3	0
1	JH	417	0	416	2	0
1	JI	417	0	416	1	0
1	JJ	417	0	416	2	0
1	JK	417	0	417	3	0
1	KA	417	0	416	3	0
1	KB	417	0	416	1	0
1	KC	417	0	416	2	0
1	KD	417	0	417	1	0
1	KE	417	0	416	3	0
1	KF	417	0	417	3	0
1	KG	417	0	416	3	0
1	KH	417	0	417	4	0
1	KI	417	0	416	3	0
1	KJ	417	0	417	2	0
1	KK	417	0	417	2	0
1	LA	417	0	416	2	0
1	LB	417	0	416	3	0
1	LC	417	0	416	3	0
1	LD	417	0	417	2	0
1	LE	417	0	416	2	0
1	LF	417	0	416	4	0
1	LG	417	0	416	3	0
1	LH	417	0	417	2	0
1	LI	417	0	417	2	0
1	LJ	417	0	416	1	0
1	LK	417	0	417	2	0
1	MA	417	0	416	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	416	5	0
1	MD	417	0	417	3	0
1	ME	417	0	416	2	0
1	MF	417	0	416	4	0
1	MG	417	0	416	4	0
1	MH	417	0	417	3	0
1	MI	417	0	417	3	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	4	0
1	ND	417	0	417	4	0
1	NE	417	0	417	4	0
1	NF	417	0	416	2	0
1	NG	417	0	416	3	0
1	NH	417	0	416	4	0
1	NI	417	0	416	2	0
1	NJ	417	0	416	3	0
1	NK	417	0	417	3	0
1	OA	417	0	416	1	0
1	OB	417	0	416	1	0
1	OC	417	0	417	1	0
1	OD	417	0	416	2	0
1	OE	417	0	417	3	0
1	OF	417	0	416	3	0
1	OG	417	0	417	2	0
1	OH	417	0	417	1	0
1	OI	417	0	416	2	0
1	OJ	417	0	416	2	0
1	OK	417	0	417	1	0
1	PA	417	0	416	2	0
1	PB	417	0	416	2	0
1	PC	417	0	417	1	0
1	PD	417	0	417	2	0
1	PE	417	0	417	2	0
1	PF	417	0	416	1	0
1	PG	417	0	417	1	0
1	PH	417	0	417	2	0
1	PI	417	0	416	2	0
1	PJ	417	0	416	3	0
1	PK	417	0	417	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	417	0	416	7	0
1	QB	417	0	416	5	0
1	QC	417	0	416	3	0
1	QD	417	0	417	2	0
1	QE	417	0	417	2	0
1	QF	417	0	417	3	0
1	QG	417	0	416	2	0
1	QH	417	0	417	3	0
1	QI	417	0	416	4	0
1	QJ	417	0	417	3	0
1	QK	417	0	417	3	0
1	RA	417	0	416	2	0
1	RB	417	0	417	5	0
1	RC	417	0	417	5	0
1	RD	417	0	417	3	0
1	RE	417	0	417	3	0
1	RF	417	0	416	2	0
1	RG	417	0	416	2	0
1	RH	417	0	416	3	0
1	RI	417	0	416	2	0
1	RJ	417	0	416	2	0
1	RK	417	0	417	2	0
1	SA	417	0	416	1	0
1	SB	417	0	416	3	0
1	SC	417	0	416	4	0
1	SD	417	0	417	2	0
1	SE	417	0	416	2	0
1	SF	417	0	416	2	0
1	SG	417	0	417	1	0
1	SH	417	0	417	2	0
1	SI	417	0	416	4	0
1	SJ	417	0	416	2	0
1	SK	417	0	417	1	0
1	TA	417	0	416	3	0
1	TB	417	0	417	3	0
1	TC	417	0	417	1	0
1	TD	417	0	416	3	0
1	TE	417	0	416	3	0
1	TF	417	0	416	1	0
1	TG	417	0	417	1	0
1	TH	417	0	416	3	0
1	TI	417	0	417	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TJ	417	0	416	3	0
1	TK	417	0	417	5	0
1	UA	417	0	416	4	0
1	UB	417	0	416	4	0
1	UC	417	0	416	3	0
1	UD	417	0	416	4	0
1	UE	417	0	417	3	0
1	UF	417	0	416	1	0
1	UG	417	0	416	4	0
1	UH	417	0	416	4	0
1	UI	417	0	416	2	0
1	UJ	417	0	416	3	0
1	UK	417	0	417	3	0
1	VA	417	0	416	3	0
1	VB	417	0	417	2	0
1	VC	417	0	417	1	0
1	VD	417	0	416	2	0
1	VE	417	0	416	1	0
1	VF	417	0	416	2	0
1	VG	417	0	417	2	0
1	VH	417	0	417	2	0
1	VI	417	0	416	3	0
1	VJ	417	0	416	3	0
1	VK	417	0	417	3	0
1	WA	417	0	416	3	0
1	WB	417	0	417	5	0
1	WC	417	0	416	2	0
1	WD	417	0	416	4	0
1	WE	417	0	416	2	0
1	WF	417	0	416	1	0
1	WG	417	0	417	2	0
1	WH	417	0	416	2	0
1	WI	417	0	416	1	0
1	WJ	417	0	416	2	0
1	WK	417	0	417	2	0
1	XA	417	0	416	1	0
1	XB	417	0	416	3	0
1	XC	417	0	416	2	0
1	XD	417	0	416	2	0
1	XE	417	0	417	3	0
1	XF	417	0	417	4	0
1	XG	417	0	416	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XH	417	0	416	3	0
1	XI	417	0	417	2	0
1	XJ	417	0	416	2	0
1	XK	417	0	417	2	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	FC	1	0	0	0	0
2	FD	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	JA	1	0	0	0	0
2	JB	1	0	0	0	0
2	JG	1	0	0	0	0
2	JH	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	KC	1	0	0	0	0
2	KD	1	0	0	0	0
2	KE	1	0	0	0	0
2	KF	1	0	0	0	0
2	LE	1	0	0	0	0
2	LF	1	0	0	0	0
2	LG	1	0	0	0	0
2	LH	1	0	0	0	0
2	LI	1	0	0	0	0
2	LJ	1	0	0	0	0
2	MA	1	0	0	0	0
2	MB	1	0	0	0	0
2	NC	1	0	0	0	0
2	ND	1	0	0	0	0
2	NE	1	0	0	0	0
2	NF	1	0	0	0	0
2	OA	1	0	0	0	0
2	OB	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	PA	1	0	0	0	0
2	PB	1	0	0	0	0
2	PC	1	0	0	0	0
2	PD	1	0	0	0	0
2	QG	1	0	0	0	0
2	QH	1	0	0	0	0
2	RC	1	0	0	0	0
2	RD	1	0	0	0	0
2	RE	1	0	0	0	0
2	RF	1	0	0	0	0
2	SE	1	0	0	0	0
2	SF	1	0	0	0	0
2	TE	1	0	0	0	0
2	TF	1	0	0	0	0
2	TI	1	0	0	0	0
2	TJ	1	0	0	0	0
2	WA	1	0	0	0	0
2	WB	1	0	0	0	0
All	All	110208	0	109918	539	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 (539) 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:WB:42:LEU:HD11	1:WC:52:ALA:HB1	1.83	0.60
1:IH:7:PHE:O	1:II:65:HIS:NE2	2.35	0.60
1:WA:39:GLY:O	1:WB:71:GLU:N	2.32	0.59
1:MH:7:PHE:O	1:MI:65:HIS:NE2	2.36	0.58
1:QA:7:PHE:O	1:QB:65:HIS:NE2	2.36	0.57
1:WA:7:PHE:O	1:WB:65:HIS:NE2	2.37	0.56
1:EC:42:LEU:HD11	1:ED:52:ALA:HB1	1.88	0.56
1:LB:7:PHE:O	1:LC:65:HIS:NE2	2.38	0.56
1:HA:65:HIS:NE2	1:HK:7:PHE:O	2.38	0.55
1:OE:7:PHE:O	1:OF:65:HIS:NE2	2.37	0.55
1:CD:7:PHE:O	1:CE:65:HIS:NE2	2.37	0.55
1:XC:42:LEU:HD11	1:XD:52:ALA:HB1	1.88	0.55
1:RA:42:LEU:HD11	1:RB:52:ALA:HB1	1.90	0.54
1:KA:65:HIS:NE2	1:KK:7:PHE:O	2.37	0.54
1:KH:7:PHE:O	1:KI:65:HIS:NE2	2.40	0.54
1:LH:7:PHE:O	1:LI:65:HIS:NE2	2.36	0.53
1:IF:39:GLY:O	1:IG:71:GLU:N	2.36	0.53
1:MC:42:LEU:HD11	1:MD:52:ALA:HB1	1.92	0.52
1:MB:7:PHE:O	1:MC:65:HIS:NE2	2.42	0.52
1:BE:7:PHE:O	1:BF:65:HIS:NE2	2.42	0.52
1:QI:42:LEU:HD11	1:QJ:52:ALA:HB1	1.91	0.52
1:QH:7:PHE:O	1:QI:65:HIS:NE2	2.42	0.51
1:NJ:7:PHE:O	1:NK:65:HIS:NE2	2.39	0.51
1:QE:7:PHE:O	1:QF:65:HIS:NE2	2.41	0.51
1:BJ:7:PHE:O	1:BK:65:HIS:NE2	2.43	0.50
1:HE:7:PHE:O	1:HF:65:HIS:NE2	2.44	0.50
1:UA:65:HIS:NE2	1:UK:7:PHE:O	2.44	0.50
1:SC:42:LEU:HD11	1:SD:52:ALA:HB1	1.94	0.50
1:NB:7:PHE:O	1:NC:65:HIS:NE2	2.40	0.50
1:TH:7:PHE:O	1:TI:65:HIS:NE2	2.43	0.50
1:SH:7:PHE:O	1:SI:65:HIS:NE2	2.39	0.50
1:TA:52:ALA:HB1	1:TK:42:LEU:HD11	1.93	0.49
1:IA:65:HIS:NE2	1:IK:7:PHE:O	2.43	0.49
1:FE:7:PHE:O	1:FF:65:HIS:NE2	2.44	0.49
1:KE:7:PHE:O	1:KF:65:HIS:NE2	2.44	0.49
1:LF:7:PHE:O	1:LG:65:HIS:NE2	2.35	0.49
1:SE:7:PHE:O	1:SF:65:HIS:NE2	2.43	0.49
1:XE:39:GLY:O	1:XF:71:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:7:PHE:O	1:CB:65:HIS:NE2	2.44	0.48
1:HC:42:LEU:HD11	1:HD:52:ALA:HB1	1.94	0.48
1:DA:65:HIS:NE2	1:DK:7:PHE:O	2.44	0.48
1:NH:7:PHE:O	1:NI:65:HIS:NE2	2.46	0.48
1:UH:7:PHE:O	1:UI:65:HIS:NE2	2.46	0.48
1:BA:65:HIS:NE2	1:BK:7:PHE:O	2.43	0.48
1:MF:7:PHE:O	1:MG:65:HIS:NE2	2.40	0.48
1:RC:42:LEU:HD11	1:RD:52:ALA:HB1	1.96	0.47
1:EF:7:PHE:O	1:EG:65:HIS:NE2	2.40	0.47
1:GA:65:HIS:NE2	1:GK:7:PHE:O	2.45	0.47
1:FH:7:PHE:O	1:FI:65:HIS:NE2	2.43	0.47
1:VA:52:ALA:HB1	1:VK:42:LEU:HD11	1.96	0.47
1:BD:7:PHE:O	1:BE:65:HIS:NE2	2.46	0.47
1:CG:7:PHE:O	1:CH:65:HIS:NE2	2.45	0.47
1:FC:42:LEU:HD11	1:FD:52:ALA:HB1	1.97	0.46
1:LE:7:PHE:O	1:LF:65:HIS:NE2	2.47	0.46
1:BG:7:PHE:O	1:BH:65:HIS:NE2	2.43	0.46
1:JF:7:PHE:O	1:JG:65:HIS:NE2	2.42	0.46
1:AA:52:ALA:HB1	1:AK:42:LEU:HD11	1.96	0.46
1:BH:7:PHE:O	1:BI:65:HIS:NE2	2.44	0.46
1:RG:7:PHE:O	1:RH:65:HIS:NE2	2.45	0.46
1:GG:7:PHE:O	1:GH:65:HIS:NE2	2.43	0.46
1:NB:39:GLY:O	1:NC:71:GLU:N	2.37	0.46
1:XG:42:LEU:HD11	1:XH:52:ALA:HB1	1.98	0.46
1:KG:42:LEU:HD11	1:KH:52:ALA:HB1	1.98	0.46
1:MI:42:LEU:HD11	1:MJ:52:ALA:HB1	1.97	0.46
1:FB:7:PHE:O	1:FC:65:HIS:NE2	2.45	0.45
1:HH:7:PHE:O	1:HI:65:HIS:NE2	2.48	0.45
1:LA:42:LEU:HD11	1:LB:52:ALA:HB1	1.99	0.45
1:DH:7:PHE:O	1:DI:65:HIS:NE2	2.44	0.45
1:GE:7:PHE:O	1:GF:65:HIS:NE2	2.47	0.45
1:RD:7:PHE:O	1:RE:65:HIS:NE2	2.47	0.45
1:AD:42:LEU:HD11	1:AE:52:ALA:HB1	1.99	0.45
1:NC:42:LEU:HD11	1:ND:52:ALA:HB1	1.98	0.45
1:EH:7:PHE:O	1:EI:65:HIS:NE2	2.45	0.45
1:GJ:7:PHE:O	1:GK:65:HIS:NE2	2.45	0.45
1:GC:42:LEU:HD11	1:GD:52:ALA:HB1	1.98	0.45
1:ME:7:PHE:O	1:MF:65:HIS:NE2	2.45	0.45
1:FA:42:LEU:HD11	1:FB:52:ALA:HB1	1.99	0.45
1:QC:42:LEU:HD11	1:QD:52:ALA:HB1	1.99	0.45
1:XE:7:PHE:O	1:XF:65:HIS:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:7:PHE:O	1:HC:65:HIS:NE2	2.45	0.44
1:NG:7:PHE:O	1:NH:65:HIS:NE2	2.47	0.44
1:UD:7:PHE:O	1:UE:65:HIS:NE2	2.43	0.44
1:UC:42:LEU:HD11	1:UD:52:ALA:HB1	1.99	0.44
1:CJ:7:PHE:O	1:CK:65:HIS:NE2	2.46	0.44
1:EI:42:LEU:HD11	1:EJ:52:ALA:HB1	2.00	0.44
1:HG:7:PHE:O	1:HH:65:HIS:NE2	2.48	0.44
1:GD:7:PHE:O	1:GE:65:HIS:NE2	2.48	0.43
1:HJ:7:PHE:O	1:HK:65:HIS:NE2	2.48	0.43
1:TJ:7:PHE:O	1:TK:65:HIS:NE2	2.44	0.43
1:AE:7:PHE:O	1:AF:65:HIS:NE2	2.48	0.43
1:CA:65:HIS:NE2	1:CK:7:PHE:O	2.49	0.43
1:GE:60:TYR:OH	1:GE:62:GLN:NE2	2.49	0.43
1:PK:61:ILE:HB	1:PK:68:ILE:HG22	2.01	0.43
1:CH:61:ILE:HB	1:CH:68:ILE:HG22	2.01	0.43
1:DI:61:ILE:HB	1:DI:68:ILE:HG22	2.01	0.43
1:GD:61:ILE:HB	1:GD:68:ILE:HG22	2.01	0.43
1:IH:61:ILE:HB	1:IH:68:ILE:HG22	2.01	0.43
1:JG:61:ILE:HB	1:JG:68:ILE:HG22	2.01	0.43
1:KD:61:ILE:HB	1:KD:68:ILE:HG22	2.01	0.43
1:MD:60:TYR:OH	1:MD:62:GLN:NE2	2.49	0.43
1:UA:60:TYR:OH	1:UA:62:GLN:NE2	2.49	0.43
1:UG:60:TYR:OH	1:UG:62:GLN:NE2	2.49	0.43
1:XH:61:ILE:HB	1:XH:68:ILE:HG22	2.01	0.43
1:AF:61:ILE:HB	1:AF:68:ILE:HG22	2.01	0.43
1:AH:7:PHE:O	1:AI:65:HIS:NE2	2.46	0.43
1:DI:42:LEU:HD11	1:DJ:52:ALA:HB1	2.01	0.43
1:FI:61:ILE:HB	1:FI:68:ILE:HG22	2.01	0.43
1:GA:61:ILE:HB	1:GA:68:ILE:HG22	2.01	0.43
1:HA:61:ILE:HB	1:HA:68:ILE:HG22	2.01	0.43
1:HH:61:ILE:HB	1:HH:68:ILE:HG22	2.01	0.43
1:IB:61:ILE:HB	1:IB:68:ILE:HG22	2.01	0.43
1:JH:61:ILE:HB	1:JH:68:ILE:HG22	2.01	0.43
1:JJ:61:ILE:HB	1:JJ:68:ILE:HG22	2.01	0.43
1:KC:61:ILE:HB	1:KC:68:ILE:HG22	2.01	0.43
1:LD:61:ILE:HB	1:LD:68:ILE:HG22	2.01	0.43
1:MA:42:LEU:HD11	1:MB:52:ALA:HB1	2.01	0.43
1:MA:65:HIS:NE2	1:MK:7:PHE:O	2.46	0.43
1:ME:61:ILE:HB	1:ME:68:ILE:HG22	2.01	0.43
1:PJ:61:ILE:HB	1:PJ:68:ILE:HG22	2.01	0.43
1:QA:45:GLN:OE1	1:QB:46:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:61:ILE:HB	1:QB:68:ILE:HG22	2.01	0.43
1:QC:61:ILE:HB	1:QC:68:ILE:HG22	2.01	0.43
1:RJ:7:PHE:O	1:RK:65:HIS:NE2	2.48	0.43
1:SB:61:ILE:HB	1:SB:68:ILE:HG22	2.01	0.43
1:TK:61:ILE:HB	1:TK:68:ILE:HG22	2.01	0.43
1:UJ:7:PHE:O	1:UK:65:HIS:NE2	2.48	0.43
1:VK:61:ILE:HB	1:VK:68:ILE:HG22	2.01	0.43
1:WF:61:ILE:HB	1:WF:68:ILE:HG22	2.01	0.43
1:XJ:61:ILE:HB	1:XJ:68:ILE:HG22	2.01	0.43
1:BI:61:ILE:HB	1:BI:68:ILE:HG22	2.01	0.43
1:CB:61:ILE:HB	1:CB:68:ILE:HG22	2.01	0.43
1:DA:61:ILE:HB	1:DA:68:ILE:HG22	2.01	0.43
1:EB:61:ILE:HB	1:EB:68:ILE:HG22	2.01	0.43
1:FA:61:ILE:HB	1:FA:68:ILE:HG22	2.01	0.43
1:FC:61:ILE:HB	1:FC:68:ILE:HG22	2.01	0.43
1:GH:61:ILE:HB	1:GH:68:ILE:HG22	2.01	0.43
1:HD:61:ILE:HB	1:HD:68:ILE:HG22	2.01	0.43
1:IE:61:ILE:HB	1:IE:68:ILE:HG22	2.01	0.43
1:IF:61:ILE:HB	1:IF:68:ILE:HG22	2.01	0.43
1:KB:61:ILE:HB	1:KB:68:ILE:HG22	2.01	0.43
1:LG:61:ILE:HB	1:LG:68:ILE:HG22	2.01	0.43
1:MD:61:ILE:HB	1:MD:68:ILE:HG22	2.01	0.43
1:NK:61:ILE:HB	1:NK:68:ILE:HG22	2.01	0.43
1:OH:61:ILE:HB	1:OH:68:ILE:HG22	2.01	0.43
1:QD:61:ILE:HB	1:QD:68:ILE:HG22	2.01	0.43
1:QE:61:ILE:HB	1:QE:68:ILE:HG22	2.01	0.43
1:SB:7:PHE:O	1:SC:65:HIS:NE2	2.45	0.43
1:TJ:61:ILE:HB	1:TJ:68:ILE:HG22	2.01	0.43
1:UK:61:ILE:HB	1:UK:68:ILE:HG22	2.01	0.43
1:VF:61:ILE:HB	1:VF:68:ILE:HG22	2.01	0.43
1:VH:61:ILE:HB	1:VH:68:ILE:HG22	2.01	0.43
1:WJ:7:PHE:O	1:WK:65:HIS:NE2	2.45	0.43
1:XA:61:ILE:HB	1:XA:68:ILE:HG22	2.01	0.43
1:XG:61:ILE:HB	1:XG:68:ILE:HG22	2.01	0.43
1:AA:61:ILE:HB	1:AA:68:ILE:HG22	2.01	0.43
1:AH:60:TYR:OH	1:AH:62:GLN:NE2	2.49	0.43
1:AK:61:ILE:HB	1:AK:68:ILE:HG22	2.01	0.43
1:BE:61:ILE:HB	1:BE:68:ILE:HG22	2.01	0.43
1:CE:61:ILE:HB	1:CE:68:ILE:HG22	2.01	0.43
1:CF:61:ILE:HB	1:CF:68:ILE:HG22	2.01	0.43
1:DC:61:ILE:HB	1:DC:68:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:61:ILE:HB	1:EA:68:ILE:HG22	2.01	0.43
1:EI:61:ILE:HB	1:EI:68:ILE:HG22	2.01	0.43
1:GE:61:ILE:HB	1:GE:68:ILE:HG22	2.01	0.43
1:HE:61:ILE:HB	1:HE:68:ILE:HG22	2.01	0.43
1:JK:61:ILE:HB	1:JK:68:ILE:HG22	2.01	0.43
1:KE:61:ILE:HB	1:KE:68:ILE:HG22	2.01	0.43
1:LA:61:ILE:HB	1:LA:68:ILE:HG22	2.01	0.43
1:LC:61:ILE:HB	1:LC:68:ILE:HG22	2.01	0.43
1:LE:61:ILE:HB	1:LE:68:ILE:HG22	2.01	0.43
1:MA:61:ILE:HB	1:MA:68:ILE:HG22	2.01	0.43
1:MB:61:ILE:HB	1:MB:68:ILE:HG22	2.01	0.43
1:MC:61:ILE:HB	1:MC:68:ILE:HG22	2.01	0.43
1:NA:60:TYR:OH	1:NA:62:GLN:NE2	2.49	0.43
1:NE:61:ILE:HB	1:NE:68:ILE:HG22	2.01	0.43
1:OF:61:ILE:HB	1:OF:68:ILE:HG22	2.01	0.43
1:OK:61:ILE:HB	1:OK:68:ILE:HG22	2.01	0.43
1:RA:61:ILE:HB	1:RA:68:ILE:HG22	2.01	0.43
1:RH:61:ILE:HB	1:RH:68:ILE:HG22	2.01	0.43
1:RI:61:ILE:HB	1:RI:68:ILE:HG22	2.01	0.43
1:SA:61:ILE:HB	1:SA:68:ILE:HG22	2.01	0.43
1:SI:42:LEU:HD11	1:SJ:52:ALA:HB1	2.01	0.43
1:SI:61:ILE:HB	1:SI:68:ILE:HG22	2.01	0.43
1:UE:61:ILE:HB	1:UE:68:ILE:HG22	2.01	0.43
1:WA:61:ILE:HB	1:WA:68:ILE:HG22	2.01	0.43
1:XK:61:ILE:HB	1:XK:68:ILE:HG22	2.01	0.43
1:AC:61:ILE:HB	1:AC:68:ILE:HG22	2.01	0.43
1:AD:61:ILE:HB	1:AD:68:ILE:HG22	2.01	0.43
1:BA:61:ILE:HB	1:BA:68:ILE:HG22	2.01	0.43
1:BF:61:ILE:HB	1:BF:68:ILE:HG22	2.01	0.43
1:BH:61:ILE:HB	1:BH:68:ILE:HG22	2.01	0.43
1:DE:61:ILE:HB	1:DE:68:ILE:HG22	2.01	0.43
1:JA:61:ILE:HB	1:JA:68:ILE:HG22	2.01	0.43
1:LD:60:TYR:OH	1:LD:62:GLN:NE2	2.49	0.43
1:MG:61:ILE:HB	1:MG:68:ILE:HG22	2.01	0.43
1:ND:61:ILE:HB	1:ND:68:ILE:HG22	2.01	0.43
1:NH:61:ILE:HB	1:NH:68:ILE:HG22	2.01	0.43
1:OI:61:ILE:HB	1:OI:68:ILE:HG22	2.01	0.43
1:RE:61:ILE:HB	1:RE:68:ILE:HG22	2.01	0.43
1:UH:61:ILE:HB	1:UH:68:ILE:HG22	2.01	0.43
1:VI:61:ILE:HB	1:VI:68:ILE:HG22	2.01	0.43
1:WC:61:ILE:HB	1:WC:68:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WD:61:ILE:HB	1:WD:68:ILE:HG22	2.01	0.43
1:WH:61:ILE:HB	1:WH:68:ILE:HG22	2.01	0.43
1:WK:61:ILE:HB	1:WK:68:ILE:HG22	2.01	0.43
1:AH:61:ILE:HB	1:AH:68:ILE:HG22	2.01	0.43
1:DD:61:ILE:HB	1:DD:68:ILE:HG22	2.01	0.43
1:FD:61:ILE:HB	1:FD:68:ILE:HG22	2.01	0.43
1:GI:61:ILE:HB	1:GI:68:ILE:HG22	2.01	0.43
1:HI:60:TYR:OH	1:HI:62:GLN:NE2	2.49	0.43
1:HI:61:ILE:HB	1:HI:68:ILE:HG22	2.01	0.43
1:JJ:60:TYR:OH	1:JJ:62:GLN:NE2	2.49	0.43
1:KA:61:ILE:HB	1:KA:68:ILE:HG22	2.01	0.43
1:NE:7:PHE:O	1:NF:65:HIS:NE2	2.48	0.43
1:PA:52:ALA:HB1	1:PK:42:LEU:HD11	1.99	0.43
1:PB:60:TYR:OH	1:PB:62:GLN:NE2	2.49	0.43
1:QA:61:ILE:HB	1:QA:68:ILE:HG22	2.01	0.43
1:RF:61:ILE:HB	1:RF:68:ILE:HG22	2.01	0.43
1:TE:61:ILE:HB	1:TE:68:ILE:HG22	2.01	0.43
1:TF:61:ILE:HB	1:TF:68:ILE:HG22	2.01	0.43
1:WJ:61:ILE:HB	1:WJ:68:ILE:HG22	2.01	0.43
1:XI:61:ILE:HB	1:XI:68:ILE:HG22	2.01	0.43
1:AB:7:PHE:O	1:AC:65:HIS:NE2	2.48	0.42
1:DB:61:ILE:HB	1:DB:68:ILE:HG22	2.01	0.42
1:DH:61:ILE:HB	1:DH:68:ILE:HG22	2.01	0.42
1:DK:61:ILE:HB	1:DK:68:ILE:HG22	2.01	0.42
1:FB:61:ILE:HB	1:FB:68:ILE:HG22	2.01	0.42
1:FE:61:ILE:HB	1:FE:68:ILE:HG22	2.01	0.42
1:GI:60:TYR:OH	1:GI:62:GLN:NE2	2.49	0.42
1:HB:61:ILE:HB	1:HB:68:ILE:HG22	2.01	0.42
1:IA:61:ILE:HB	1:IA:68:ILE:HG22	2.01	0.42
1:IG:61:ILE:HB	1:IG:68:ILE:HG22	2.01	0.42
1:JF:61:ILE:HB	1:JF:68:ILE:HG22	2.01	0.42
1:LB:61:ILE:HB	1:LB:68:ILE:HG22	2.01	0.42
1:MC:60:TYR:OH	1:MC:62:GLN:NE2	2.49	0.42
1:NF:61:ILE:HB	1:NF:68:ILE:HG22	2.01	0.42
1:PE:61:ILE:HB	1:PE:68:ILE:HG22	2.01	0.42
1:PF:61:ILE:HB	1:PF:68:ILE:HG22	2.01	0.42
1:UF:61:ILE:HB	1:UF:68:ILE:HG22	2.01	0.42
1:WH:60:TYR:OH	1:WH:62:GLN:NE2	2.49	0.42
1:AG:61:ILE:HB	1:AG:68:ILE:HG22	2.01	0.42
1:AJ:61:ILE:HB	1:AJ:68:ILE:HG22	2.01	0.42
1:CG:61:ILE:HB	1:CG:68:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:42:LEU:HD11	1:DD:52:ALA:HB1	2.01	0.42
1:IK:61:ILE:HB	1:IK:68:ILE:HG22	2.01	0.42
1:JA:52:ALA:HB1	1:JK:42:LEU:HD11	2.01	0.42
1:JI:61:ILE:HB	1:JI:68:ILE:HG22	2.01	0.42
1:KK:61:ILE:HB	1:KK:68:ILE:HG22	2.01	0.42
1:LH:61:ILE:HB	1:LH:68:ILE:HG22	2.01	0.42
1:MH:61:ILE:HB	1:MH:68:ILE:HG22	2.01	0.42
1:OF:60:TYR:OH	1:OF:62:GLN:NE2	2.49	0.42
1:PB:61:ILE:HB	1:PB:68:ILE:HG22	2.01	0.42
1:SJ:61:ILE:HB	1:SJ:68:ILE:HG22	2.01	0.42
1:TI:60:TYR:OH	1:TI:62:GLN:NE2	2.49	0.42
1:UD:61:ILE:HB	1:UD:68:ILE:HG22	2.01	0.42
1:VA:61:ILE:HB	1:VA:68:ILE:HG22	2.01	0.42
1:WD:60:TYR:OH	1:WD:62:GLN:NE2	2.49	0.42
1:XF:61:ILE:HB	1:XF:68:ILE:HG22	2.01	0.42
1:CA:61:ILE:HB	1:CA:68:ILE:HG22	2.01	0.42
1:CI:61:ILE:HB	1:CI:68:ILE:HG22	2.01	0.42
1:DE:60:TYR:OH	1:DE:62:GLN:NE2	2.49	0.42
1:ED:61:ILE:HB	1:ED:68:ILE:HG22	2.01	0.42
1:FH:61:ILE:HB	1:FH:68:ILE:HG22	2.01	0.42
1:FK:61:ILE:HB	1:FK:68:ILE:HG22	2.01	0.42
1:GB:61:ILE:HB	1:GB:68:ILE:HG22	2.01	0.42
1:HG:61:ILE:HB	1:HG:68:ILE:HG22	2.01	0.42
1:JG:42:LEU:HD11	1:JH:52:ALA:HB1	2.01	0.42
1:KI:61:ILE:HB	1:KI:68:ILE:HG22	2.01	0.42
1:OA:61:ILE:HB	1:OA:68:ILE:HG22	2.01	0.42
1:OE:61:ILE:HB	1:OE:68:ILE:HG22	2.01	0.42
1:OJ:61:ILE:HB	1:OJ:68:ILE:HG22	2.01	0.42
1:PC:61:ILE:HB	1:PC:68:ILE:HG22	2.01	0.42
1:PH:61:ILE:HB	1:PH:68:ILE:HG22	2.01	0.42
1:QA:42:LEU:HD11	1:QB:52:ALA:HB1	2.02	0.42
1:QK:61:ILE:HB	1:QK:68:ILE:HG22	2.01	0.42
1:TA:61:ILE:HB	1:TA:68:ILE:HG22	2.01	0.42
1:TB:60:TYR:OH	1:TB:62:GLN:NE2	2.49	0.42
1:TB:61:ILE:HB	1:TB:68:ILE:HG22	2.01	0.42
1:UB:61:ILE:HB	1:UB:68:ILE:HG22	2.01	0.42
1:VF:60:TYR:OH	1:VF:62:GLN:NE2	2.49	0.42
1:VG:61:ILE:HB	1:VG:68:ILE:HG22	2.01	0.42
1:XJ:60:TYR:OH	1:XJ:62:GLN:NE2	2.49	0.42
1:AD:60:TYR:OH	1:AD:62:GLN:NE2	2.49	0.42
1:BJ:61:ILE:HB	1:BJ:68:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:39:GLY:O	1:CG:71:GLU:N	2.47	0.42
1:CK:61:ILE:HB	1:CK:68:ILE:HG22	2.01	0.42
1:EJ:61:ILE:HB	1:EJ:68:ILE:HG22	2.01	0.42
1:GF:61:ILE:HB	1:GF:68:ILE:HG22	2.01	0.42
1:GG:61:ILE:HB	1:GG:68:ILE:HG22	2.01	0.42
1:NB:61:ILE:HB	1:NB:68:ILE:HG22	2.01	0.42
1:ND:7:PHE:O	1:NE:65:HIS:NE2	2.49	0.42
1:OG:61:ILE:HB	1:OG:68:ILE:HG22	2.01	0.42
1:QG:61:ILE:HB	1:QG:68:ILE:HG22	2.01	0.42
1:QI:61:ILE:HB	1:QI:68:ILE:HG22	2.01	0.42
1:RJ:61:ILE:HB	1:RJ:68:ILE:HG22	2.01	0.42
1:SB:60:TYR:OH	1:SB:62:GLN:NE2	2.49	0.42
1:SC:61:ILE:HB	1:SC:68:ILE:HG22	2.01	0.42
1:SD:61:ILE:HB	1:SD:68:ILE:HG22	2.01	0.42
1:TC:61:ILE:HB	1:TC:68:ILE:HG22	2.01	0.42
1:TH:61:ILE:HB	1:TH:68:ILE:HG22	2.01	0.42
1:UA:42:LEU:HD11	1:UB:52:ALA:HB1	2.00	0.42
1:VG:60:TYR:OH	1:VG:62:GLN:NE2	2.49	0.42
1:VJ:7:PHE:O	1:VK:65:HIS:NE2	2.49	0.42
1:AA:7:PHE:O	1:AB:65:HIS:NE2	2.47	0.42
1:CC:61:ILE:HB	1:CC:68:ILE:HG22	2.01	0.42
1:DD:60:TYR:OH	1:DD:62:GLN:NE2	2.49	0.42
1:EC:61:ILE:HB	1:EC:68:ILE:HG22	2.01	0.42
1:EE:61:ILE:HB	1:EE:68:ILE:HG22	2.01	0.42
1:EG:61:ILE:HB	1:EG:68:ILE:HG22	2.01	0.42
1:HC:61:ILE:HB	1:HC:68:ILE:HG22	2.01	0.42
1:II:61:ILE:HB	1:II:68:ILE:HG22	2.01	0.42
1:JB:61:ILE:HB	1:JB:68:ILE:HG22	2.01	0.42
1:OD:61:ILE:HB	1:OD:68:ILE:HG22	2.01	0.42
1:OJ:60:TYR:OH	1:OJ:62:GLN:NE2	2.49	0.42
1:SE:61:ILE:HB	1:SE:68:ILE:HG22	2.01	0.42
1:TJ:60:TYR:OH	1:TJ:62:GLN:NE2	2.49	0.42
1:UG:7:PHE:O	1:UH:65:HIS:NE2	2.50	0.42
1:VE:61:ILE:HB	1:VE:68:ILE:HG22	2.01	0.42
1:VJ:60:TYR:OH	1:VJ:62:GLN:NE2	2.49	0.42
1:VJ:61:ILE:HB	1:VJ:68:ILE:HG22	2.01	0.42
1:WG:61:ILE:HB	1:WG:68:ILE:HG22	2.01	0.42
1:XB:61:ILE:HB	1:XB:68:ILE:HG22	2.01	0.42
1:XD:61:ILE:HB	1:XD:68:ILE:HG22	2.01	0.42
1:AJ:7:PHE:O	1:AK:65:HIS:NE2	2.46	0.42
1:CF:60:TYR:OH	1:CF:62:GLN:NE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:60:TYR:OH	1:EB:62:GLN:NE2	2.49	0.42
1:FE:60:TYR:OH	1:FE:62:GLN:NE2	2.49	0.42
1:KF:7:PHE:O	1:KG:65:HIS:NE2	2.46	0.42
1:KG:61:ILE:HB	1:KG:68:ILE:HG22	2.01	0.42
1:LC:60:TYR:OH	1:LC:62:GLN:NE2	2.49	0.42
1:MI:61:ILE:HB	1:MI:68:ILE:HG22	2.01	0.42
1:NJ:61:ILE:HB	1:NJ:68:ILE:HG22	2.01	0.42
1:OB:61:ILE:HB	1:OB:68:ILE:HG22	2.01	0.42
1:OG:60:TYR:OH	1:OG:62:GLN:NE2	2.49	0.42
1:PA:61:ILE:HB	1:PA:68:ILE:HG22	2.01	0.42
1:PI:60:TYR:OH	1:PI:62:GLN:NE2	2.49	0.42
1:QI:60:TYR:OH	1:QI:62:GLN:NE2	2.49	0.42
1:UJ:61:ILE:HB	1:UJ:68:ILE:HG22	2.01	0.42
1:VD:61:ILE:HB	1:VD:68:ILE:HG22	2.01	0.42
1:WD:42:LEU:HD11	1:WE:52:ALA:HB1	2.01	0.42
1:AB:61:ILE:HB	1:AB:68:ILE:HG22	2.01	0.42
1:EK:61:ILE:HB	1:EK:68:ILE:HG22	2.01	0.42
1:FD:60:TYR:OH	1:FD:62:GLN:NE2	2.49	0.42
1:GK:61:ILE:HB	1:GK:68:ILE:HG22	2.01	0.42
1:IC:61:ILE:HB	1:IC:68:ILE:HG22	2.01	0.42
1:JA:7:PHE:O	1:JB:65:HIS:NE2	2.46	0.42
1:JD:61:ILE:HB	1:JD:68:ILE:HG22	2.01	0.42
1:LI:61:ILE:HB	1:LI:68:ILE:HG22	2.01	0.42
1:NA:61:ILE:HB	1:NA:68:ILE:HG22	2.01	0.42
1:PJ:60:TYR:OH	1:PJ:62:GLN:NE2	2.49	0.42
1:RB:61:ILE:HB	1:RB:68:ILE:HG22	2.01	0.42
1:AI:61:ILE:HB	1:AI:68:ILE:HG22	2.01	0.42
1:BD:61:ILE:HB	1:BD:68:ILE:HG22	2.01	0.42
1:CH:7:PHE:O	1:CI:65:HIS:NE2	2.49	0.42
1:GC:61:ILE:HB	1:GC:68:ILE:HG22	2.01	0.42
1:HF:61:ILE:HB	1:HF:68:ILE:HG22	2.01	0.42
1:IA:71:GLU:N	1:IK:39:GLY:O	2.39	0.42
1:KC:60:TYR:OH	1:KC:62:GLN:NE2	2.49	0.42
1:KI:60:TYR:OH	1:KI:62:GLN:NE2	2.49	0.42
1:QC:60:TYR:OH	1:QC:62:GLN:NE2	2.49	0.42
1:RH:7:PHE:O	1:RI:65:HIS:NE2	2.49	0.42
1:VB:61:ILE:HB	1:VB:68:ILE:HG22	2.01	0.42
1:AE:61:ILE:HB	1:AE:68:ILE:HG22	2.01	0.42
1:BB:61:ILE:HB	1:BB:68:ILE:HG22	2.01	0.42
1:DG:61:ILE:HB	1:DG:68:ILE:HG22	2.01	0.42
1:FF:61:ILE:HB	1:FF:68:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FG:61:ILE:HB	1:FG:68:ILE:HG22	2.01	0.42
1:GB:7:PHE:O	1:GC:65:HIS:NE2	2.50	0.42
1:HK:61:ILE:HB	1:HK:68:ILE:HG22	2.01	0.42
1:JB:60:TYR:OH	1:JB:62:GLN:NE2	2.49	0.42
1:JF:60:TYR:OH	1:JF:62:GLN:NE2	2.49	0.42
1:MK:61:ILE:HB	1:MK:68:ILE:HG22	2.01	0.42
1:QH:60:TYR:OH	1:QH:62:GLN:NE2	2.49	0.42
1:SG:61:ILE:HB	1:SG:68:ILE:HG22	2.01	0.42
1:SK:61:ILE:HB	1:SK:68:ILE:HG22	2.01	0.42
1:WB:61:ILE:HB	1:WB:68:ILE:HG22	2.01	0.42
1:WE:61:ILE:HB	1:WE:68:ILE:HG22	2.01	0.42
1:XE:61:ILE:HB	1:XE:68:ILE:HG22	2.01	0.42
1:AG:6:ASP:HB3	1:AG:7:PHE:H	1.77	0.42
1:BB:6:ASP:HB3	1:BB:7:PHE:H	1.77	0.42
1:BC:60:TYR:OH	1:BC:62:GLN:NE2	2.49	0.42
1:EA:65:HIS:NE2	1:EK:7:PHE:O	2.44	0.42
1:GB:60:TYR:OH	1:GB:62:GLN:NE2	2.49	0.42
1:HJ:61:ILE:HB	1:HJ:68:ILE:HG22	2.01	0.42
1:IE:7:PHE:O	1:IF:65:HIS:NE2	2.50	0.42
1:IF:60:TYR:OH	1:IF:62:GLN:NE2	2.49	0.42
1:JE:61:ILE:HB	1:JE:68:ILE:HG22	2.01	0.42
1:JK:60:TYR:OH	1:JK:62:GLN:NE2	2.49	0.42
1:MF:61:ILE:HB	1:MF:68:ILE:HG22	2.01	0.42
1:OD:60:TYR:OH	1:OD:62:GLN:NE2	2.49	0.42
1:OE:6:ASP:HB3	1:OE:7:PHE:H	1.77	0.42
1:RD:61:ILE:HB	1:RD:68:ILE:HG22	2.01	0.42
1:TK:6:ASP:HB3	1:TK:7:PHE:H	1.77	0.42
1:UA:61:ILE:HB	1:UA:68:ILE:HG22	2.01	0.42
1:UJ:6:ASP:HB3	1:UJ:7:PHE:H	1.77	0.42
1:WI:61:ILE:HB	1:WI:68:ILE:HG22	2.01	0.42
1:XB:60:TYR:OH	1:XB:62:GLN:NE2	2.49	0.42
1:XF:60:TYR:OH	1:XF:62:GLN:NE2	2.49	0.42
1:DF:61:ILE:HB	1:DF:68:ILE:HG22	2.01	0.41
1:DG:60:TYR:OH	1:DG:62:GLN:NE2	2.49	0.41
1:DJ:61:ILE:HB	1:DJ:68:ILE:HG22	2.01	0.41
1:DK:60:TYR:OH	1:DK:62:GLN:NE2	2.49	0.41
1:EF:61:ILE:HB	1:EF:68:ILE:HG22	2.01	0.41
1:GJ:61:ILE:HB	1:GJ:68:ILE:HG22	2.01	0.41
1:KF:61:ILE:HB	1:KF:68:ILE:HG22	2.01	0.41
1:KH:61:ILE:HB	1:KH:68:ILE:HG22	2.01	0.41
1:KJ:61:ILE:HB	1:KJ:68:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LK:61:ILE:HB	1:LK:68:ILE:HG22	2.01	0.41
1:MJ:61:ILE:HB	1:MJ:68:ILE:HG22	2.01	0.41
1:NA:65:HIS:NE2	1:NK:7:PHE:O	2.47	0.41
1:QA:42:LEU:HD12	1:QB:53:ILE:O	2.20	0.41
1:QF:61:ILE:HB	1:QF:68:ILE:HG22	2.01	0.41
1:QH:61:ILE:HB	1:QH:68:ILE:HG22	2.01	0.41
1:QJ:61:ILE:HB	1:QJ:68:ILE:HG22	2.01	0.41
1:RC:61:ILE:HB	1:RC:68:ILE:HG22	2.01	0.41
1:TI:61:ILE:HB	1:TI:68:ILE:HG22	2.01	0.41
1:VD:60:TYR:OH	1:VD:62:GLN:NE2	2.49	0.41
1:XK:60:TYR:OH	1:XK:62:GLN:NE2	2.49	0.41
1:CD:61:ILE:HB	1:CD:68:ILE:HG22	2.01	0.41
1:CJ:61:ILE:HB	1:CJ:68:ILE:HG22	2.01	0.41
1:FJ:61:ILE:HB	1:FJ:68:ILE:HG22	2.01	0.41
1:ID:61:ILE:HB	1:ID:68:ILE:HG22	2.01	0.41
1:IJ:61:ILE:HB	1:IJ:68:ILE:HG22	2.01	0.41
1:KH:60:TYR:OH	1:KH:62:GLN:NE2	2.49	0.41
1:LF:61:ILE:HB	1:LF:68:ILE:HG22	2.01	0.41
1:MF:60:TYR:OH	1:MF:62:GLN:NE2	2.49	0.41
1:NG:61:ILE:HB	1:NG:68:ILE:HG22	2.01	0.41
1:NI:61:ILE:HB	1:NI:68:ILE:HG22	2.01	0.41
1:PG:61:ILE:HB	1:PG:68:ILE:HG22	2.01	0.41
1:RC:60:TYR:OH	1:RC:62:GLN:NE2	2.49	0.41
1:TE:6:ASP:HB3	1:TE:7:PHE:H	1.77	0.41
1:VI:60:TYR:OH	1:VI:62:GLN:NE2	2.49	0.41
1:XB:6:ASP:HB3	1:XB:7:PHE:H	1.77	0.41
1:BF:60:TYR:OH	1:BF:62:GLN:NE2	2.49	0.41
1:BK:61:ILE:HB	1:BK:68:ILE:HG22	2.01	0.41
1:EE:42:LEU:HD11	1:EF:52:ALA:HB1	2.02	0.41
1:JC:61:ILE:HB	1:JC:68:ILE:HG22	2.01	0.41
1:LJ:61:ILE:HB	1:LJ:68:ILE:HG22	2.01	0.41
1:NG:6:ASP:HB3	1:NG:7:PHE:H	1.77	0.41
1:OC:61:ILE:HB	1:OC:68:ILE:HG22	2.01	0.41
1:PD:61:ILE:HB	1:PD:68:ILE:HG22	2.01	0.41
1:PI:61:ILE:HB	1:PI:68:ILE:HG22	2.01	0.41
1:PK:6:ASP:HB3	1:PK:7:PHE:H	1.77	0.41
1:SF:61:ILE:HB	1:SF:68:ILE:HG22	2.01	0.41
1:TD:7:PHE:O	1:TE:65:HIS:NE2	2.48	0.41
1:TG:61:ILE:HB	1:TG:68:ILE:HG22	2.01	0.41
1:UI:61:ILE:HB	1:UI:68:ILE:HG22	2.01	0.41
1:VC:61:ILE:HB	1:VC:68:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XC:61:ILE:HB	1:XC:68:ILE:HG22	2.01	0.41
1:FG:60:TYR:OH	1:FG:62:GLN:NE2	2.49	0.41
1:GJ:60:TYR:OH	1:GJ:62:GLN:NE2	2.49	0.41
1:HB:60:TYR:OH	1:HB:62:GLN:NE2	2.49	0.41
1:MG:60:TYR:OH	1:MG:62:GLN:NE2	2.49	0.41
1:PJ:7:PHE:O	1:PK:65:HIS:NE2	2.47	0.41
1:RB:6:ASP:HB3	1:RB:7:PHE:H	1.77	0.41
1:RF:60:TYR:OH	1:RF:62:GLN:NE2	2.49	0.41
1:TD:61:ILE:HB	1:TD:68:ILE:HG22	2.01	0.41
1:UG:61:ILE:HB	1:UG:68:ILE:HG22	2.01	0.41
1:XH:7:PHE:O	1:XI:65:HIS:NE2	2.43	0.41
1:AC:42:LEU:HD11	1:AD:52:ALA:HB1	2.03	0.41
1:BE:60:TYR:OH	1:BE:62:GLN:NE2	2.49	0.41
1:JB:6:ASP:HB3	1:JB:7:PHE:H	1.77	0.41
1:RE:60:TYR:OH	1:RE:62:GLN:NE2	2.49	0.41
1:WG:6:ASP:HB3	1:WG:7:PHE:H	1.77	0.41
1:BC:61:ILE:HB	1:BC:68:ILE:HG22	2.01	0.41
1:CI:60:TYR:OH	1:CI:62:GLN:NE2	2.49	0.41
1:EH:61:ILE:HB	1:EH:68:ILE:HG22	2.01	0.41
1:FK:60:TYR:OH	1:FK:62:GLN:NE2	2.49	0.41
1:KJ:60:TYR:OH	1:KJ:62:GLN:NE2	2.49	0.41
1:NH:60:TYR:OH	1:NH:62:GLN:NE2	2.49	0.41
1:OI:60:TYR:OH	1:OI:62:GLN:NE2	2.49	0.41
1:QF:7:PHE:O	1:QG:65:HIS:NE2	2.48	0.41
1:SH:61:ILE:HB	1:SH:68:ILE:HG22	2.01	0.41
1:CJ:6:ASP:HB3	1:CJ:7:PHE:H	1.77	0.41
1:EA:7:PHE:O	1:EB:65:HIS:NE2	2.46	0.41
1:HF:60:TYR:OH	1:HF:62:GLN:NE2	2.49	0.41
1:IA:60:TYR:OH	1:IA:62:GLN:NE2	2.49	0.41
1:LG:60:TYR:OH	1:LG:62:GLN:NE2	2.49	0.41
1:NC:61:ILE:HB	1:NC:68:ILE:HG22	2.01	0.41
1:NE:60:TYR:OH	1:NE:62:GLN:NE2	2.49	0.41
1:PE:6:ASP:HB3	1:PE:7:PHE:H	1.77	0.41
1:UC:61:ILE:HB	1:UC:68:ILE:HG22	2.01	0.41
1:BB:60:TYR:OH	1:BB:62:GLN:NE2	2.49	0.41
1:NJ:6:ASP:HB3	1:NJ:7:PHE:H	1.77	0.41
1:QJ:60:TYR:OH	1:QJ:62:GLN:NE2	2.49	0.41
1:RK:61:ILE:HB	1:RK:68:ILE:HG22	2.01	0.41
1:BG:61:ILE:HB	1:BG:68:ILE:HG22	2.01	0.41
1:HJ:60:TYR:OH	1:HJ:62:GLN:NE2	2.49	0.41
1:II:60:TYR:OH	1:II:62:GLN:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LF:60:TYR:OH	1:LF:62:GLN:NE2	2.49	0.41
1:MB:39:GLY:O	1:MC:71:GLU:N	2.48	0.41
1:RB:60:TYR:OH	1:RB:62:GLN:NE2	2.49	0.41
1:RC:6:ASP:HB3	1:RC:7:PHE:H	1.77	0.41
1:RG:61:ILE:HB	1:RG:68:ILE:HG22	2.01	0.41
1:TA:42:LEU:HD11	1:TB:52:ALA:HB1	2.03	0.41
1:UB:7:PHE:O	1:UC:65:HIS:NE2	2.49	0.41
1:UH:60:TYR:OH	1:UH:62:GLN:NE2	2.49	0.41
1:VH:7:PHE:O	1:VI:65:HIS:NE2	2.50	0.41
1:WD:6:ASP:HB3	1:WD:7:PHE:H	1.77	0.41
1:AD:6:ASP:HB3	1:AD:7:PHE:H	1.77	0.41
1:CA:60:TYR:OH	1:CA:62:GLN:NE2	2.49	0.41
1:UB:6:ASP:HB3	1:UB:7:PHE:H	1.77	0.41
1:UD:60:TYR:OH	1:UD:62:GLN:NE2	2.49	0.41
1:UE:60:TYR:OH	1:UE:62:GLN:NE2	2.49	0.41
1:VA:7:PHE:O	1:VB:65:HIS:NE2	2.52	0.41
1:EC:60:TYR:OH	1:EC:62:GLN:NE2	2.49	0.40
1:HE:6:ASP:HB3	1:HE:7:PHE:H	1.77	0.40
1:QA:60:TYR:OH	1:QA:62:GLN:NE2	2.49	0.40
1:QK:60:TYR:OH	1:QK:62:GLN:NE2	2.49	0.40
1:SC:60:TYR:OH	1:SC:62:GLN:NE2	2.49	0.40
1:TH:6:ASP:HB3	1:TH:7:PHE:H	1.77	0.40
1:BC:6:ASP:HB3	1:BC:7:PHE:H	1.77	0.40
1:BJ:6:ASP:HB3	1:BJ:7:PHE:H	1.77	0.40
1:GF:60:TYR:OH	1:GF:62:GLN:NE2	2.49	0.40
1:GG:60:TYR:OH	1:GG:62:GLN:NE2	2.49	0.40
1:SI:6:ASP:HB3	1:SI:7:PHE:H	1.77	0.40
1:UG:6:ASP:HB3	1:UG:7:PHE:H	1.77	0.40
1:WB:60:TYR:OH	1:WB:62:GLN:NE2	2.49	0.40
1:AB:60:TYR:OH	1:AB:62:GLN:NE2	2.49	0.40
1:FH:60:TYR:OH	1:FH:62:GLN:NE2	2.49	0.40
1:HB:39:GLY:O	1:HC:71:GLU:N	2.46	0.40
1:HD:7:PHE:O	1:HE:65:HIS:NE2	2.50	0.40
1:HD:60:TYR:OH	1:HD:62:GLN:NE2	2.49	0.40
1:HG:60:TYR:OH	1:HG:62:GLN:NE2	2.49	0.40
1:KE:60:TYR:OH	1:KE:62:GLN:NE2	2.49	0.40
1:ND:60:TYR:OH	1:ND:62:GLN:NE2	2.49	0.40
1:QA:65:HIS:NE2	1:QK:7:PHE:O	2.51	0.40
1:RB:7:PHE:O	1:RC:65:HIS:NE2	2.51	0.40
1:GF:6:ASP:HB3	1:GF:7:PHE:H	1.77	0.40
1:JA:39:GLY:O	1:JB:71:GLU:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:60:TYR:OH	1:KA:62:GLN:NE2	2.49	0.40
1:LK:6:ASP:HB3	1:LK:7:PHE:H	1.77	0.40
1:TD:60:TYR:OH	1:TD:62:GLN:NE2	2.49	0.40
1:TK:60:TYR:OH	1:TK:62:GLN:NE2	2.49	0.40
1:CI:42:LEU:HD11	1:CJ:52:ALA:HB1	2.04	0.40
1:GD:60:TYR:OH	1:GD:62:GLN:NE2	2.49	0.40
1:MG:7:PHE:O	1:MH:65:HIS:NE2	2.53	0.40
1:PD:60:TYR:OH	1:PD:62:GLN:NE2	2.49	0.40
1:PH:6:ASP:HB3	1:PH:7:PHE:H	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	ED	45	GLN
1	QK	45	GLN
1	SD	45	GLN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

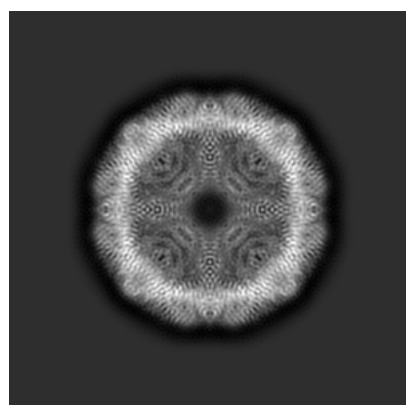
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4443. These allow visual inspection of the internal detail of the map and identification of artifacts.

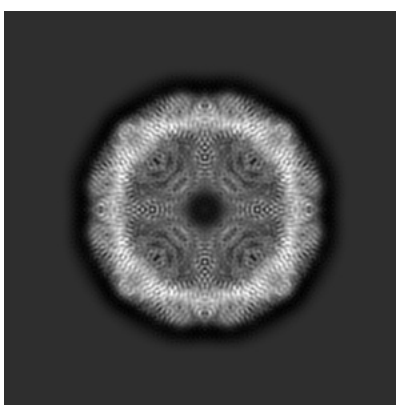
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

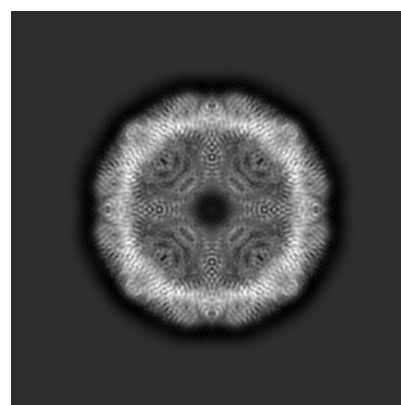
6.1.1 Primary map



X



Y

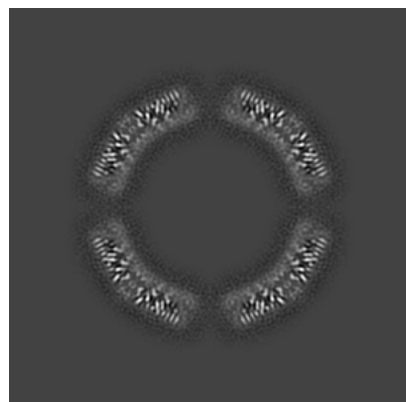


Z

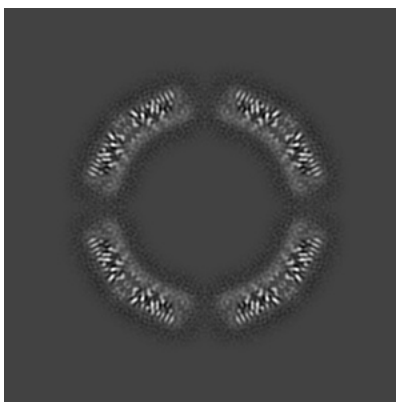
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

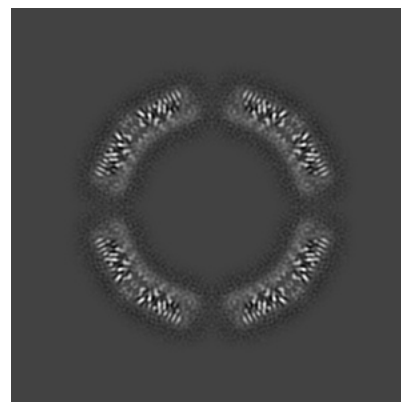
6.2.1 Primary map



X Index: 110



Y Index: 110

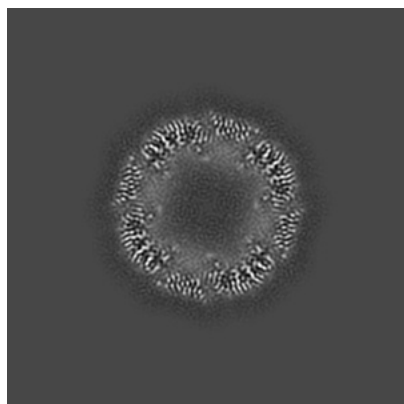


Z Index: 110

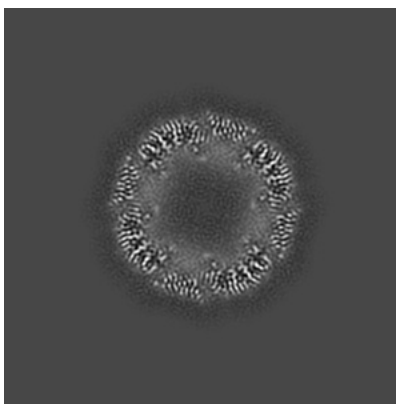
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

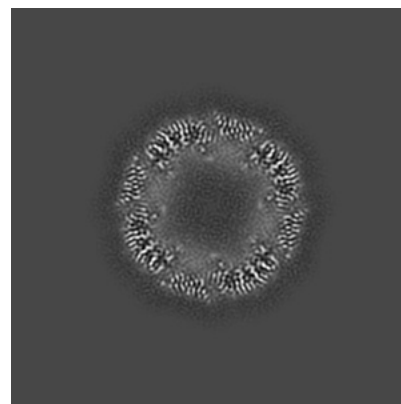
6.3.1 Primary map



X Index: 67



Y Index: 67

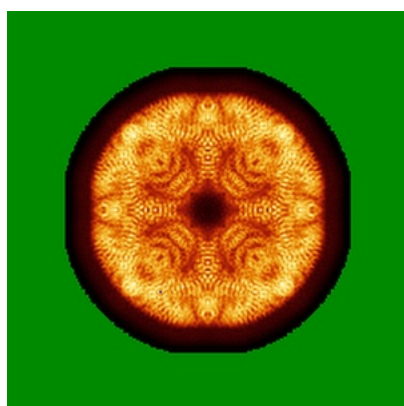


Z Index: 67

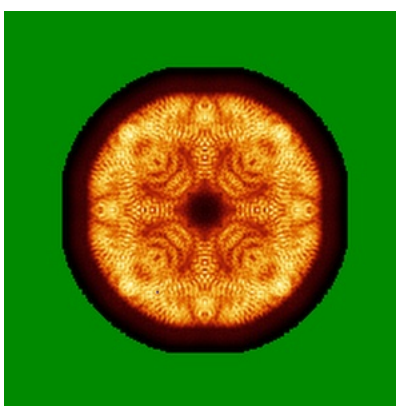
The images above show the largest variance slices of the map in three orthogonal directions.

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

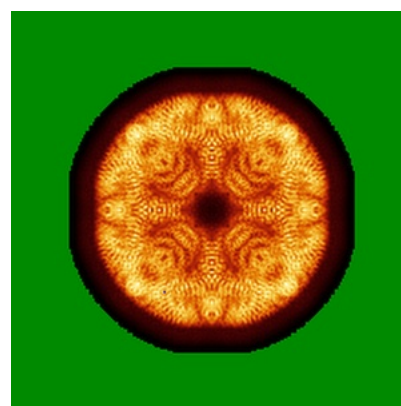
6.4.1 Primary map



X



Y

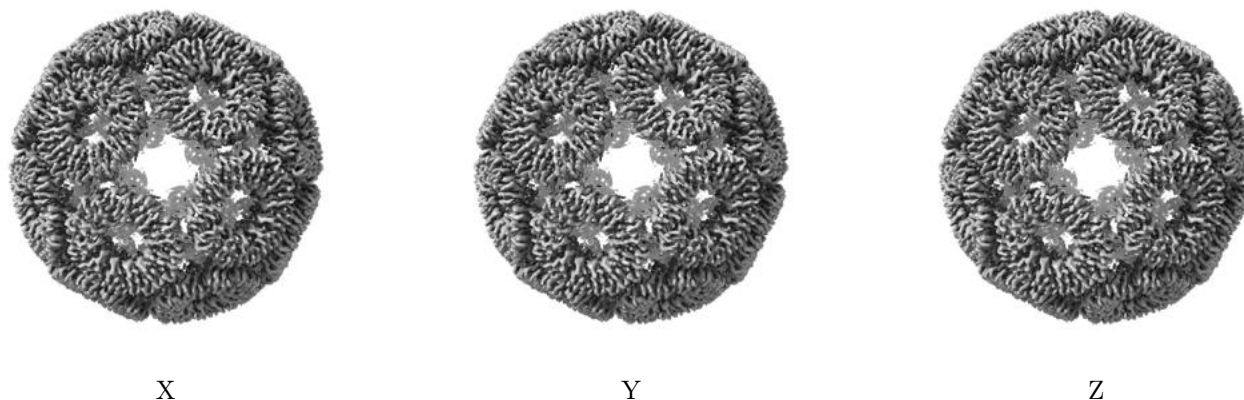


Z

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.

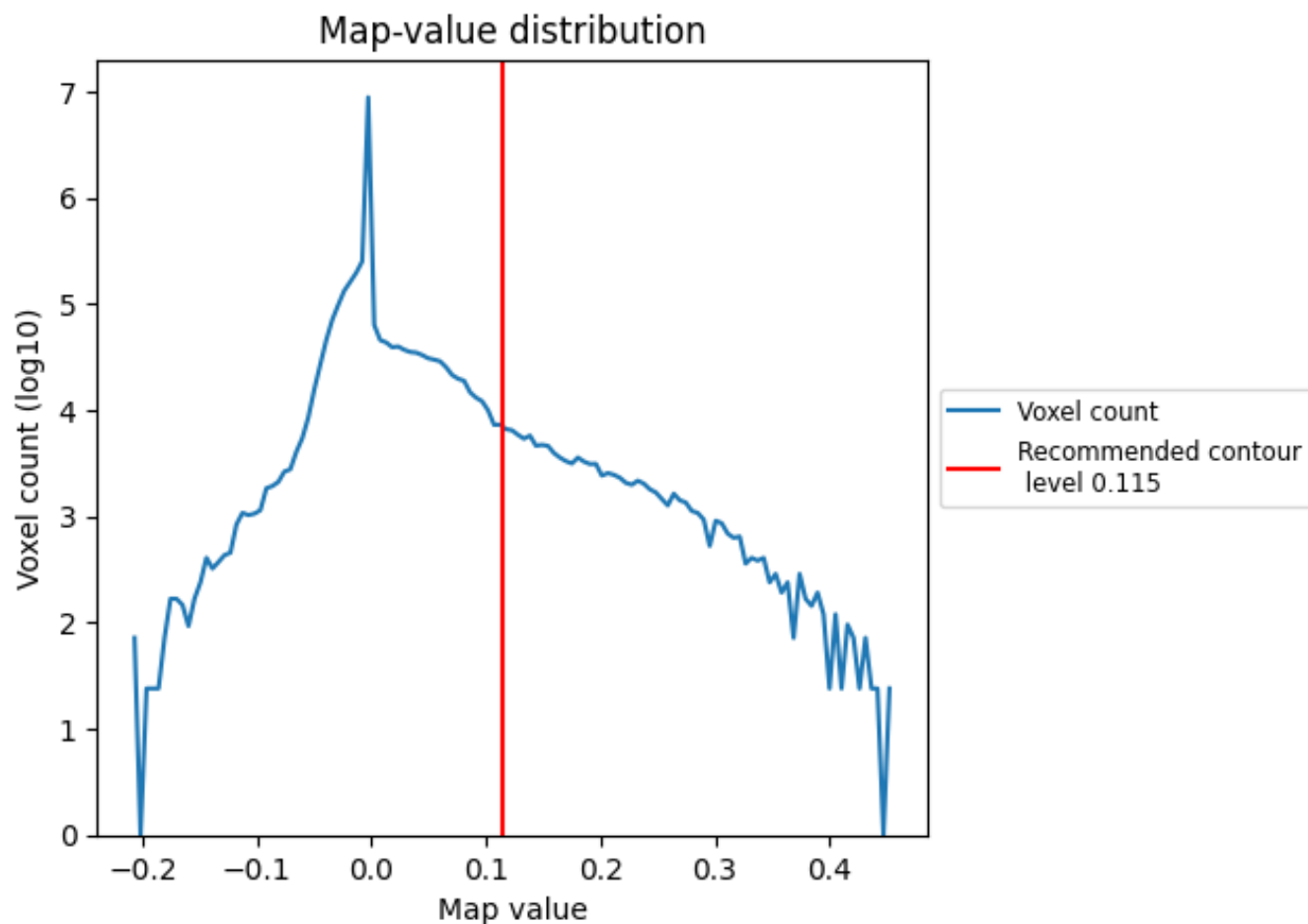
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

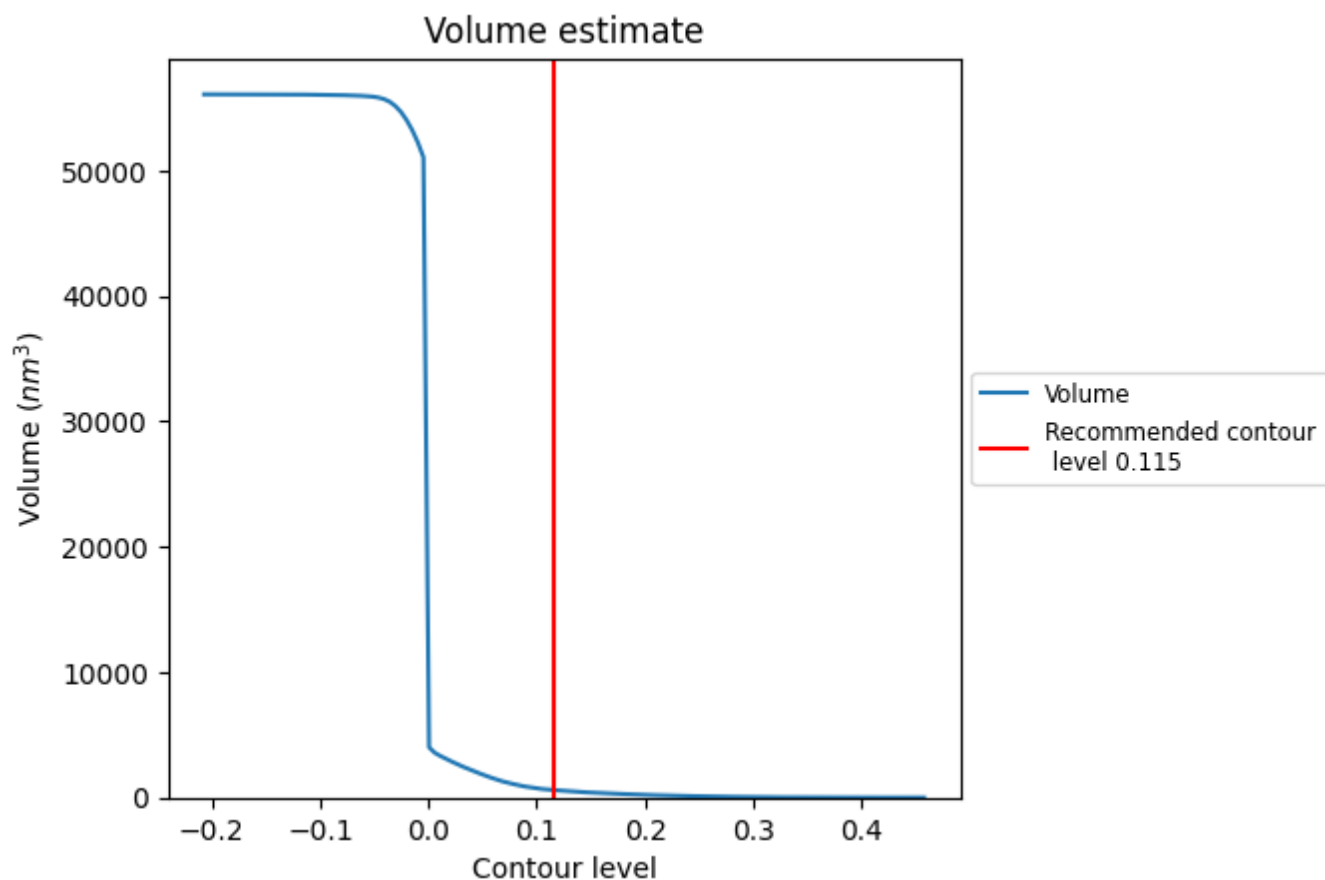
This section contains the results of statistical analysis of the map.

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.

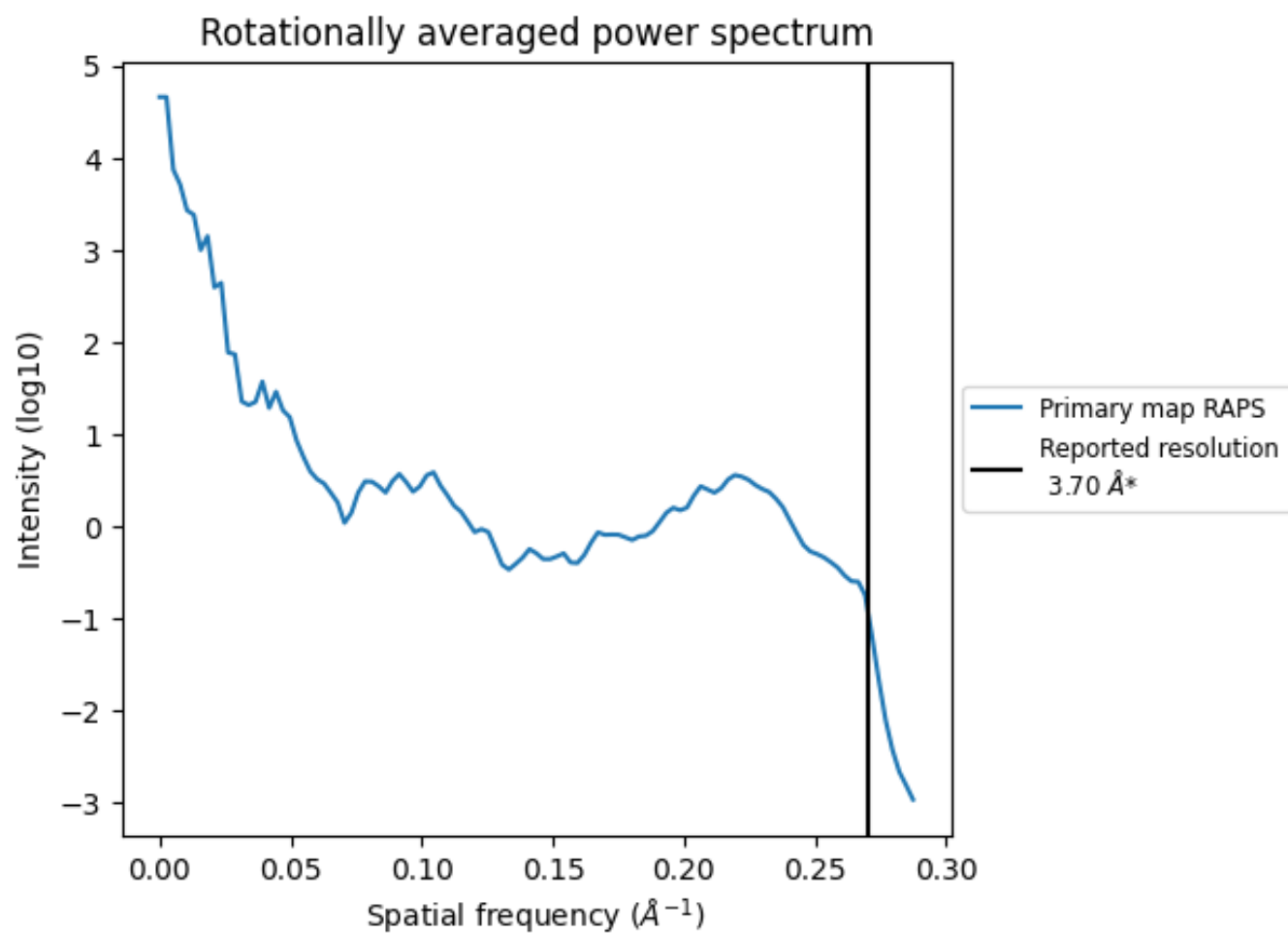
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm³; this corresponds to an approximate mass of 545 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 ⓘ

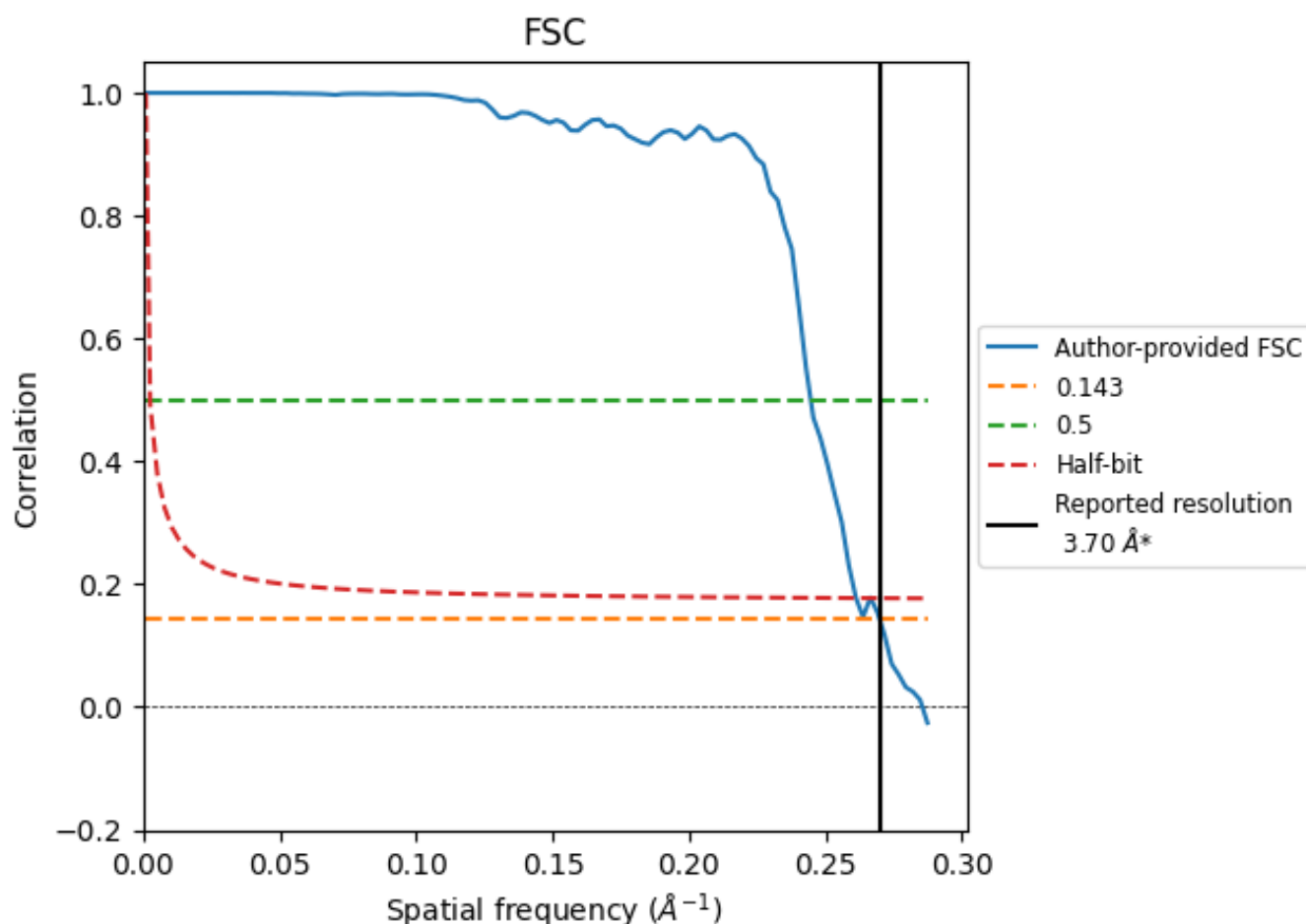


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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](#)

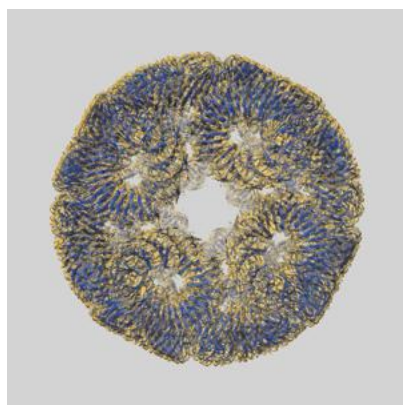
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.09	3.83
Unmasked-calculated*	-	-	-

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

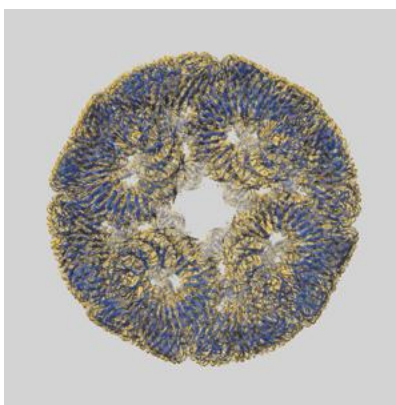
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4443 and PDB model 6RVV. Per-residue inclusion information can be found in section 3 on page 46.

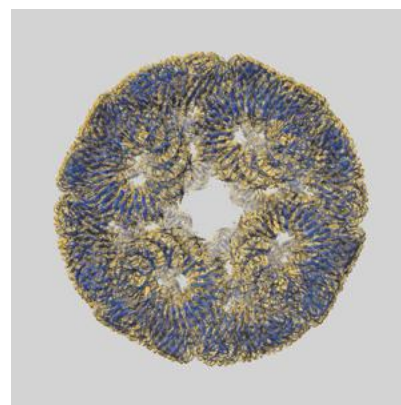
9.1 Map-model overlay [i](#)



X



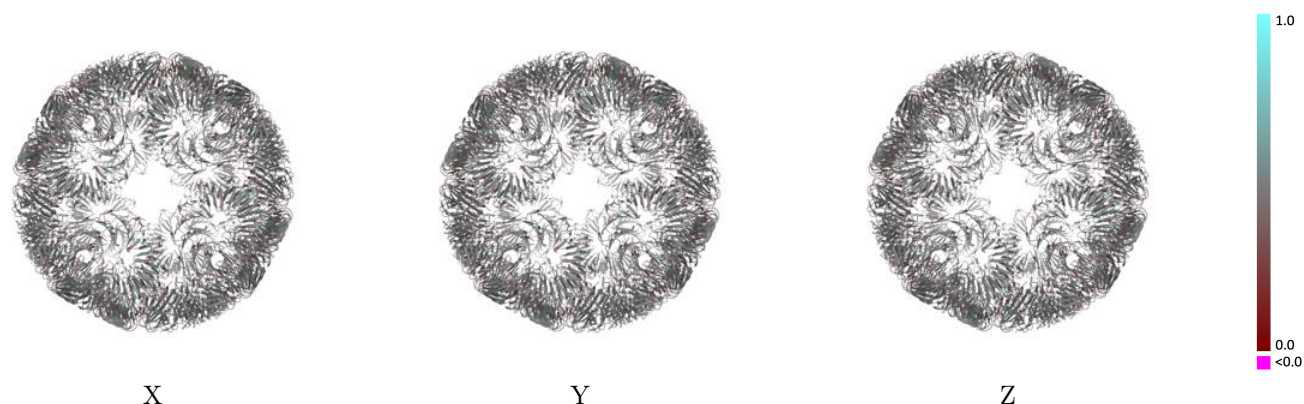
Y



Z

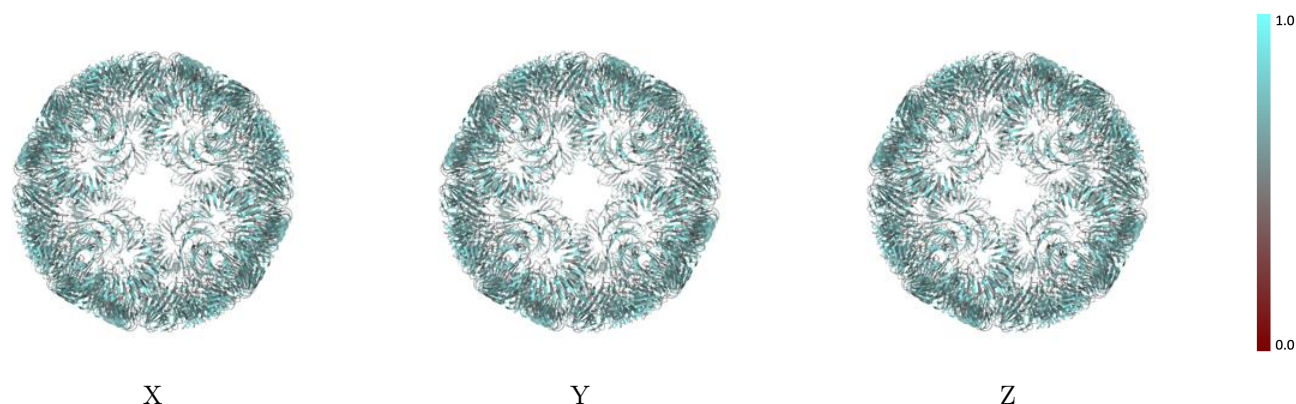
The images above show the 3D surface view of the map at the recommended contour level 0.115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



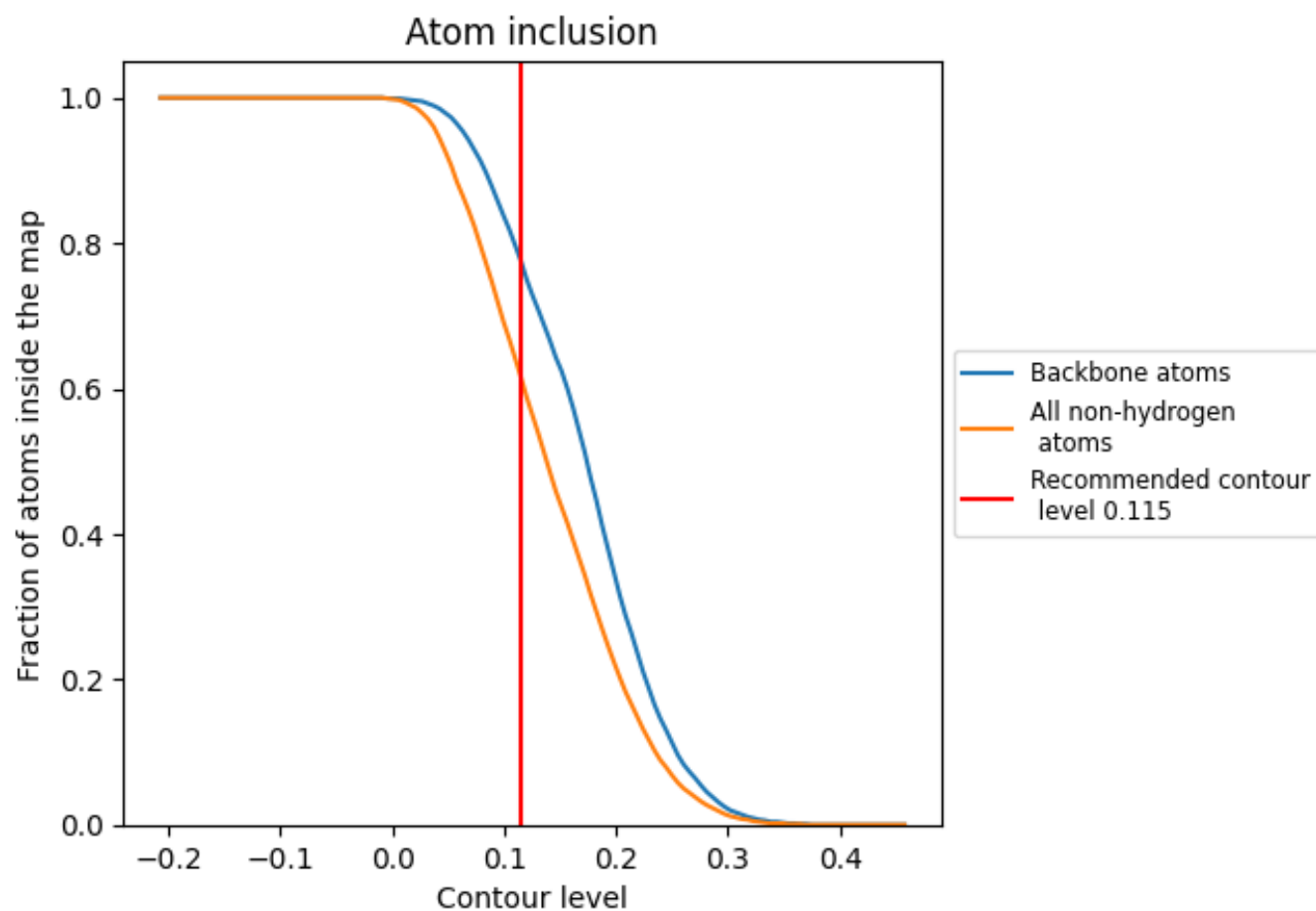
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 62% 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	 0.6150	 0.4450
AA	 0.6070	 0.4520
AB	 0.5860	 0.4450
AC	 0.6120	 0.4540
AD	 0.6120	 0.4410
AE	 0.6340	 0.4470
AF	 0.6310	 0.4470
AG	 0.6310	 0.4420
AH	 0.6260	 0.4550
AI	 0.6190	 0.4380
AJ	 0.6050	 0.4350
AK	 0.6060	 0.4430
BA	 0.6050	 0.4530
BB	 0.5980	 0.4440
BC	 0.6070	 0.4490
BD	 0.6120	 0.4390
BE	 0.6310	 0.4440
BF	 0.6290	 0.4480
BG	 0.6310	 0.4460
BH	 0.6260	 0.4640
BI	 0.6220	 0.4440
BJ	 0.5980	 0.4410
BK	 0.6060	 0.4400
CA	 0.6170	 0.4510
CB	 0.5860	 0.4430
CC	 0.6120	 0.4510
CD	 0.6050	 0.4350
CE	 0.6290	 0.4480
CF	 0.6460	 0.4510
CG	 0.6300	 0.4460
CH	 0.6280	 0.4610
CI	 0.6220	 0.4410
CJ	 0.6100	 0.4400
CK	 0.6010	 0.4400
DA	 0.6120	 0.4530



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Chain	Atom inclusion	Q-score
DB	 0.5900	 0.4400
DC	 0.6170	 0.4460
DD	 0.6100	 0.4320
DE	 0.6190	 0.4480
DF	 0.6430	 0.4460
DG	 0.6190	 0.4420
DH	 0.6340	 0.4550
DI	 0.6190	 0.4420
DJ	 0.6020	 0.4390
DK	 0.6090	 0.4440
EA	 0.6110	 0.4520
EB	 0.5940	 0.4400
EC	 0.6060	 0.4500
ED	 0.6140	 0.4330
EE	 0.6170	 0.4500
EF	 0.6240	 0.4510
EG	 0.6170	 0.4390
EH	 0.6290	 0.4570
EI	 0.6190	 0.4430
EJ	 0.6050	 0.4420
EK	 0.6060	 0.4420
FA	 0.6070	 0.4530
FB	 0.5880	 0.4400
FC	 0.6100	 0.4520
FD	 0.6150	 0.4370
FE	 0.6170	 0.4480
FF	 0.6460	 0.4490
FG	 0.6360	 0.4410
FH	 0.6260	 0.4590
FI	 0.6190	 0.4450
FJ	 0.6050	 0.4440
FK	 0.5990	 0.4440
GA	 0.6140	 0.4520
GB	 0.5890	 0.4390
GC	 0.6120	 0.4450
GD	 0.6120	 0.4360
GE	 0.6300	 0.4460
GF	 0.6230	 0.4500
GG	 0.6220	 0.4450
GH	 0.6220	 0.4570
GI	 0.6170	 0.4370
GJ	 0.5950	 0.4400

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Chain	Atom inclusion	Q-score
GK	 0.5920	 0.4360
HA	 0.6100	 0.4520
HB	 0.6020	 0.4430
HC	 0.6070	 0.4450
HD	 0.6100	 0.4340
HE	 0.6330	 0.4470
HF	 0.6230	 0.4510
HG	 0.6190	 0.4420
HH	 0.6290	 0.4580
HI	 0.6150	 0.4390
HJ	 0.5980	 0.4380
HK	 0.5920	 0.4410
IA	 0.6170	 0.4500
IB	 0.5900	 0.4460
IC	 0.6110	 0.4510
ID	 0.6140	 0.4370
IE	 0.6290	 0.4500
IF	 0.6260	 0.4540
IG	 0.6310	 0.4400
IH	 0.6220	 0.4580
II	 0.6310	 0.4380
IJ	 0.6050	 0.4360
IK	 0.5970	 0.4400
JA	 0.6120	 0.4530
JB	 0.5880	 0.4430
JC	 0.6140	 0.4500
JD	 0.6160	 0.4420
JE	 0.6280	 0.4480
JF	 0.6260	 0.4520
JG	 0.6340	 0.4410
JH	 0.6360	 0.4590
JI	 0.6330	 0.4400
JJ	 0.5940	 0.4370
JK	 0.6110	 0.4400
KA	 0.6110	 0.4490
KB	 0.5920	 0.4390
KC	 0.6100	 0.4490
KD	 0.6170	 0.4360
KE	 0.6260	 0.4490
KF	 0.6360	 0.4470
KG	 0.6230	 0.4420
KH	 0.6330	 0.4610

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Chain	Atom inclusion	Q-score
KI	 0.6330	 0.4410
KJ	 0.6110	 0.4370
KK	 0.6010	 0.4390
LA	 0.6110	 0.4500
LB	 0.5870	 0.4390
LC	 0.6160	 0.4460
LD	 0.6160	 0.4330
LE	 0.6260	 0.4500
LF	 0.6150	 0.4480
LG	 0.6170	 0.4380
LH	 0.6260	 0.4570
LI	 0.6220	 0.4410
LJ	 0.6100	 0.4320
LK	 0.6060	 0.4400
MA	 0.6100	 0.4510
MB	 0.5950	 0.4400
MC	 0.6090	 0.4480
MD	 0.6160	 0.4380
ME	 0.6280	 0.4500
MF	 0.6330	 0.4510
MG	 0.6210	 0.4410
MH	 0.6210	 0.4600
MI	 0.6260	 0.4390
MJ	 0.6060	 0.4380
MK	 0.5990	 0.4380
NA	 0.6160	 0.4510
NB	 0.5920	 0.4450
NC	 0.6100	 0.4510
ND	 0.6120	 0.4350
NE	 0.6310	 0.4450
NF	 0.6310	 0.4500
NG	 0.6280	 0.4430
NH	 0.6280	 0.4580
NI	 0.6210	 0.4380
NJ	 0.5970	 0.4360
NK	 0.5990	 0.4410
OA	 0.6100	 0.4530
OB	 0.5950	 0.4420
OC	 0.6090	 0.4530
OD	 0.6210	 0.4370
OE	 0.6280	 0.4470
OF	 0.6420	 0.4420

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Chain	Atom inclusion	Q-score
OG	 0.6240	 0.4400
OH	 0.6310	 0.4560
OI	 0.6240	 0.4400
OJ	 0.6070	 0.4330
OK	 0.6060	 0.4440
PA	 0.6070	 0.4480
PB	 0.6020	 0.4430
PC	 0.6070	 0.4490
PD	 0.6170	 0.4390
PE	 0.6330	 0.4470
PF	 0.6330	 0.4460
PG	 0.6180	 0.4430
PH	 0.6260	 0.4570
PI	 0.6180	 0.4390
PJ	 0.6060	 0.4360
PK	 0.6060	 0.4370
QA	 0.6110	 0.4550
QB	 0.5920	 0.4390
QC	 0.6110	 0.4510
QD	 0.6140	 0.4350
QE	 0.6230	 0.4480
QF	 0.6330	 0.4510
QG	 0.6260	 0.4410
QH	 0.6260	 0.4570
QI	 0.6260	 0.4400
QJ	 0.6180	 0.4360
QK	 0.6090	 0.4450
RA	 0.6110	 0.4490
RB	 0.6090	 0.4320
RC	 0.6070	 0.4460
RD	 0.6070	 0.4360
RE	 0.6260	 0.4470
RF	 0.6410	 0.4510
RG	 0.6280	 0.4450
RH	 0.6260	 0.4620
RI	 0.6230	 0.4420
RJ	 0.6090	 0.4380
RK	 0.6060	 0.4430
SA	 0.6140	 0.4500
SB	 0.5890	 0.4410
SC	 0.6060	 0.4470
SD	 0.6180	 0.4360

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Chain	Atom inclusion	Q-score
SE	 0.6150	 0.4500
SF	 0.6410	 0.4450
SG	 0.6180	 0.4390
SH	 0.6300	 0.4600
SI	 0.6210	 0.4440
SJ	 0.5970	 0.4380
SK	 0.5970	 0.4370
TA	 0.6090	 0.4470
TB	 0.5920	 0.4400
TC	 0.6060	 0.4500
TD	 0.6090	 0.4380
TE	 0.6430	 0.4440
TF	 0.6360	 0.4460
TG	 0.6260	 0.4420
TH	 0.6280	 0.4540
TI	 0.6260	 0.4350
TJ	 0.6070	 0.4320
TK	 0.5970	 0.4370
UA	 0.6180	 0.4480
UB	 0.6060	 0.4370
UC	 0.6110	 0.4440
UD	 0.6110	 0.4350
UE	 0.6260	 0.4480
UF	 0.6330	 0.4540
UG	 0.6180	 0.4440
UH	 0.6300	 0.4600
UI	 0.6210	 0.4400
UJ	 0.6010	 0.4380
UK	 0.6040	 0.4390
VA	 0.6140	 0.4470
VB	 0.5920	 0.4440
VC	 0.6060	 0.4490
VD	 0.6140	 0.4400
VE	 0.6300	 0.4500
VF	 0.6380	 0.4500
VG	 0.6260	 0.4440
VH	 0.6280	 0.4590
VI	 0.6210	 0.4400
VJ	 0.6060	 0.4350
VK	 0.6090	 0.4370
WA	 0.6000	 0.4470
WB	 0.5950	 0.4370

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Chain	Atom inclusion	Q-score
WC	 0.6040	 0.4440
WD	 0.6140	 0.4370
WE	 0.6380	 0.4440
WF	 0.6280	 0.4500
WG	 0.6210	 0.4400
WH	 0.6260	 0.4570
WI	 0.6110	 0.4370
WJ	 0.6060	 0.4360
WK	 0.6060	 0.4380
XA	 0.6040	 0.4520
XB	 0.5850	 0.4390
XC	 0.6060	 0.4480
XD	 0.6160	 0.4390
XE	 0.6300	 0.4390
XF	 0.6330	 0.4470
XG	 0.6350	 0.4390
XH	 0.6300	 0.4560
XI	 0.6280	 0.4370
XJ	 0.6010	 0.4310
XK	 0.6010	 0.4420