wwPDB EM Validation Summary Report

Jun 23, 2024 – 05:19 PM EDT

PDB ID	:	6Q3G
EMDB ID	:	EMD-4459
Title	:	Structure of native bacteriophage P68
Authors	:	Dominik, H.; Karel, S.; Fuzik, T.; Plevka, P.
Deposited on	:	2018-12-04
Resolution	:	3.80 Å(reported)
Based on initial models	:	6IAT, 6IAW, 6IAB, 6IAC

This is a wwPDB EM Validation Summary 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:

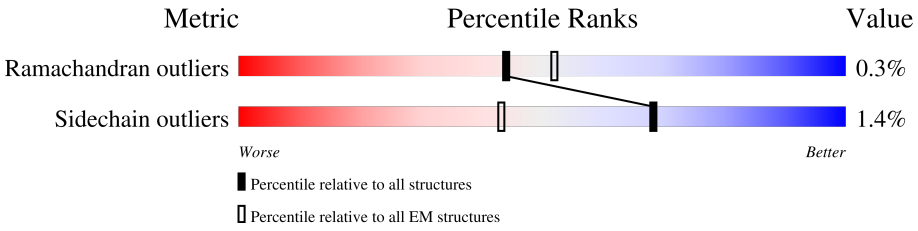
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.80 Å.

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



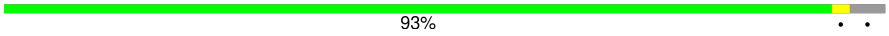
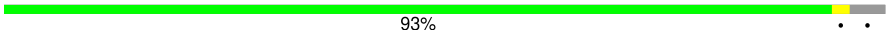
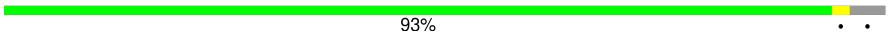
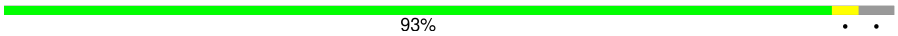
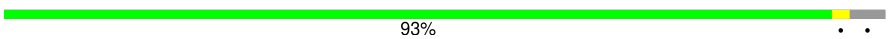
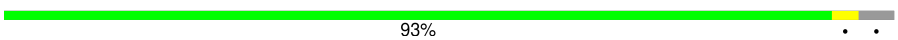
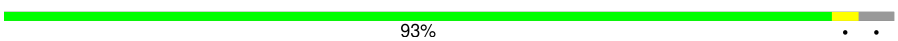
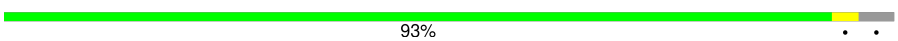
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A1	408	93%
1	A3	408	93%
1	A4	408	93%
1	A6	408	93%
1	A7	408	93%
1	A8	408	93%
1	AD	408	82% 13%
1	AE	408	92% 6%
1	AG	408	93%
1	AJ	408	82% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AK	408	
1	AL	408	
1	AP	408	
1	AQ	408	
1	AR	408	
1	AS	408	
1	B1	408	
1	B3	408	
1	B4	408	
1	B6	408	
1	B7	408	
1	B8	408	
1	BD	408	
1	BE	408	
1	BG	408	
1	BJ	408	
1	BK	408	
1	BL	408	
1	BP	408	
1	BQ	408	
1	BR	408	
1	BS	408	
1	C1	408	
1	C3	408	
1	C4	408	

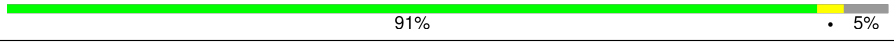
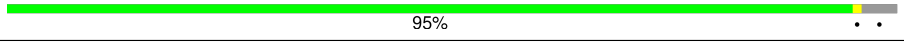
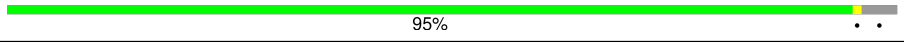
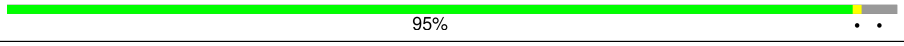
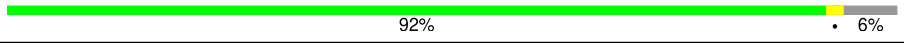
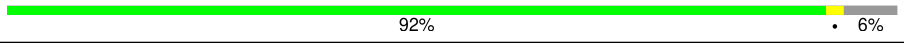
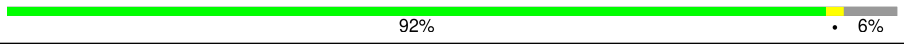
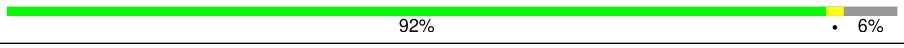
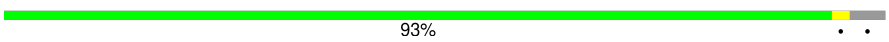
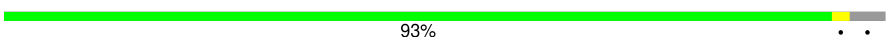
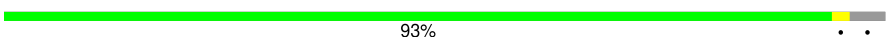
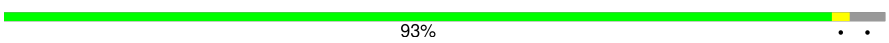
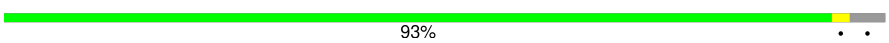
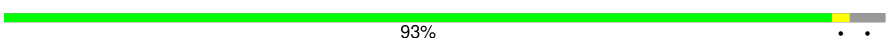
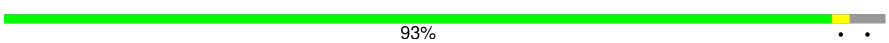
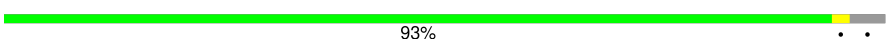
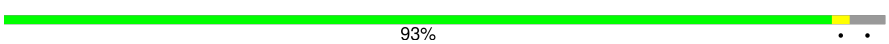
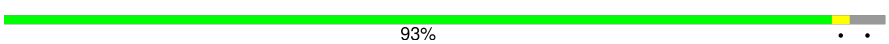
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	C6	408	92% • 6%
1	C7	408	92% • 6%
1	C8	408	92% • 6%
1	CD	408	92% • 5%
1	CE	408	92% • 6%
1	CG	408	92% • 6%
1	CJ	408	92% • 5%
1	CK	408	92% • 5%
1	CL	408	92% • 6%
1	CP	408	92% • 5%
1	CQ	408	92% • 6%
1	CR	408	92% • 6%
1	CS	408	91% • 5%
1	D1	408	95% • •
1	D3	408	95% • •
1	D4	408	95% • •
1	D6	408	95% • •
1	D7	408	95% • •
1	D8	408	95% • •
1	DD	408	91% • 5%
1	DE	408	95% • •
1	DG	408	95% • •
1	DJ	408	91% • 5%
1	DK	408	91% • 5%
1	DL	408	95% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DP	408	
1	DQ	408	
1	DR	408	
1	FE	408	
1	I1	408	
1	I3	408	
1	I4	408	
1	I6	408	
1	I7	408	
1	I8	408	
1	IG	408	
1	IL	408	
1	IQ	408	
1	IR	408	
1	IS	408	
1	J1	408	
1	J3	408	
1	J4	408	
1	J6	408	
1	J7	408	
1	J8	408	
1	JG	408	
1	JL	408	
1	JQ	408	
1	JR	408	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	JS	408	91% • 6%
1	K1	408	92% • 6%
1	K3	408	92% • 6%
1	K4	408	92% • 6%
1	K6	408	92% • 6%
1	K7	408	92% • 6%
1	K8	408	92% • 6%
1	KD	408	91% • 6%
1	KE	408	92% • 6%
1	KG	408	92% • 6%
1	KJ	408	91% • 6%
1	KK	408	91% • 6%
1	KL	408	92% • 6%
1	KP	408	91% • 6%
1	KQ	408	92% • 6%
1	KR	408	92% • 6%
1	KS	408	92% • 5%
1	L1	408	95% • •
1	L3	408	95% • •
1	L4	408	95% • •
1	L6	408	95% • •
1	L7	408	95% • •
1	L8	408	95% • •
1	LD	408	92% • 5%
1	LE	408	93% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	LG	408	95%
1	LJ	408	92% 5%
1	LK	408	92% 5%
1	LL	408	95%
1	LP	408	92% 5%
1	LQ	408	95%
1	LR	408	95%
1	ME	408	92% 6%
1	NE	408	95%
1	Q1	408	92% 6%
1	Q3	408	92% 6%
1	Q4	408	92% 6%
1	Q6	408	92% 6%
1	Q7	408	92% 6%
1	Q8	408	92% 6%
1	QG	408	92% 6%
1	QL	408	92% 6%
1	QQ	408	92% 6%
1	QR	408	92% 6%
1	R1	408	93%
1	R3	408	93%
1	R4	408	93%
1	R6	408	93%
1	R7	408	93%
1	R8	408	93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	RG	408	93%
1	RL	408	93%
1	RQ	408	93%
1	RR	408	93%
1	S1	408	92% 6%
1	S3	408	92% 6%
1	S4	408	92% 6%
1	S6	408	92% 6%
1	S7	408	92% 6%
1	S8	408	92% 6%
1	SE	408	92% 6%
1	SG	408	92% 6%
1	SL	408	92% 6%
1	SQ	408	92% 6%
1	SR	408	92% 6%
1	T1	408	95%
1	T3	408	95%
1	T4	408	95%
1	T6	408	95%
1	T7	408	95%
1	T8	408	95%
1	TE	408	93%
1	TG	408	95%
1	TL	408	95%
1	TQ	408	95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	TR	408	95%
1	UE	408	92% 6%
1	VE	408	95%
1	X1	408	92% 6%
1	X4	408	92% 6%
1	Y1	408	93%
1	Y3	408	95%
1	Y4	408	93%
1	Y6	408	92% 6%
1	Y7	408	92% 6%
1	Y8	408	92% 6%
1	YG	408	92% 6%
1	YL	408	92% 6%
1	YQ	408	95%
1	YR	408	92% 6%
1	Z1	408	92% 6%
1	Z4	408	92% 6%
1	Z6	408	93%
1	Z7	408	93%
1	Z8	408	93%
1	ZG	408	93%
1	ZL	408	93%
1	ZR	408	93%
1	a1	408	95%
1	a4	408	95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a6	408	92% 6%
1	a7	408	92% 6%
1	a8	408	92% 6%
1	aE	408	92% 6%
1	aG	408	92% 6%
1	aL	408	92% 6%
1	aR	408	92% 6%
1	b3	408	95%
1	b6	408	95%
1	b7	408	95%
1	b8	408	95%
1	bE	408	93%
1	bG	408	95%
1	bL	408	95%
1	bQ	408	92% 6%
1	bR	408	95%
1	cE	408	92% 6%
1	cQ	408	93%
1	dE	408	95%
1	dQ	408	92% 6%
1	eQ	408	95%
1	f1	408	92% 6%
1	f4	408	92% 6%
1	g1	408	93%
1	g4	408	93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	g6	408	92% · 6%
1	g7	408	92% · 6%
1	g8	408	92% · 6%
1	gG	408	92% · 6%
1	gL	408	95% · ·
1	gR	408	92% · 6%
1	h1	408	92% · 6%
1	h4	408	92% · 6%
1	h6	408	93% · ·
1	h7	408	93% · ·
1	h8	408	93% · ·
1	hG	408	93% · ·
1	hR	408	93% · ·
1	i1	408	95% · ·
1	i4	408	95% · ·
1	i6	408	92% · 6%
1	i7	408	92% · 6%
1	i8	408	92% · 6%
1	iG	408	92% · 6%
1	iR	408	92% · 6%
1	j6	408	95% · ·
1	j7	408	95% · ·
1	j8	408	95% · ·
1	jG	408	95% · ·
1	jR	408	95% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	DS	60	85% 7% 8%
2	E1	60	78% 10% • 10%
2	E3	60	78% 10% • 10%
2	E4	60	78% 10% • 10%
2	E6	60	78% 10% • 10%
2	E7	60	78% 10% • 10%
2	E8	60	78% 10% • 10%
2	ED	60	85% 7% 8%
2	EE	60	78% 10% • 10%
2	EG	60	78% 10% • 10%
2	EJ	60	85% 7% 8%
2	EK	60	85% 7% 8%
2	EL	60	78% 10% • 10%
2	EP	60	85% 7% 8%
2	EQ	60	78% 10% • 10%
2	ER	60	78% 10% • 10%
2	ES	60	82% 8% • 8%
2	F1	60	83% 7% • 8%
2	F3	60	83% 7% • 8%
2	F4	60	83% 7% • 8%
2	F6	60	83% 7% • 8%
2	F7	60	83% 7% • 8%
2	F8	60	83% 7% • 8%
2	FD	60	82% 8% • 8%
2	FG	60	83% 7% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	FJ	60	82% 8% • 8%
2	FK	60	82% 8% • 8%
2	FL	60	83% 7% • 8%
2	FP	60	82% 8% • 8%
2	FQ	60	83% 7% • 8%
2	FR	60	83% 7% • 8%
2	FS	60	45% 5% 50%
2	G1	60	37% 8% 55%
2	G3	60	37% 8% 55%
2	G4	60	37% 8% 55%
2	G6	60	37% 8% 55%
2	G7	60	37% 8% 55%
2	G8	60	37% 8% 55%
2	GD	60	45% 5% 50%
2	GE	60	37% 8% 55%
2	GG	60	37% 8% 55%
2	GJ	60	45% 5% 50%
2	GK	60	45% 5% 50%
2	GL	60	37% 8% 55%
2	GP	60	45% 5% 50%
2	GQ	60	37% 8% 55%
2	GR	60	37% 8% 55%
2	GS	60	90% 10%
2	H1	60	87% 5% 8%
2	H3	60	87% 5% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H4	60	87% 5% 8%
2	H6	60	87% 5% 8%
2	H7	60	87% 5% 8%
2	H8	60	87% 5% 8%
2	HD	60	90% 10%
2	HE	60	83% 7% 8%
2	HG	60	87% 5% 8%
2	HJ	60	90% 10%
2	HK	60	90% 10%
2	HL	60	87% 5% 8%
2	HP	60	90% 10%
2	HQ	60	87% 5% 8%
2	HR	60	87% 5% 8%
2	IE	60	37% 8% 55%
2	JE	60	87% 5% 8%
2	LS	60	83% 8% 8%
2	M1	60	78% 10% 10%
2	M3	60	78% 10% 10%
2	M4	60	78% 10% 10%
2	M6	60	78% 10% 10%
2	M7	60	78% 10% 10%
2	M8	60	78% 10% 10%
2	MD	60	83% 8% 8%
2	MG	60	78% 10% 10%
2	MJ	60	83% 8% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	MK	60	83% 8% 8%
2	ML	60	78% 10% 10%
2	MP	60	83% 8% 8%
2	MQ	60	78% 10% 10%
2	MR	60	78% 10% 10%
2	MS	60	85% 5% 8%
2	N1	60	83% 7% 8%
2	N3	60	83% 7% 8%
2	N4	60	83% 7% 8%
2	N6	60	83% 7% 8%
2	N7	60	83% 7% 8%
2	N8	60	83% 7% 8%
2	ND	60	85% 5% 8%
2	NG	60	83% 7% 8%
2	NJ	60	85% 5% 8%
2	NK	60	85% 5% 8%
2	NL	60	83% 7% 8%
2	NP	60	85% 5% 8%
2	NQ	60	83% 7% 8%
2	NR	60	83% 7% 8%
2	O1	60	37% 8% 55%
2	O3	60	37% 8% 55%
2	O4	60	37% 8% 55%
2	O6	60	37% 8% 55%
2	O7	60	37% 8% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O8	60	37% 8% 55%
2	OE	60	78% 10% • 10%
2	OG	60	37% 8% 55%
2	OL	60	37% 8% 55%
2	OQ	60	37% 8% 55%
2	OR	60	37% 8% 55%
2	P1	60	87% 5% 8%
2	P3	60	87% 5% 8%
2	P4	60	87% 5% 8%
2	P6	60	87% 5% 8%
2	P7	60	87% 5% 8%
2	P8	60	87% 5% 8%
2	PE	60	83% 7% • 8%
2	PG	60	87% 5% 8%
2	PL	60	87% 5% 8%
2	PQ	60	87% 5% 8%
2	PR	60	87% 5% 8%
2	QE	60	37% 8% 55%
2	RE	60	87% 5% 8%
2	U1	60	83% 7% • 8%
2	U3	60	78% 10% • 10%
2	U4	60	83% 7% • 8%
2	U6	60	78% 10% • 10%
2	U7	60	78% 10% • 10%
2	U8	60	78% 10% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	UG	60	78% 10% • 10%
2	UL	60	78% 10% • 10%
2	UQ	60	78% 10% • 10%
2	UR	60	78% 10% • 10%
2	V1	60	37% 8% 55%
2	V3	60	83% 7% • 8%
2	V4	60	37% 8% 55%
2	V6	60	83% 7% • 8%
2	V7	60	83% 7% • 8%
2	V8	60	83% 7% • 8%
2	VG	60	83% 7% • 8%
2	VL	60	83% 7% • 8%
2	VQ	60	83% 7% • 8%
2	VR	60	83% 7% • 8%
2	W1	60	87% 5% 8%
2	W3	60	37% 8% 55%
2	W4	60	87% 5% 8%
2	W6	60	37% 8% 55%
2	W7	60	37% 8% 55%
2	W8	60	37% 8% 55%
2	WE	60	78% 10% • 10%
2	WG	60	37% 8% 55%
2	WL	60	37% 8% 55%
2	WQ	60	37% 8% 55%
2	WR	60	37% 8% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X3	60	87% 5% 8%
2	X6	60	87% 5% 8%
2	X7	60	87% 5% 8%
2	X8	60	87% 5% 8%
2	XE	60	83% 7% 8%
2	XG	60	87% 5% 8%
2	XL	60	87% 5% 8%
2	XQ	60	87% 5% 8%
2	XR	60	87% 5% 8%
2	YE	60	37% 8% 55%
2	Z3	60	78% 10% 10%
2	ZE	60	87% 5% 8%
2	ZQ	60	78% 10% 10%
2	a3	60	37% 8% 55%
2	aQ	60	37% 8% 55%
2	b1	60	78% 10% 10%
2	b4	60	78% 10% 10%
2	c1	60	83% 7% 8%
2	c3	60	78% 10% 10%
2	c4	60	83% 7% 8%
2	c6	60	78% 10% 10%
2	c7	60	78% 10% 10%
2	c8	60	78% 10% 10%
2	cG	60	78% 10% 10%
2	cL	60	78% 10% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	cR	60	78% 10% • 10%
2	d1	60	37% 8% 55%
2	d3	60	37% 8% 55%
2	d4	60	37% 8% 55%
2	d6	60	83% 7% • 8%
2	d7	60	83% 7% • 8%
2	d8	60	83% 7% • 8%
2	dG	60	83% 7% • 8%
2	dL	60	83% 7% • 8%
2	dR	60	83% 7% • 8%
2	e1	60	87% 5% 8%
2	e4	60	87% 5% 8%
2	e6	60	37% 8% 55%
2	e7	60	37% 8% 55%
2	e8	60	37% 8% 55%
2	eE	60	78% 10% • 10%
2	eG	60	37% 8% 55%
2	eL	60	37% 8% 55%
2	eR	60	37% 8% 55%
2	f6	60	87% 5% 8%
2	f7	60	87% 5% 8%
2	f8	60	87% 5% 8%
2	fE	60	83% 7% • 8%
2	fG	60	87% 5% 8%
2	fL	60	87% 5% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	fQ	60	78% 10% • 10%
2	fR	60	87% 5% 8%
2	gE	60	37% 8% 55%
2	gQ	60	83% 7% • 8%
2	hE	60	87% 5% 8%
2	hL	60	78% 10% • 10%
2	hQ	60	37% 8% 55%
2	iL	60	37% 8% 55%
2	iQ	60	87% 5% 8%
2	j1	60	78% 10% • 10%
2	j4	60	83% 7% • 8%
2	k1	60	83% 7% • 8%
2	k4	60	37% 8% 55%
2	k6	60	78% 10% • 10%
2	k7	60	78% 10% • 10%
2	k8	60	78% 10% • 10%
2	kG	60	78% 10% • 10%
2	kR	60	83% 7% • 8%
2	l1	60	37% 8% 55%
2	l4	60	87% 5% 8%
2	l6	60	83% 7% • 8%
2	l7	60	83% 7% • 8%
2	l8	60	83% 7% • 8%
2	lG	60	83% 7% • 8%
2	lR	60	37% 8% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	m1	60	87% 5% 8%
2	m6	60	37% 8% 55%
2	m7	60	37% 8% 55%
2	m8	60	37% 8% 55%
2	mG	60	37% 8% 55%
2	mR	60	87% 5% 8%
2	n6	60	87% 5% 8%
2	n7	60	87% 5% 8%
2	n8	60	87% 5% 8%
2	nG	60	87% 5% 8%
3	A2	327	88% 8%
3	A5	327	88% 8%
3	A9	327	88% 8%
3	AA	327	88% 8%
3	AB	327	88% 8%
3	AC	327	88% 8%
3	AF	327	88% 8%
3	AH	327	88% 8%
3	AI	327	88% 8%
3	AM	327	88% 8%
3	AN	327	88% 8%
3	AO	327	88% 8%
4	B2	251	86% 12%
4	B5	251	86% 12%
4	B9	251	86% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	BA	251	86% • 12%
4	BB	251	86% • 12%
4	BC	251	86% • 12%
4	BF	251	86% • 12%
4	BH	251	86% • 12%
4	BI	251	86% • 12%
4	BM	251	86% • 12%
4	BN	251	86% • 12%
4	BO	251	86% • 12%
5	C2	647	77% 23%
5	C5	647	77% 23%
5	C9	647	77% 23%
5	CA	647	77% 23%
5	CB	647	77% 23%
5	CC	647	77% 23%
5	CF	647	77% 23%
5	CH	647	77% 23%
5	CI	647	77% 23%
5	CM	647	77% 23%
5	CN	647	77% 23%
5	CO	647	77% 23%
5	D2	647	20% 80%
5	D5	647	20% 80%
5	D9	647	20% 80%
5	DA	647	20% 80%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	DB	647	20% 80%
5	DC	647	20% 80%
5	DF	647	20% 80%
5	DH	647	20% 80%
5	DI	647	20% 80%
5	DM	647	20% 80%
5	DN	647	20% 80%
5	DO	647	20% 80%
5	E2	647	21% 79%
5	E5	647	21% 79%
5	E9	647	21% 79%
5	EA	647	21% 79%
5	EB	647	21% 79%
5	EC	647	21% 79%
5	EF	647	21% 79%
5	EH	647	21% 79%
5	EI	647	21% 79%
5	EM	647	21% 79%
5	EN	647	21% 79%
5	EO	647	21% 79%
5	F2	647	17% 83%
5	F5	647	17% 83%
5	F9	647	17% 83%
5	FA	647	17% 83%
5	FB	647	17% 83%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	FC	647	17% 83%
5	FF	647	17% 83%
5	FH	647	17% 83%
5	FI	647	17% 83%
5	FM	647	17% 83%
5	FN	647	17% 83%
5	FO	647	17% 83%
5	N2	647	77% 23%
5	N5	647	77% 23%
5	N9	647	77% 23%
5	NA	647	77% 23%
5	NB	647	77% 23%
5	NC	647	77% 23%
5	NF	647	77% 23%
5	NH	647	77% 23%
5	NI	647	77% 23%
5	NM	647	77% 23%
5	NN	647	77% 23%
5	NO	647	77% 23%
5	O2	647	77% 23%
5	O5	647	77% 23%
5	O9	647	77% 23%
5	OA	647	77% 23%
5	OB	647	77% 23%
5	OC	647	77% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	OF	647	77% 23%
5	OH	647	77% 23%
5	OI	647	77% 23%
5	OM	647	77% 23%
5	ON	647	77% 23%
5	OO	647	77% 23%
6	G2	133	14% 86%
6	G5	133	14% 86%
6	G9	133	14% 86%
6	GA	133	14% 86%
6	GB	133	14% 86%
6	GC	133	14% 86%
6	GF	133	14% 86%
6	GH	133	14% 86%
6	GI	133	14% 86%
6	GM	133	14% 86%
6	GN	133	14% 86%
6	GO	133	14% 86%
6	H2	133	14% 86%
6	H5	133	14% 86%
6	H9	133	14% 86%
6	HA	133	14% 86%
6	HB	133	14% 86%
6	HC	133	14% 86%
6	HF	133	14% 86%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	HH	133	14% 86%
6	HI	133	14% 86%
6	HM	133	14% 86%
6	HN	133	14% 86%
6	HO	133	14% 86%
6	I2	133	18% 82%
6	I5	133	18% 82%
6	I9	133	18% 82%
6	IA	133	18% 82%
6	IB	133	18% 82%
6	IC	133	18% 82%
6	IF	133	18% 82%
6	IH	133	18% 82%
6	II	133	18% 82%
6	IM	133	18% 82%
6	IN	133	18% 82%
6	IO	133	18% 82%
6	J2	133	18% 82%
6	J5	133	18% 82%
6	J9	133	18% 82%
6	JA	133	18% 82%
6	JB	133	18% 82%
6	JC	133	18% 82%
6	JF	133	18% 82%
6	JH	133	18% 82%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	JI	133	18% 82%
6	JM	133	18% 82%
6	JN	133	18% 82%
6	JO	133	18% 82%
6	K2	133	17% 83%
6	K5	133	17% 83%
6	K9	133	17% 83%
6	KA	133	17% 83%
6	KB	133	17% 83%
6	KC	133	17% 83%
6	KF	133	17% 83%
6	KH	133	17% 83%
6	KI	133	17% 83%
6	KM	133	17% 83%
6	KN	133	17% 83%
6	KO	133	17% 83%
6	L2	133	18% 82%
6	L5	133	18% 82%
6	L9	133	18% 82%
6	LA	133	18% 82%
6	LB	133	18% 82%
6	LC	133	18% 82%
6	LF	133	18% 82%
6	LH	133	18% 82%
6	LI	133	18% 82%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	LM	133	18% 82%
6	LN	133	18% 82%
6	LO	133	18% 82%
7	HS	55	100%
7	ID	55	100%
7	IJ	55	100%
7	IK	55	100%
7	IP	55	100%
7	NS	55	100%
7	OD	55	100%
7	OJ	55	100%
7	OK	55	100%
7	OP	55	100%
7	SD	55	100%
7	SJ	55	100%
7	SK	55	100%
7	SP	55	100%
7	SS	55	100%
8	PD	17	100%
8	PJ	17	100%
8	PK	17	100%
8	PP	17	100%
8	PS	17	100%
8	QD	17	94% 6%
8	QJ	17	94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	QK	17	94% 6%
8	QP	17	94% 6%
8	QS	17	94% 6%
8	RD	17	71% 29%
8	RJ	17	71% 29%
8	RK	17	71% 29%
8	RP	17	71% 29%
8	RS	17	71% 29%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 1074183 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 Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A1	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D1	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	I1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	J1	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	K1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	L1	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R1	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T1	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	X1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	Y1	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	Z1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	a1	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	f1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g1	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	h1	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	i1	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	C3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A3	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D3	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	I3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	J3	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	K3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	L3	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R3	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S3	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T3	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Y3	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	b3	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	C4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A4	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D4	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	J4	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	K4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	L4	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R4	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T4	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	X4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	Y4	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	Z4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	a4	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	f4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	g4	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	h4	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	i4	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	C6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A6	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D6	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	I6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J6	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	K6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	L6	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R6	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T6	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Y6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	Z6	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	a6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	b6	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	g6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	h6	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	i6	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	j6	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	C7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A7	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D7	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	I7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	J7	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	L7	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R7	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T7	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Y7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	Z7	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	a7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	b7	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	g7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	h7	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	i7	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	j7	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	C8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	A8	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	B8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	D8	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	I8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	J8	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	K8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L8	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Q8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	R8	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	S8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	T8	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	Y8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	Z8	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	a8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	b8	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	g8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	h8	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	i8	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	j8	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	AD	354	Total	C	N	O	S	0	0
			2821	1810	463	541	7		
1	BD	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CD	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	DD	386	Total	C	N	O	S	0	0
			3131	2017	510	596	8		
1	KD	382	Total	C	N	O	S	0	0
			3103	1997	505	593	8		
1	LD	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	DE	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	AE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BE	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	CE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	FE	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	KE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	LE	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	ME	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	NE	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	SE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	TE	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	UE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	VE	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	aE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	bE	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	cE	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	dE	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	AG	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	BG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	DG	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	IG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	JG	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	KG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	LG	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	QG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	RG	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	SG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	TG	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	YG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	ZG	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	aG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	bG	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	gG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	hG	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	iG	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	jG	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	AJ	354	Total	C	N	O	S	0	0
			2821	1810	463	541	7		
1	BJ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CJ	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	DJ	386	Total	C	N	O	S	0	0
			3131	2017	510	596	8		
1	KJ	382	Total	C	N	O	S	0	0
			3103	1997	505	593	8		
1	LJ	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	AK	354	Total	C	N	O	S	0	0
			2821	1810	463	541	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BK	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CK	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	DK	386	Total	C	N	O	S	0	0
			3131	2017	510	596	8		
1	KK	382	Total	C	N	O	S	0	0
			3103	1997	505	593	8		
1	LK	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	CL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	AL	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	BL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	DL	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	IL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	JL	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	KL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	LL	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	QL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	RL	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	SL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	TL	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	YL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	ZL	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	aL	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	bL	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	gL	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	AP	354	Total	C	N	O	S	0	0
			2821	1810	463	541	7		
1	BP	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CP	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	DP	386	Total	C	N	O	S	0	0
			3131	2017	510	596	8		
1	KP	382	Total	C	N	O	S	0	0
			3103	1997	505	593	8		
1	LP	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	CQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	AQ	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	BQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	DQ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	IQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	JQ	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	KQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	LQ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	QQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	RQ	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	SQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	TQ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	YQ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	bQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	cQ	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	dQ	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	eQ	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	CR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	AR	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	BR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	DR	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	IR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	JR	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	KR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	LR	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	QR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	RR	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	SR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	TR	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	YR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	ZR	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		
1	aR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	bR	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	gR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	hR	392	Total	C	N	O	S	0	0
			3178	2044	518	608	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	iR	385	Total	C	N	O	S	0	0
			3123	2013	508	594	8		
1	jR	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	AS	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		
1	BS	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		
1	CS	386	Total	C	N	O	S	0	0
			3131	2017	510	596	8		
1	IS	354	Total	C	N	O	S	0	0
			2821	1810	463	541	7		
1	JS	382	Total	C	N	O	S	0	0
			3103	1997	505	593	8		
1	KS	386	Total	C	N	O	S	0	0
			3135	2019	510	598	8		

- Molecule 2 is a protein called Arstotzka protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E1	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	F1	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	G1	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H1	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M1	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N1	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O1	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P1	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U1	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	V1	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	W1	55	Total	C	N	O	S	0	0
			435	260	77	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b1	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	c1	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	d1	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	e1	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	j1	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	k1	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	l1	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	m1	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	E3	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	F3	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	G3	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H3	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M3	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N3	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O3	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P3	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U3	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	V3	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	W3	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	X3	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	Z3	54	Total	C	N	O	S	0	0
			432	258	76	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a3	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	c3	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	d3	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	E4	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	F4	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	G4	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H4	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M4	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N4	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O4	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P4	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U4	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	V4	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	W4	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	b4	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	c4	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	d4	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	e4	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	j4	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	k4	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	l4	55	Total	C	N	O	S	0	0
			435	260	77	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E6	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	F6	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	G6	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H6	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M6	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N6	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O6	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P6	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U6	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	V6	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	W6	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	X6	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	c6	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	d6	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	e6	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	f6	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	k6	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	l6	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	m6	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	n6	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	E7	54	Total	C	N	O	S	0	0
			432	258	76	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F7	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	G7	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H7	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M7	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N7	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O7	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P7	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U7	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	V7	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	W7	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	X7	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	c7	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	d7	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	e7	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	f7	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	k7	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	l7	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	m7	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	n7	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	E8	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	F8	55	Total	C	N	O	S	0	0
			436	260	77	94	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G8	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H8	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	M8	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	N8	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	O8	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	P8	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	U8	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	V8	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	W8	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	X8	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	c8	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	d8	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	e8	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	f8	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	k8	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	l8	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	m8	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	n8	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	ED	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	FD	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	GD	30	Total	C	N	O	S	0	0
			237	143	39	54	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	HD	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	MD	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	ND	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	EE	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	GE	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	HE	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	IE	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	JE	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	OE	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	PE	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	QE	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	RE	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	WE	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	XE	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	YE	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	ZE	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	eE	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	fE	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	gE	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	hE	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	EG	54	Total	C	N	O	S	0	0
			432	258	76	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FG	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	GG	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	HG	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	MG	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	NG	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	OG	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	PG	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	UG	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	VG	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	WG	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	XG	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	cG	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	dG	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	eG	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	fG	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	kG	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	lG	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	mG	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	nG	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	EJ	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	FJ	55	Total	C	N	O	S	0	0
			437	260	77	95	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	GJ	30	Total	C	N	O	S	0	0
			237	143	39	54	1		
2	HJ	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	MJ	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	NJ	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	EK	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	FK	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	GK	30	Total	C	N	O	S	0	0
			237	143	39	54	1		
2	HK	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	MK	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	NK	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	EL	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	FL	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	GL	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	HL	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	ML	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	NL	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	OL	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	PL	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	UL	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	VL	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	WL	27	Total	C	N	O	S	0	0
			221	130	41	46	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	XL	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	cL	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	dL	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	eL	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	fL	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	hL	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	iL	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	EP	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	FP	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	GP	30	Total	C	N	O	S	0	0
			237	143	39	54	1		
2	HP	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	MP	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	NP	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	EQ	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	FQ	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	GQ	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	HQ	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	MQ	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	NQ	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	OQ	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	PQ	55	Total	C	N	O	S	0	0
			435	260	77	93	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UQ	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	VQ	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	WQ	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	XQ	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	ZQ	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	aQ	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	fQ	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	gQ	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	hQ	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	iQ	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	ER	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	FR	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	GR	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	HR	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	MR	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	NR	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	OR	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	PR	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	UR	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	VR	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	WR	27	Total	C	N	O	S	0	0
			221	130	41	46	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	XR	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	cR	54	Total	C	N	O	S	0	0
			432	258	76	93	5		
2	dR	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	eR	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	fR	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	kR	55	Total	C	N	O	S	0	0
			436	260	77	94	5		
2	lR	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	mR	55	Total	C	N	O	S	0	0
			435	260	77	93	5		
2	DS	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	ES	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	FS	30	Total	C	N	O	S	0	0
			237	143	39	54	1		
2	GS	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	LS	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	MS	55	Total	C	N	O	S	0	0
			437	260	77	95	5		

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	A5	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	A9	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AA	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AB	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AF	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AH	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AI	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AM	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AN	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		
3	AO	301	Total	C	N	O	S	0	0
			2353	1486	398	460	9		

- Molecule 4 is a protein called Lower collar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	B5	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	B9	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BA	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BB	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BC	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BF	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BH	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BI	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BM	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BN	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		
4	BO	220	Total	C	N	O	S	0	0
			1763	1111	294	353	5		

- Molecule 5 is a protein called Minor structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D2	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	E2	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	F2	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	C2	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	N2	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	O2	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	D5	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	E5	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	F5	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	C5	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	N5	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	O5	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	D9	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	E9	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	F9	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	C9	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	N9	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	O9	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DA	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EA	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FA	110	Total	C	N	O	S	0	0
			927	595	155	174	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CA	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NA	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OA	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DB	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EB	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FB	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CB	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NB	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OB	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DC	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EC	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FC	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CC	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NC	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OC	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DF	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EF	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FF	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CF	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NF	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OF	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DH	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EH	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FH	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CH	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NH	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OH	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DI	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EI	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FI	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CI	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NI	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OI	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DM	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EM	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FM	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CM	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NM	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OM	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DN	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EN	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FN	110	Total	C	N	O	S	0	0
			927	595	155	174	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CN	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NN	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	ON	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		
5	DO	132	Total	C	N	O	S	0	0
			1107	718	178	208	3		
5	EO	136	Total	C	N	O	S	0	0
			1173	755	192	223	3		
5	FO	110	Total	C	N	O	S	0	0
			927	595	155	174	3		
5	CO	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	NO	501	Total	C	N	O	S	0	0
			4021	2545	690	771	15		
5	OO	500	Total	C	N	O	S	0	0
			4012	2539	688	770	15		

- Molecule 6 is a protein called Tail fibre protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G2	18	Total	C	N	O	0	0
			90	54	18	18		
6	H2	18	Total	C	N	O	0	0
			90	54	18	18		
6	I2	24	Total	C	N	O	0	0
			120	72	24	24		
6	J2	24	Total	C	N	O	0	0
			120	72	24	24		
6	K2	22	Total	C	N	O	0	0
			112	67	22	23		
6	L2	24	Total	C	N	O	0	0
			120	72	24	24		
6	G5	18	Total	C	N	O	0	0
			90	54	18	18		
6	H5	18	Total	C	N	O	0	0
			90	54	18	18		
6	I5	24	Total	C	N	O	0	0
			120	72	24	24		
6	J5	24	Total	C	N	O	0	0
			120	72	24	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K5	22	Total	C	N	O	0	0
			112	67	22	23		
6	L5	24	Total	C	N	O	0	0
			120	72	24	24		
6	G9	18	Total	C	N	O	0	0
			90	54	18	18		
6	H9	18	Total	C	N	O	0	0
			90	54	18	18		
6	I9	24	Total	C	N	O	0	0
			120	72	24	24		
6	J9	24	Total	C	N	O	0	0
			120	72	24	24		
6	K9	22	Total	C	N	O	0	0
			112	67	22	23		
6	L9	24	Total	C	N	O	0	0
			120	72	24	24		
6	GA	18	Total	C	N	O	0	0
			90	54	18	18		
6	HA	18	Total	C	N	O	0	0
			90	54	18	18		
6	IA	24	Total	C	N	O	0	0
			120	72	24	24		
6	JA	24	Total	C	N	O	0	0
			120	72	24	24		
6	KA	22	Total	C	N	O	0	0
			112	67	22	23		
6	LA	24	Total	C	N	O	0	0
			120	72	24	24		
6	GB	18	Total	C	N	O	0	0
			90	54	18	18		
6	HB	18	Total	C	N	O	0	0
			90	54	18	18		
6	IB	24	Total	C	N	O	0	0
			120	72	24	24		
6	JB	24	Total	C	N	O	0	0
			120	72	24	24		
6	KB	22	Total	C	N	O	0	0
			112	67	22	23		
6	LB	24	Total	C	N	O	0	0
			120	72	24	24		
6	GC	18	Total	C	N	O	0	0
			90	54	18	18		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	HC	18	Total	C	N	O	0	0
			90	54	18	18		
6	IC	24	Total	C	N	O	0	0
			120	72	24	24		
6	JC	24	Total	C	N	O	0	0
			120	72	24	24		
6	KC	22	Total	C	N	O	0	0
			112	67	22	23		
6	LC	24	Total	C	N	O	0	0
			120	72	24	24		
6	GF	18	Total	C	N	O	0	0
			90	54	18	18		
6	HF	18	Total	C	N	O	0	0
			90	54	18	18		
6	IF	24	Total	C	N	O	0	0
			120	72	24	24		
6	JF	24	Total	C	N	O	0	0
			120	72	24	24		
6	KF	22	Total	C	N	O	0	0
			112	67	22	23		
6	LF	24	Total	C	N	O	0	0
			120	72	24	24		
6	GH	18	Total	C	N	O	0	0
			90	54	18	18		
6	HH	18	Total	C	N	O	0	0
			90	54	18	18		
6	IH	24	Total	C	N	O	0	0
			120	72	24	24		
6	JH	24	Total	C	N	O	0	0
			120	72	24	24		
6	KH	22	Total	C	N	O	0	0
			112	67	22	23		
6	LH	24	Total	C	N	O	0	0
			120	72	24	24		
6	GI	18	Total	C	N	O	0	0
			90	54	18	18		
6	HI	18	Total	C	N	O	0	0
			90	54	18	18		
6	II	24	Total	C	N	O	0	0
			120	72	24	24		
6	JI	24	Total	C	N	O	0	0
			120	72	24	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	KI	22	Total	C	N	O	0	0
			112	67	22	23		
6	LI	24	Total	C	N	O	0	0
			120	72	24	24		
6	GM	18	Total	C	N	O	0	0
			90	54	18	18		
6	HM	18	Total	C	N	O	0	0
			90	54	18	18		
6	IM	24	Total	C	N	O	0	0
			120	72	24	24		
6	JM	24	Total	C	N	O	0	0
			120	72	24	24		
6	KM	22	Total	C	N	O	0	0
			112	67	22	23		
6	LM	24	Total	C	N	O	0	0
			120	72	24	24		
6	GN	18	Total	C	N	O	0	0
			90	54	18	18		
6	HN	18	Total	C	N	O	0	0
			90	54	18	18		
6	IN	24	Total	C	N	O	0	0
			120	72	24	24		
6	JN	24	Total	C	N	O	0	0
			120	72	24	24		
6	KN	22	Total	C	N	O	0	0
			112	67	22	23		
6	LN	24	Total	C	N	O	0	0
			120	72	24	24		
6	GO	18	Total	C	N	O	0	0
			90	54	18	18		
6	HO	18	Total	C	N	O	0	0
			90	54	18	18		
6	IO	24	Total	C	N	O	0	0
			120	72	24	24		
6	JO	24	Total	C	N	O	0	0
			120	72	24	24		
6	KO	22	Total	C	N	O	0	0
			112	67	22	23		
6	LO	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 7 is a protein called Head fiber protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	ID	55	Total 275	C 165	N 55	O 55	0	0
7	OD	55	Total 275	C 165	N 55	O 55	0	0
7	SD	55	Total 275	C 165	N 55	O 55	0	0
7	IJ	55	Total 275	C 165	N 55	O 55	0	0
7	OJ	55	Total 275	C 165	N 55	O 55	0	0
7	SJ	55	Total 275	C 165	N 55	O 55	0	0
7	IK	55	Total 275	C 165	N 55	O 55	0	0
7	OK	55	Total 275	C 165	N 55	O 55	0	0
7	SK	55	Total 275	C 165	N 55	O 55	0	0
7	IP	55	Total 275	C 165	N 55	O 55	0	0
7	OP	55	Total 275	C 165	N 55	O 55	0	0
7	SP	55	Total 275	C 165	N 55	O 55	0	0
7	HS	55	Total 275	C 165	N 55	O 55	0	0
7	NS	55	Total 275	C 165	N 55	O 55	0	0
7	SS	55	Total 275	C 165	N 55	O 55	0	0

- Molecule 8 is a protein called Inner core protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	PD	17	Total 85	C 51	N 17	O 17	0	0
8	QD	16	Total 79	C 47	N 16	O 16	0	0
8	RD	12	Total 54	C 30	N 12	O 12	0	0
8	PJ	17	Total 85	C 51	N 17	O 17	0	0
8	QJ	16	Total 79	C 47	N 16	O 16	0	0

Continued on next page...

Continued from previous page...

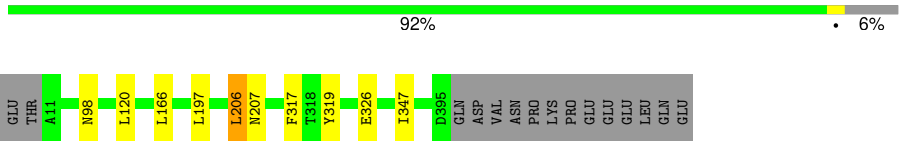
Mol	Chain	Residues	Atoms				AltConf	Trace
8	RJ	12	Total	C	N	O	0	0
			54	30	12	12		
8	PK	17	Total	C	N	O	0	0
			85	51	17	17		
8	QK	16	Total	C	N	O	0	0
			79	47	16	16		
8	RK	12	Total	C	N	O	0	0
			54	30	12	12		
8	PP	17	Total	C	N	O	0	0
			85	51	17	17		
8	QP	16	Total	C	N	O	0	0
			79	47	16	16		
8	RP	12	Total	C	N	O	0	0
			54	30	12	12		
8	PS	17	Total	C	N	O	0	0
			85	51	17	17		
8	QS	16	Total	C	N	O	0	0
			79	47	16	16		
8	RS	12	Total	C	N	O	0	0
			54	30	12	12		

3 Residue-property plots (i)

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

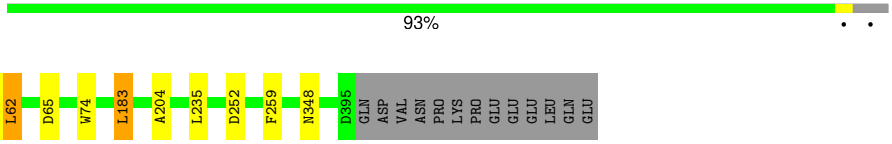
• Molecule 1: Major head protein

Chain C1:



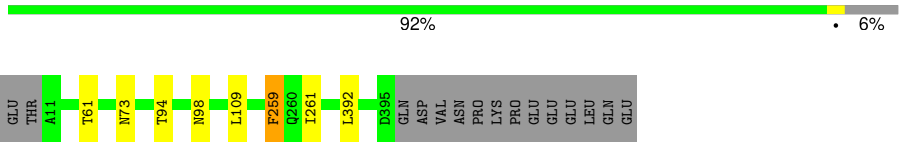
• Molecule 1: Major head protein

Chain A1:



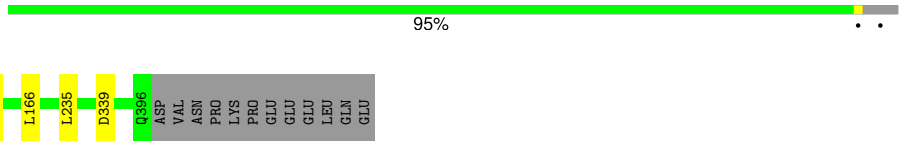
• Molecule 1: Major head protein

Chain B1:



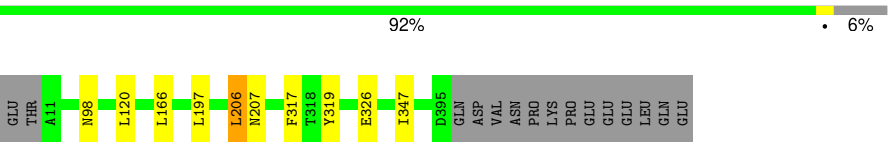
• Molecule 1: Major head protein

Chain D1:



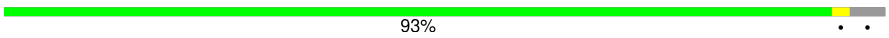
• Molecule 1: Major head protein

Chain I1:



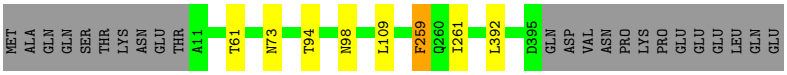
• Molecule 1: Major head protein

Chain J1:



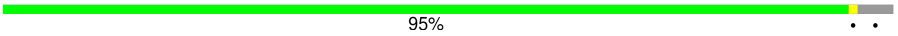
• Molecule 1: Major head protein

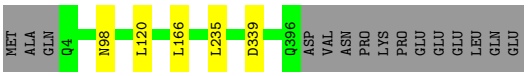
Chain K1:



• Molecule 1: Major head protein

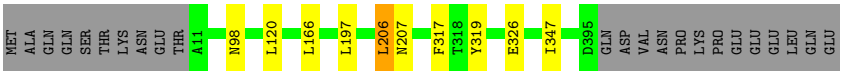
Chain L1:





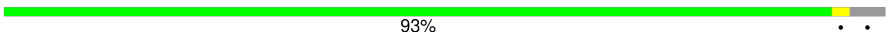
• Molecule 1: Major head protein

Chain Q1:



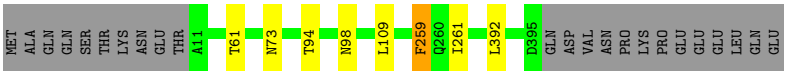
• Molecule 1: Major head protein

Chain R1:



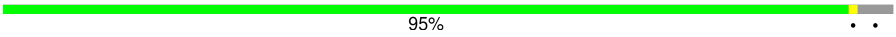
• Molecule 1: Major head protein

Chain S1:



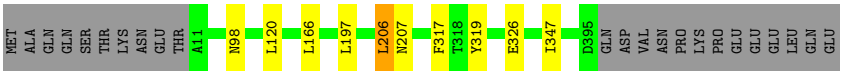
• Molecule 1: Major head protein

Chain T1:



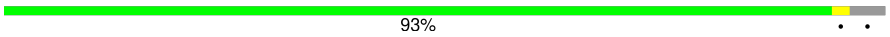
• Molecule 1: Major head protein

Chain X1:



• Molecule 1: Major head protein

Chain Y1:

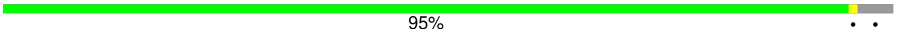


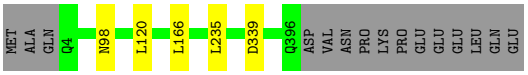
• Molecule 1: Major head protein

Chain Z1:

• Molecule 1: Major head protein

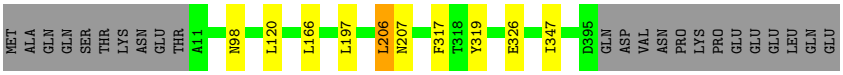
Chain a1:





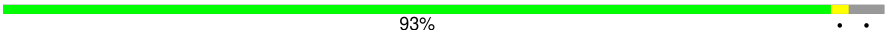
• Molecule 1: Major head protein

Chain f1:



• Molecule 1: Major head protein

Chain g1:

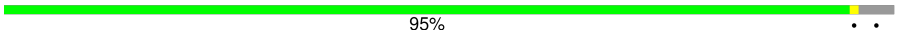


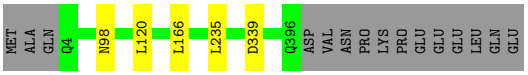
• Molecule 1: Major head protein

Chain h1:

• Molecule 1: Major head protein

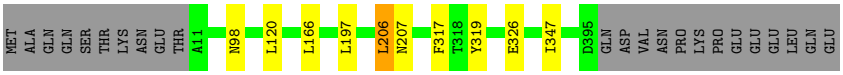
Chain i1:





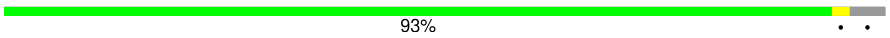
• Molecule 1: Major head protein

Chain C3:



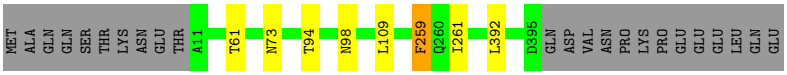
• Molecule 1: Major head protein

Chain A3:



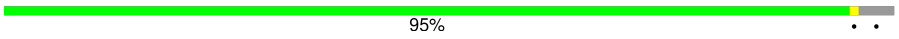
• Molecule 1: Major head protein

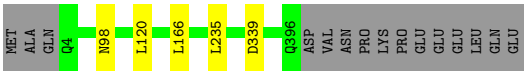
Chain B3:



• Molecule 1: Major head protein

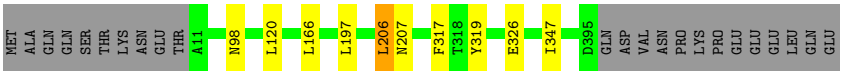
Chain D3:





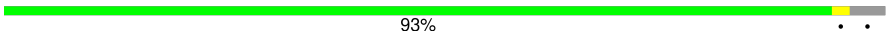
• Molecule 1: Major head protein

Chain I3:



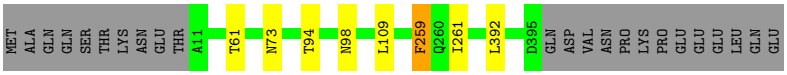
• Molecule 1: Major head protein

Chain J3:



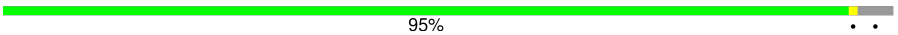
• Molecule 1: Major head protein

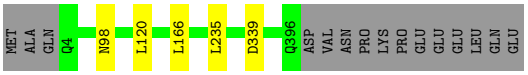
Chain K3:



• Molecule 1: Major head protein

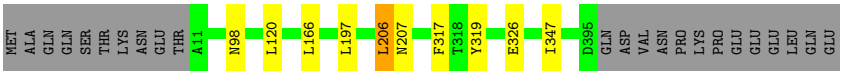
Chain L3:





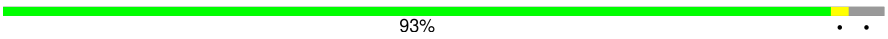
• Molecule 1: Major head protein

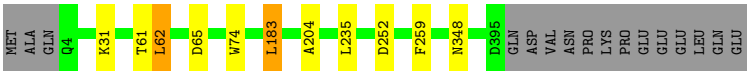
Chain Q3:



• Molecule 1: Major head protein

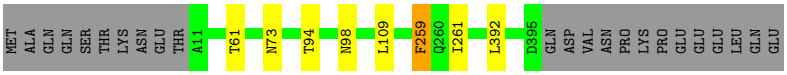
Chain R3:





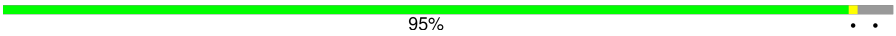
• Molecule 1: Major head protein

Chain S3:



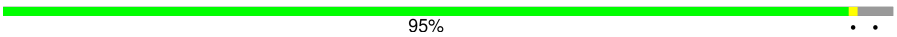
• Molecule 1: Major head protein

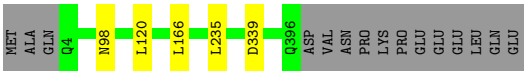
Chain T3:



• Molecule 1: Major head protein

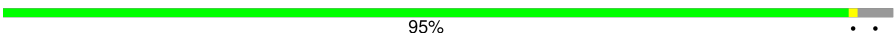
Chain Y3:

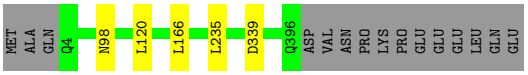




• Molecule 1: Major head protein

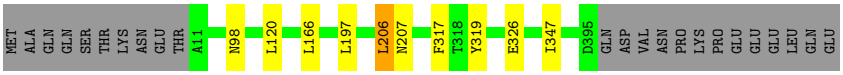
Chain b3:





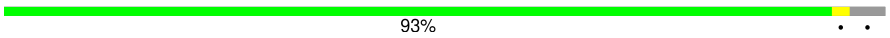
• Molecule 1: Major head protein

Chain C4:



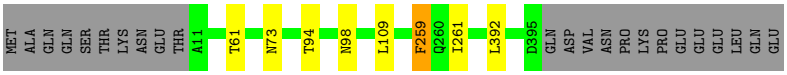
• Molecule 1: Major head protein

Chain A4:



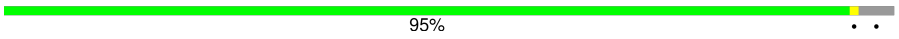
• Molecule 1: Major head protein

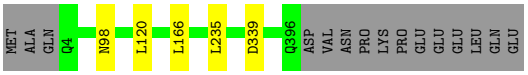
Chain B4:



• Molecule 1: Major head protein

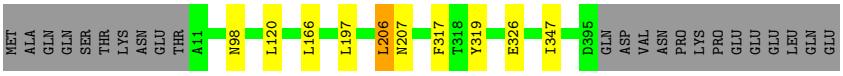
Chain D4:





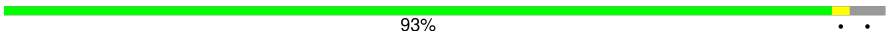
• Molecule 1: Major head protein

Chain I4:



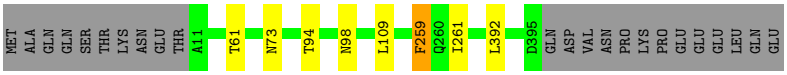
• Molecule 1: Major head protein

Chain J4:



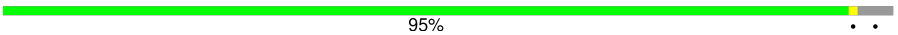
• Molecule 1: Major head protein

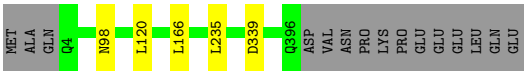
Chain K4:



• Molecule 1: Major head protein

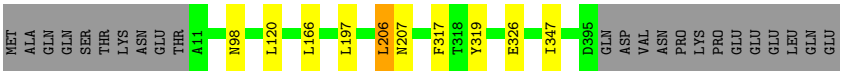
Chain L4:





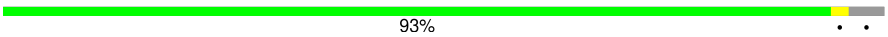
• Molecule 1: Major head protein

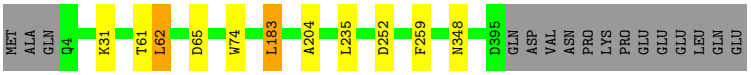
Chain Q4:



• Molecule 1: Major head protein

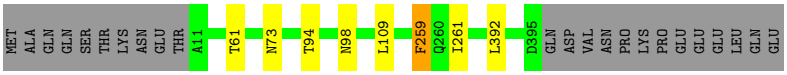
Chain R4:





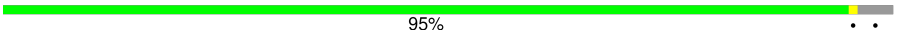
• Molecule 1: Major head protein

Chain S4:



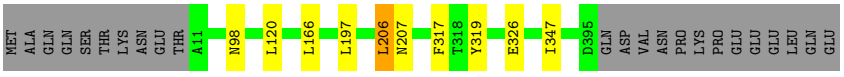
• Molecule 1: Major head protein

Chain T4:



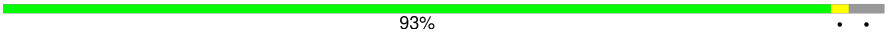
• Molecule 1: Major head protein

Chain X4:



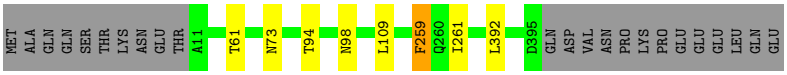
• Molecule 1: Major head protein

Chain Y4:



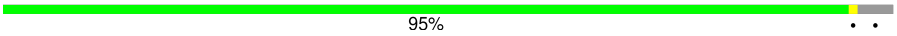
• Molecule 1: Major head protein

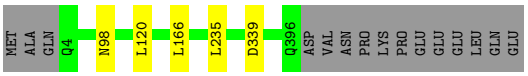
Chain Z4:



• Molecule 1: Major head protein

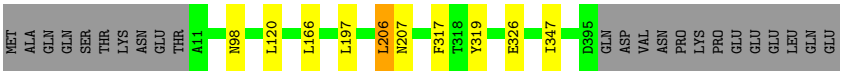
Chain a4:





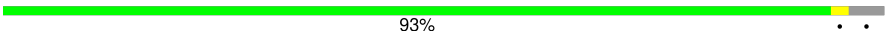
• Molecule 1: Major head protein

Chain f4:



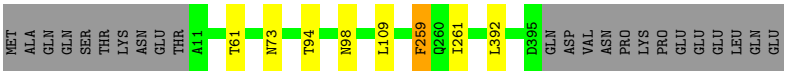
• Molecule 1: Major head protein

Chain g4:



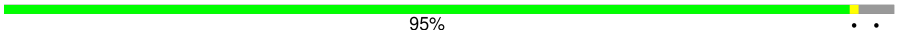
• Molecule 1: Major head protein

Chain h4:



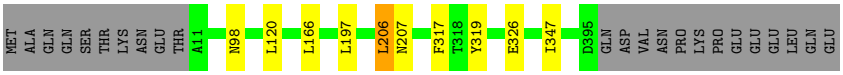
• Molecule 1: Major head protein

Chain i4:



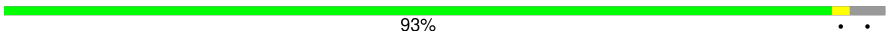
• Molecule 1: Major head protein

Chain C6:



• Molecule 1: Major head protein

Chain A6:

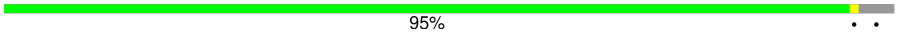


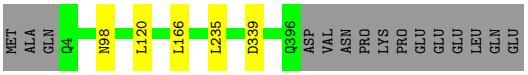
• Molecule 1: Major head protein

Chain B6:

• Molecule 1: Major head protein

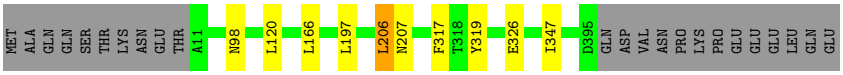
Chain D6:





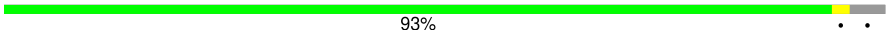
• Molecule 1: Major head protein

Chain I6:



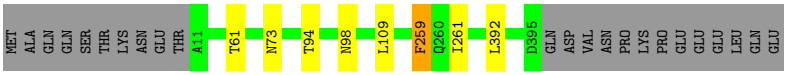
• Molecule 1: Major head protein

Chain J6:



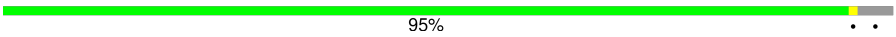
• Molecule 1: Major head protein

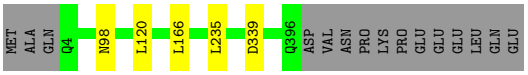
Chain K6:



• Molecule 1: Major head protein

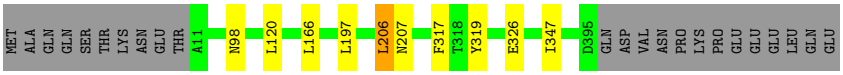
Chain L6:





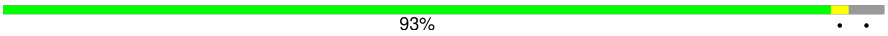
• Molecule 1: Major head protein

Chain Q6:



• Molecule 1: Major head protein

Chain R6:

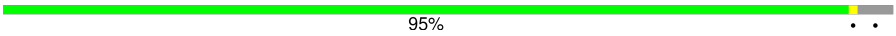


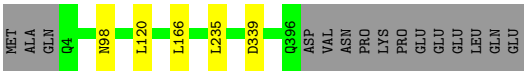
• Molecule 1: Major head protein

Chain S6:

• Molecule 1: Major head protein

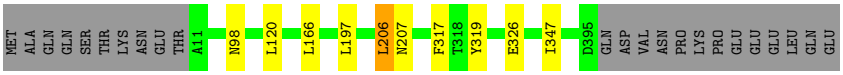
Chain T6:





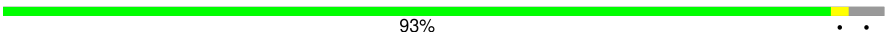
• Molecule 1: Major head protein

Chain Y6:



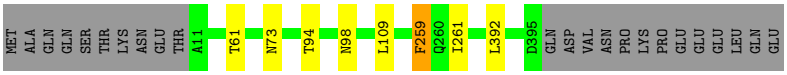
• Molecule 1: Major head protein

Chain Z6:



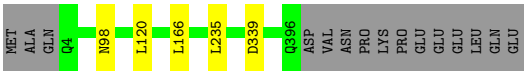
• Molecule 1: Major head protein

Chain a6:



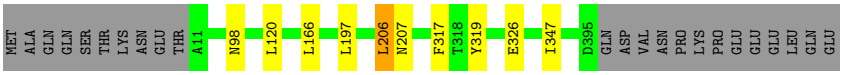
• Molecule 1: Major head protein

Chain b6:



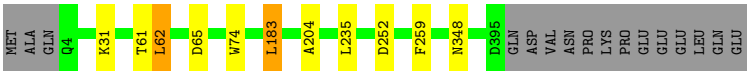
• Molecule 1: Major head protein

Chain g6:



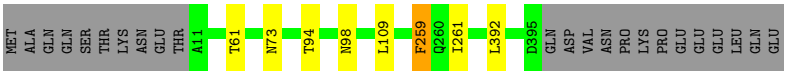
• Molecule 1: Major head protein

Chain h6:



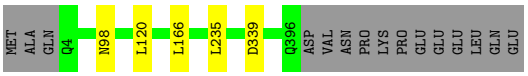
• Molecule 1: Major head protein

Chain i6:



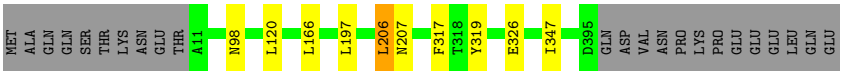
• Molecule 1: Major head protein

Chain j6:



• Molecule 1: Major head protein

Chain C7:

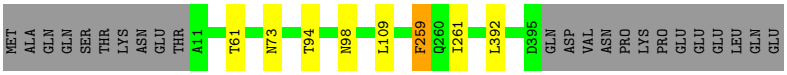


• Molecule 1: Major head protein

Chain A7:

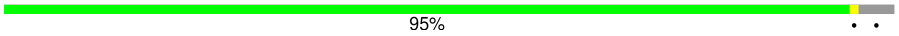
• Molecule 1: Major head protein

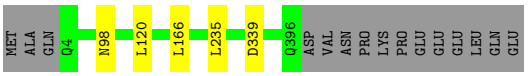
Chain B7:



• Molecule 1: Major head protein

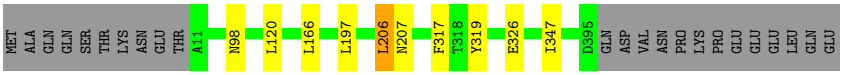
Chain D7:





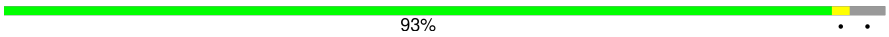
• Molecule 1: Major head protein

Chain I7:



• Molecule 1: Major head protein

Chain J7:

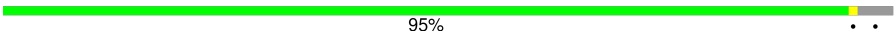


• Molecule 1: Major head protein

Chain K7:

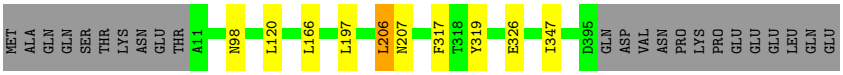
• Molecule 1: Major head protein

Chain L7:



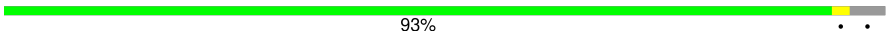
• Molecule 1: Major head protein

Chain Q7:



• Molecule 1: Major head protein

Chain R7:

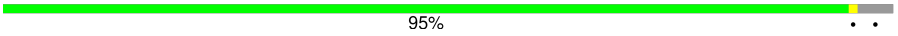


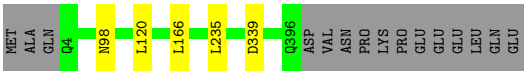
• Molecule 1: Major head protein

Chain S7:

• Molecule 1: Major head protein

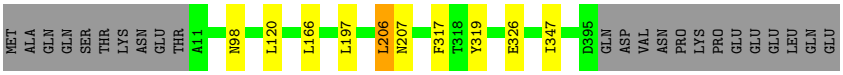
Chain T7:





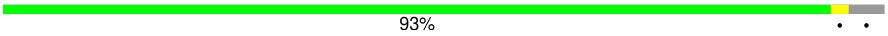
• Molecule 1: Major head protein

Chain Y7:



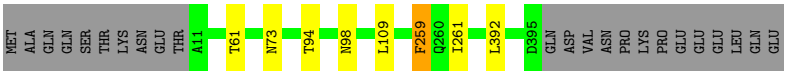
• Molecule 1: Major head protein

Chain Z7:



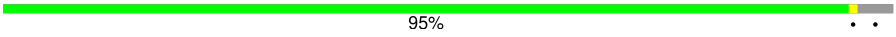
• Molecule 1: Major head protein

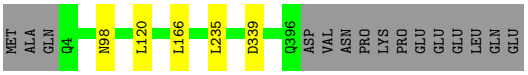
Chain a7:



• Molecule 1: Major head protein

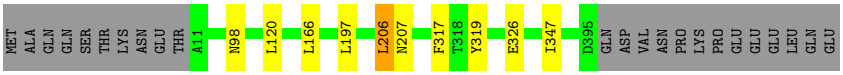
Chain b7:





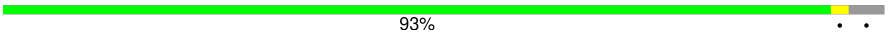
• Molecule 1: Major head protein

Chain g7:



• Molecule 1: Major head protein

Chain h7:

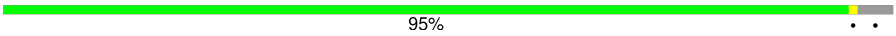


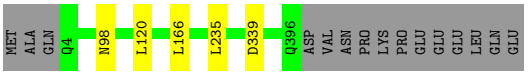
• Molecule 1: Major head protein

Chain i7:

• Molecule 1: Major head protein

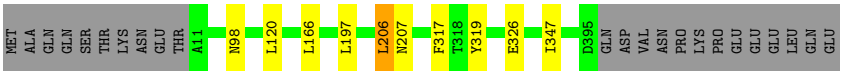
Chain j7:





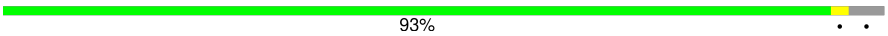
• Molecule 1: Major head protein

Chain C8:



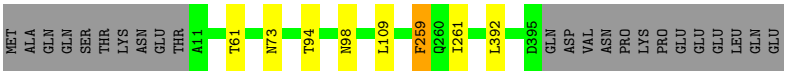
• Molecule 1: Major head protein

Chain A8:



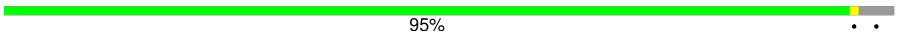
• Molecule 1: Major head protein

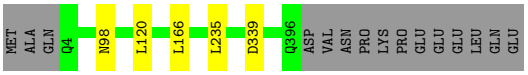
Chain B8:



• Molecule 1: Major head protein

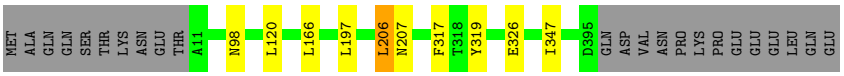
Chain D8:





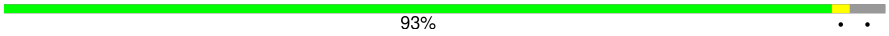
• Molecule 1: Major head protein

Chain I8:



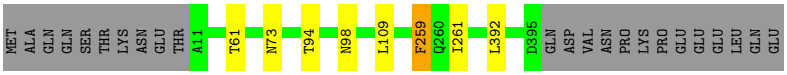
• Molecule 1: Major head protein

Chain J8:



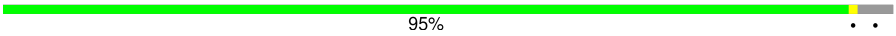
• Molecule 1: Major head protein

Chain K8:



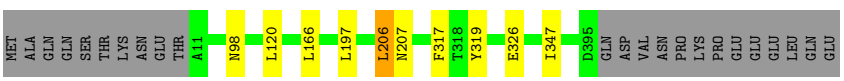
• Molecule 1: Major head protein

Chain L8:



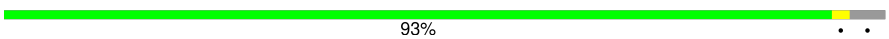
• Molecule 1: Major head protein

Chain Q8:



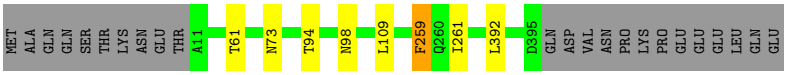
• Molecule 1: Major head protein

Chain R8:



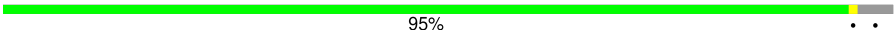
• Molecule 1: Major head protein

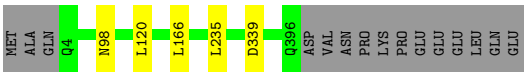
Chain S8:



• Molecule 1: Major head protein

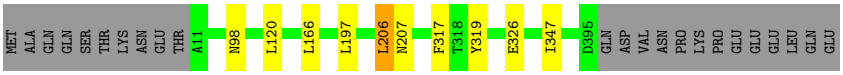
Chain T8:





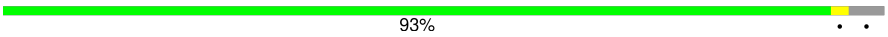
• Molecule 1: Major head protein

Chain Y8:



• Molecule 1: Major head protein

Chain Z8:

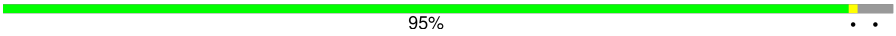


• Molecule 1: Major head protein

Chain a8:

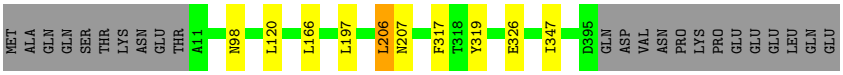
• Molecule 1: Major head protein

Chain b8:



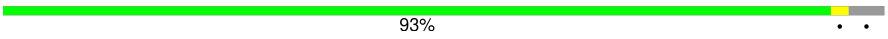
• Molecule 1: Major head protein

Chain g8:



• Molecule 1: Major head protein

Chain h8:

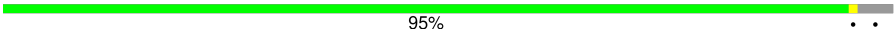


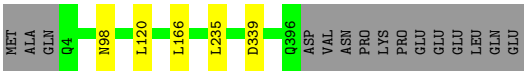
• Molecule 1: Major head protein

Chain i8:

• Molecule 1: Major head protein

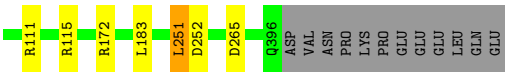
Chain j8:





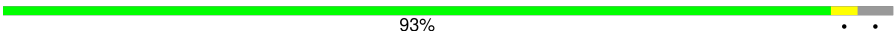
• Molecule 1: Major head protein

Chain AD:



• Molecule 1: Major head protein

Chain BD:

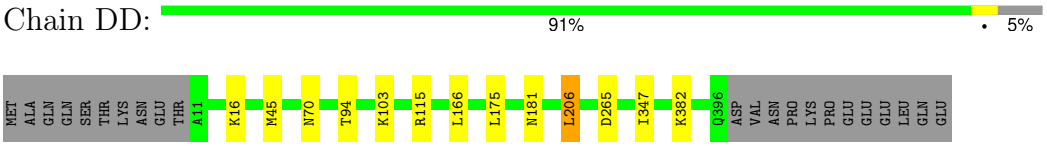


• Molecule 1: Major head protein

Chain CD:

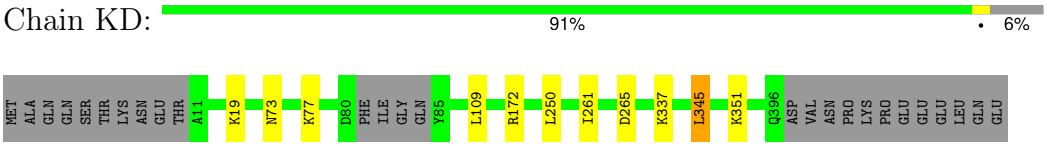
• Molecule 1: Major head protein

Chain DD:



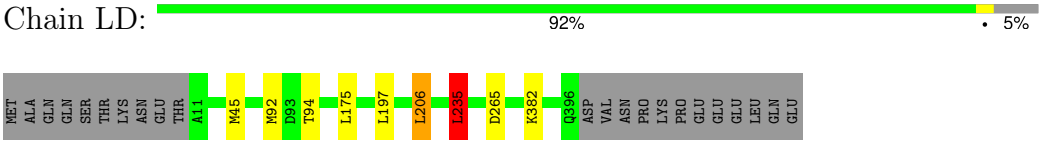
• Molecule 1: Major head protein

Chain KD:



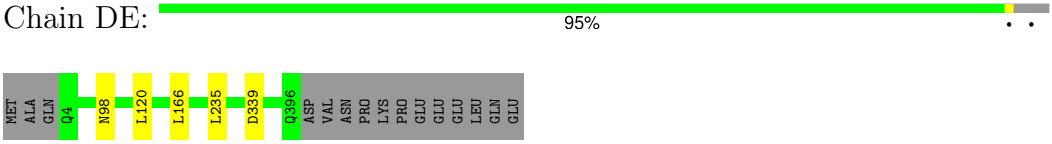
• Molecule 1: Major head protein

Chain LD:



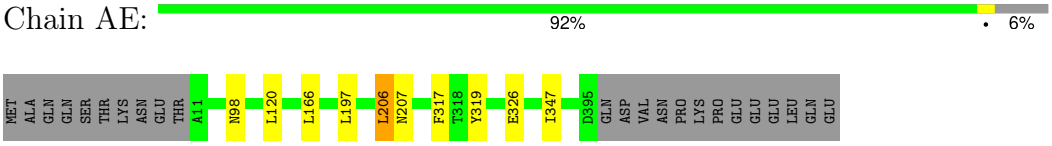
• Molecule 1: Major head protein

Chain DE:



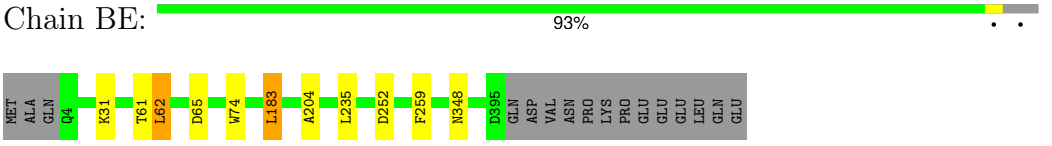
• Molecule 1: Major head protein

Chain AE:



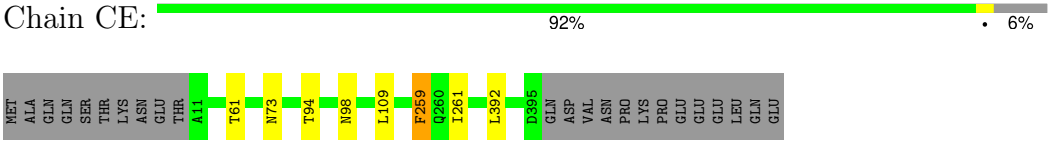
• Molecule 1: Major head protein

Chain BE:



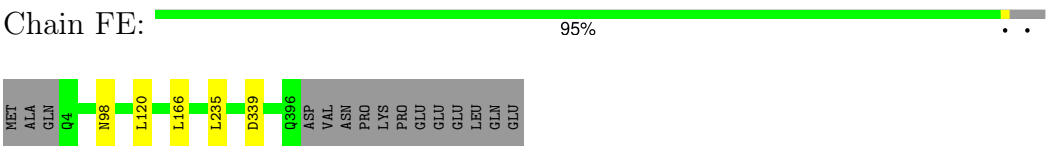
• Molecule 1: Major head protein

Chain CE:



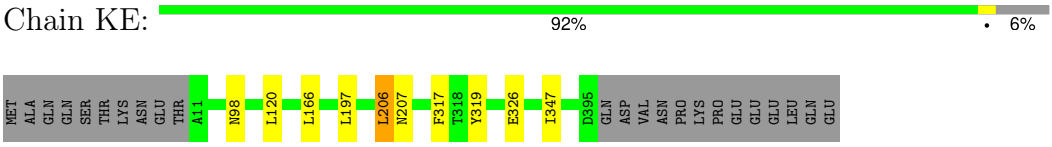
• Molecule 1: Major head protein

Chain FE:



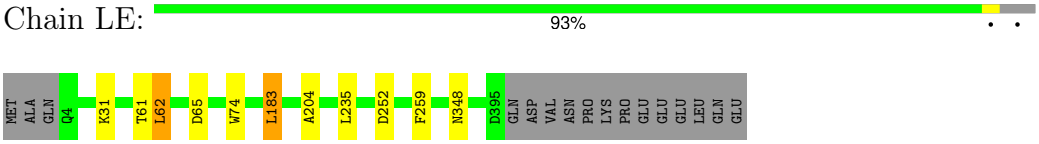
• Molecule 1: Major head protein

Chain KE:



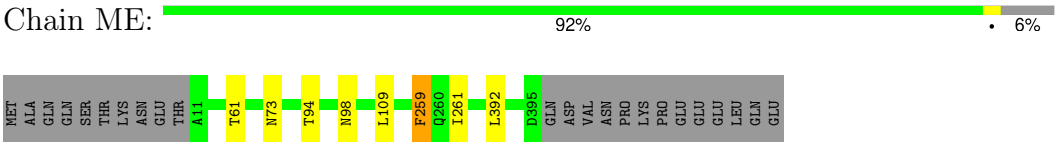
• Molecule 1: Major head protein

Chain LE:



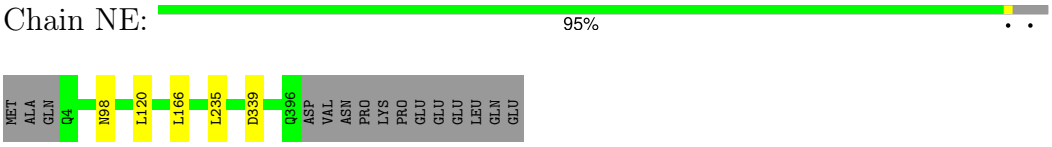
• Molecule 1: Major head protein

Chain ME:



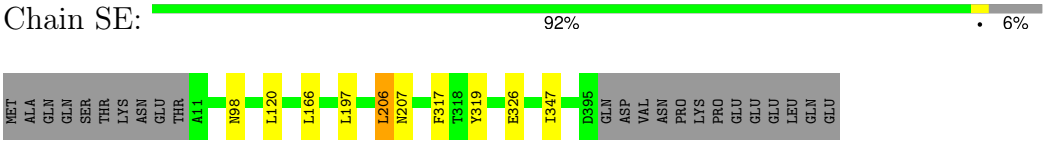
• Molecule 1: Major head protein

Chain NE:



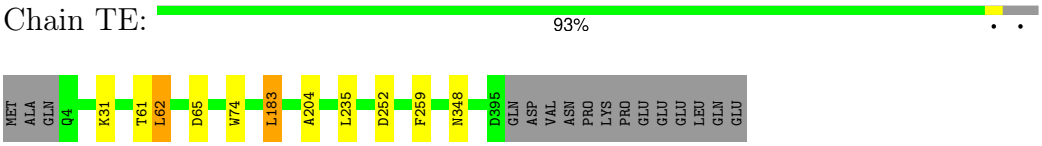
• Molecule 1: Major head protein

Chain SE:



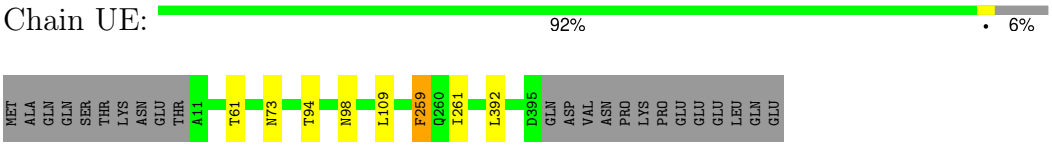
• Molecule 1: Major head protein

Chain TE:



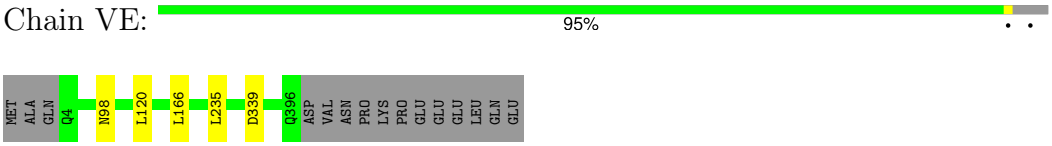
• Molecule 1: Major head protein

Chain UE:



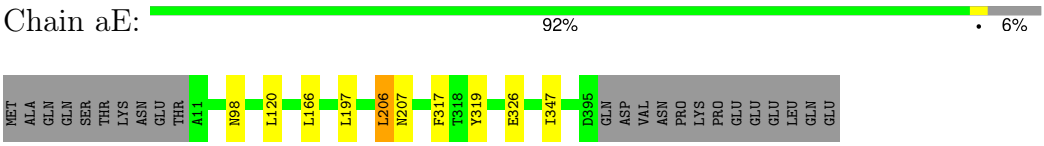
• Molecule 1: Major head protein

Chain VE:



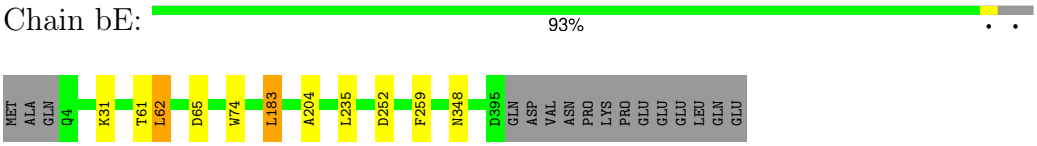
• Molecule 1: Major head protein

Chain aE:



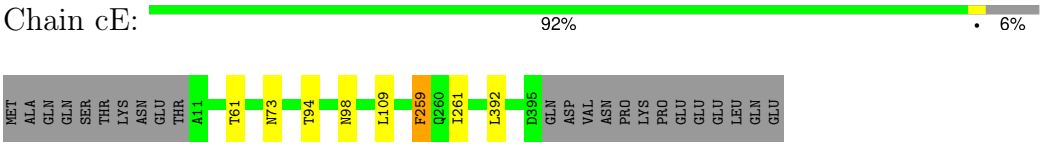
• Molecule 1: Major head protein

Chain bE:



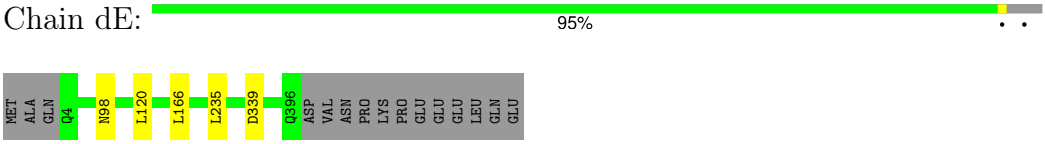
• Molecule 1: Major head protein

Chain cE:



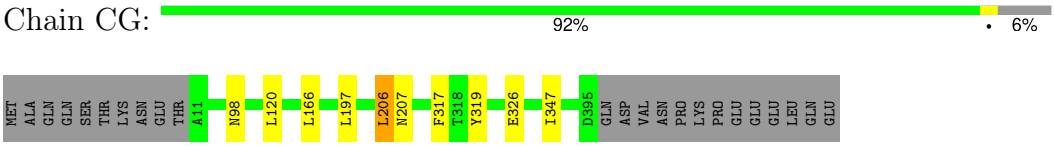
• Molecule 1: Major head protein

Chain dE:



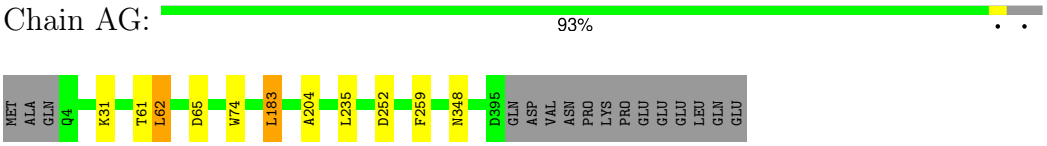
• Molecule 1: Major head protein

Chain CG:



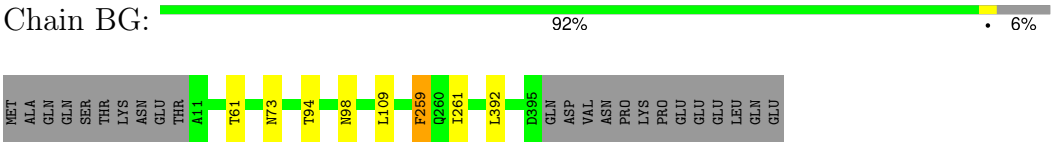
• Molecule 1: Major head protein

Chain AG:



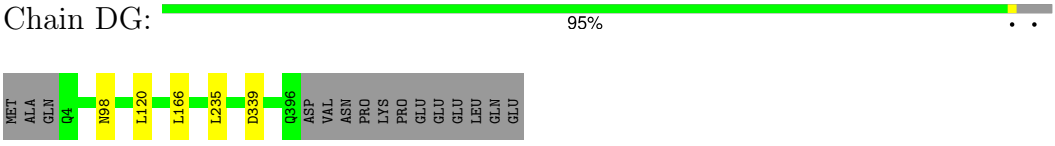
• Molecule 1: Major head protein

Chain BG:



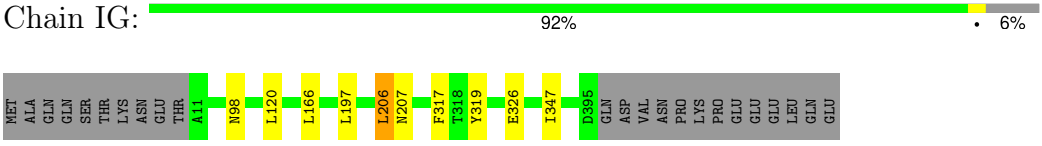
• Molecule 1: Major head protein

Chain DG:



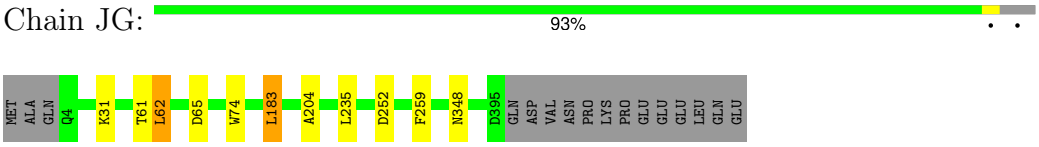
• Molecule 1: Major head protein

Chain IG:



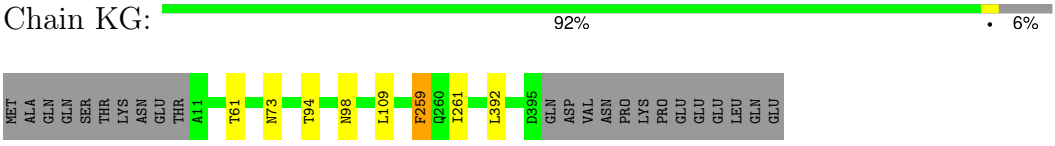
• Molecule 1: Major head protein

Chain JG:



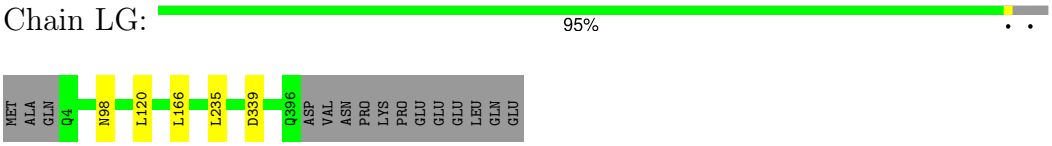
• Molecule 1: Major head protein

Chain KG:



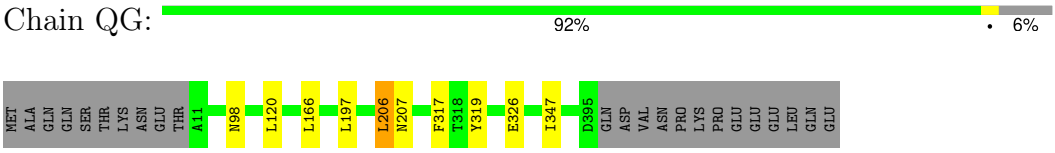
• Molecule 1: Major head protein

Chain LG:



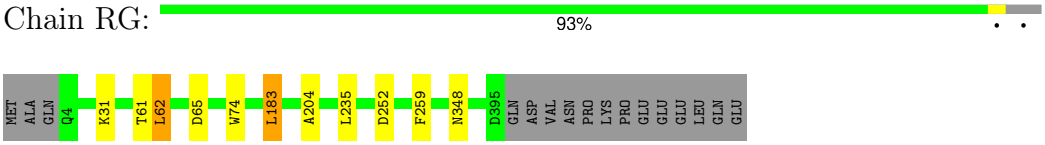
• Molecule 1: Major head protein

Chain QG:



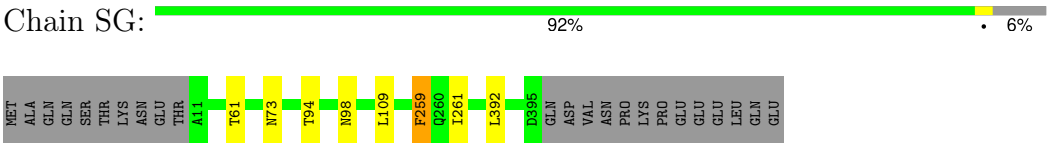
• Molecule 1: Major head protein

Chain RG:



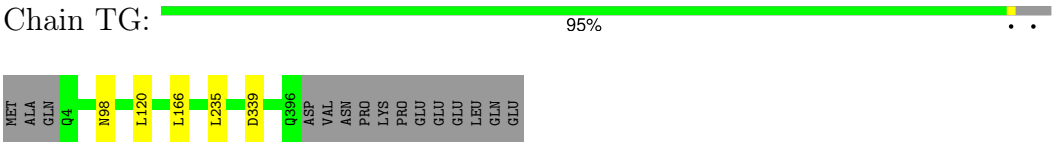
• Molecule 1: Major head protein

Chain SG:



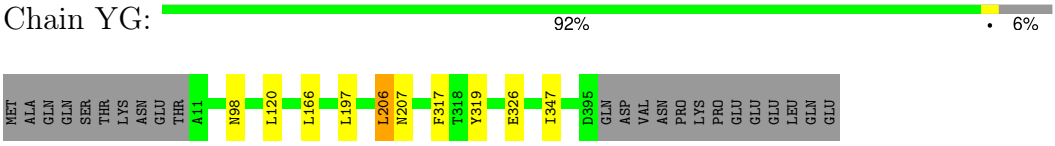
• Molecule 1: Major head protein

Chain TG:



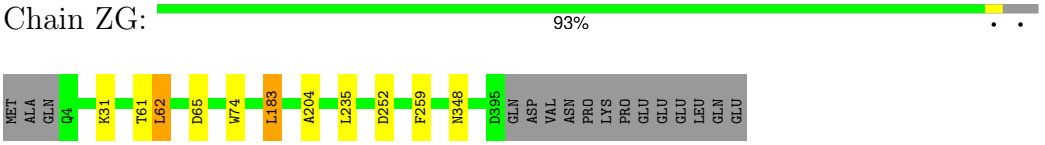
• Molecule 1: Major head protein

Chain YG:



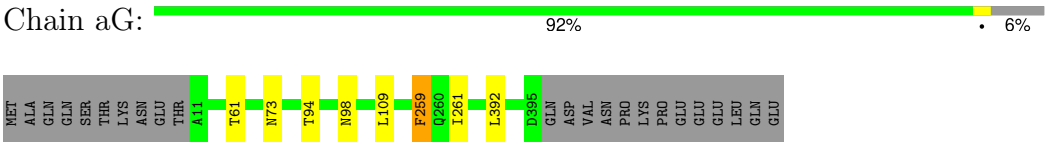
• Molecule 1: Major head protein

Chain ZG:



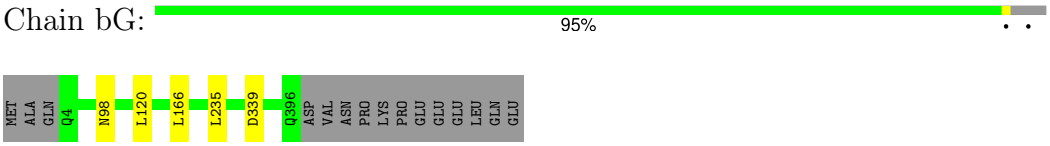
• Molecule 1: Major head protein

Chain aG:



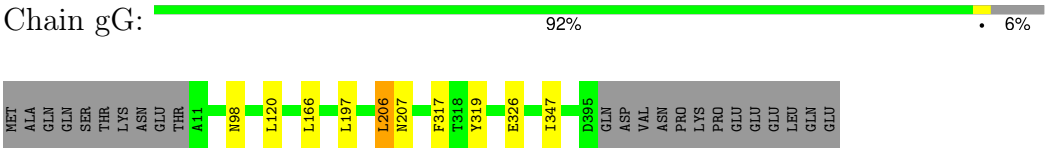
• Molecule 1: Major head protein

Chain bG:



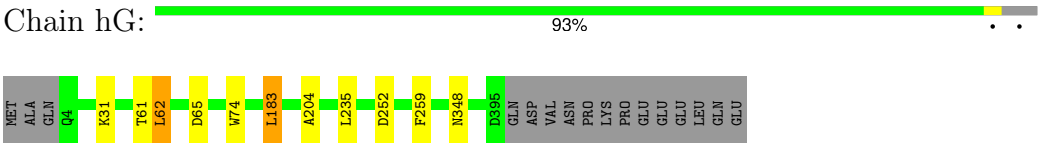
• Molecule 1: Major head protein

Chain gG:



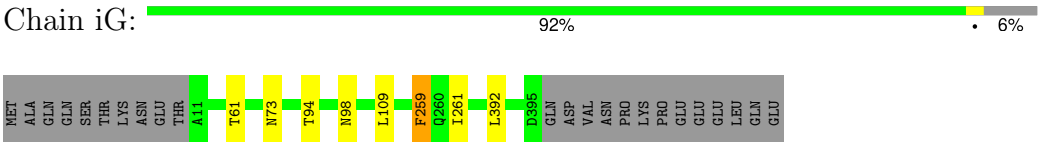
• Molecule 1: Major head protein

Chain hG:



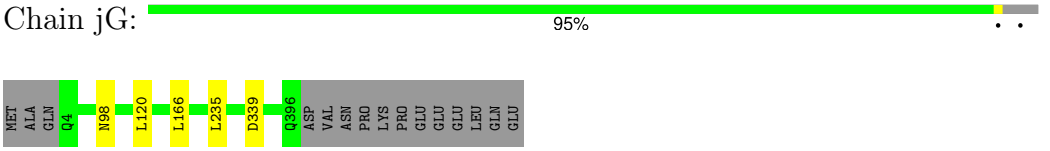
• Molecule 1: Major head protein

Chain iG:



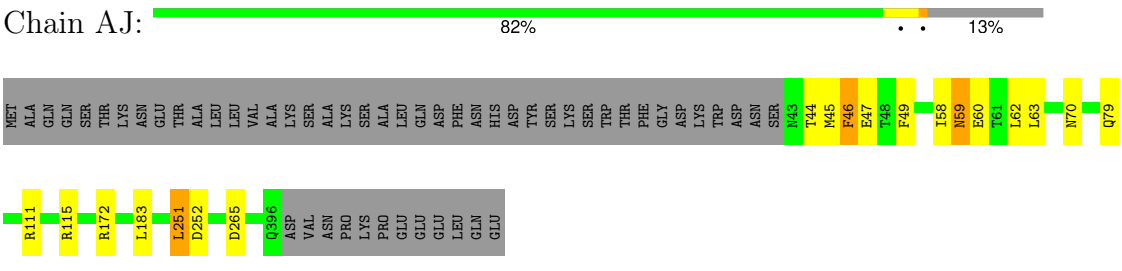
• Molecule 1: Major head protein

Chain jG:



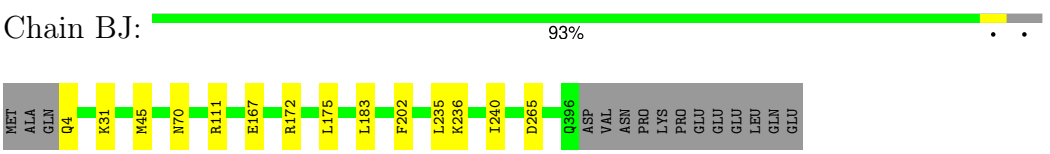
• Molecule 1: Major head protein

Chain AJ:



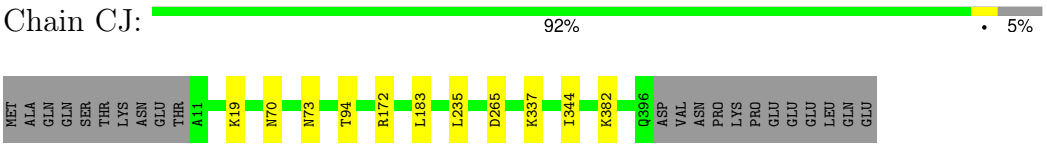
• Molecule 1: Major head protein

Chain BJ:



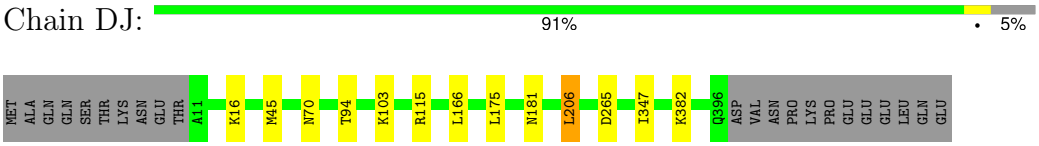
• Molecule 1: Major head protein

Chain CJ:



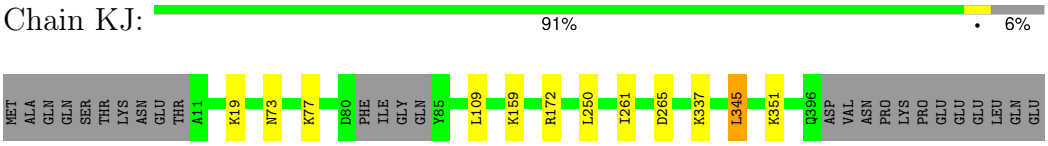
• Molecule 1: Major head protein

Chain DJ:



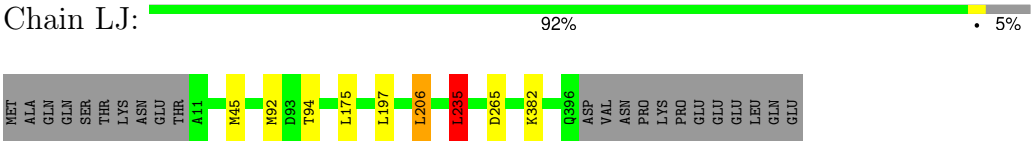
• Molecule 1: Major head protein

Chain KJ:



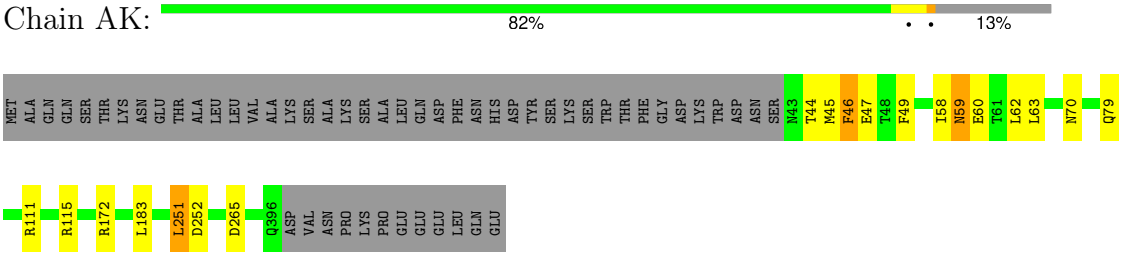
• Molecule 1: Major head protein

Chain LJ:



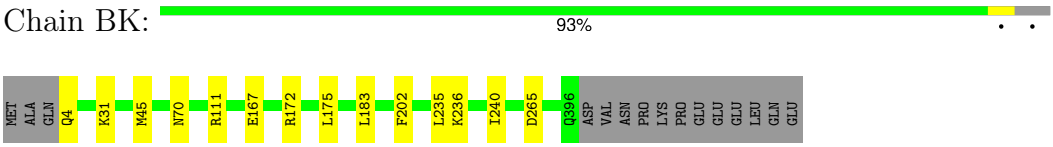
• Molecule 1: Major head protein

Chain AK:



• Molecule 1: Major head protein

Chain BK:



• Molecule 1: Major head protein

Chain CK:

• Molecule 1: Major head protein

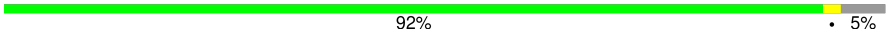
Chain DK:

• Molecule 1: Major head protein

Chain KK:

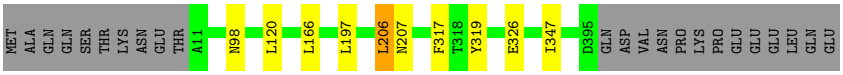
• Molecule 1: Major head protein

Chain LK:



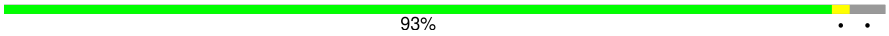
• Molecule 1: Major head protein

Chain CL:



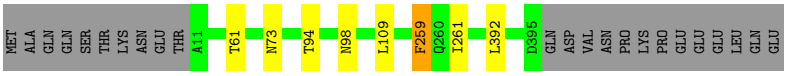
• Molecule 1: Major head protein

Chain AL:



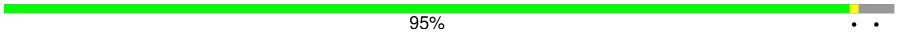
• Molecule 1: Major head protein

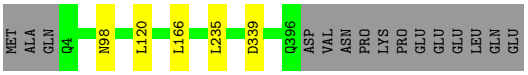
Chain BL:



• Molecule 1: Major head protein

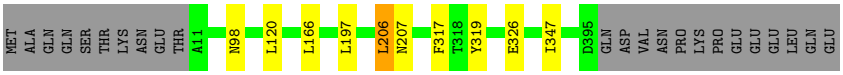
Chain DL:





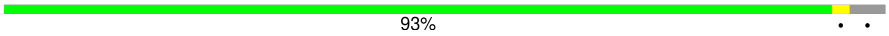
• Molecule 1: Major head protein

Chain IL:



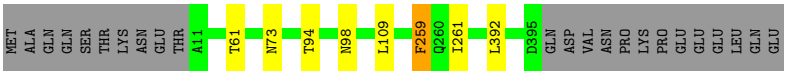
• Molecule 1: Major head protein

Chain JL:



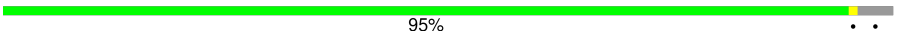
• Molecule 1: Major head protein

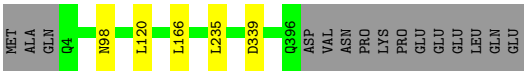
Chain KL:



• Molecule 1: Major head protein

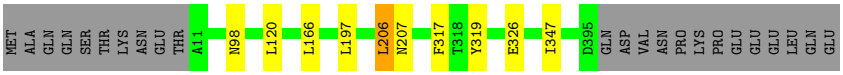
Chain LL:





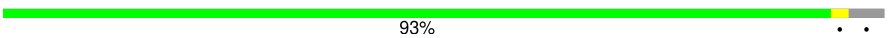
• Molecule 1: Major head protein

Chain QL:



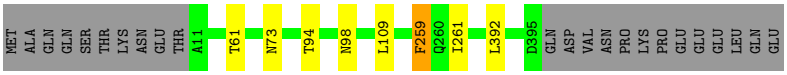
• Molecule 1: Major head protein

Chain RL:



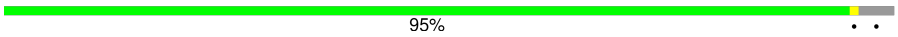
• Molecule 1: Major head protein

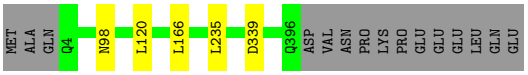
Chain SL:



• Molecule 1: Major head protein

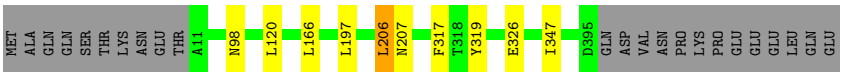
Chain TL:





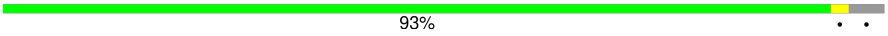
• Molecule 1: Major head protein

Chain YL:



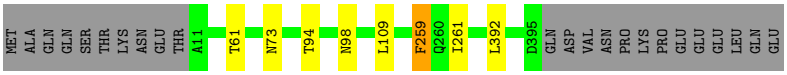
• Molecule 1: Major head protein

Chain ZL:



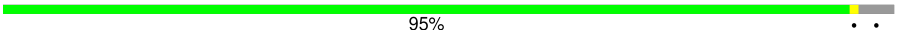
• Molecule 1: Major head protein

Chain aL:



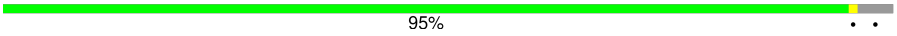
• Molecule 1: Major head protein

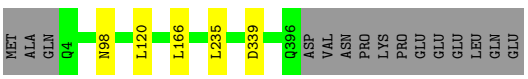
Chain bL:



• Molecule 1: Major head protein

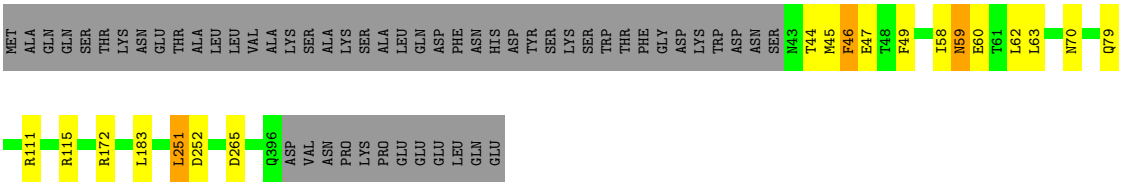
Chain gL:





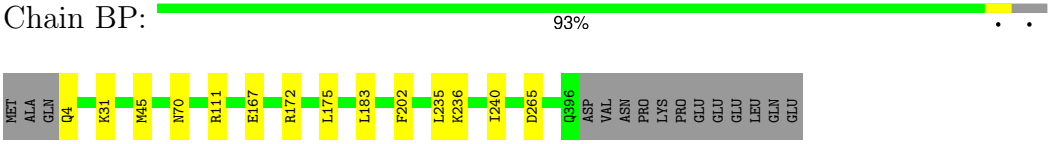
• Molecule 1: Major head protein

Chain AP:



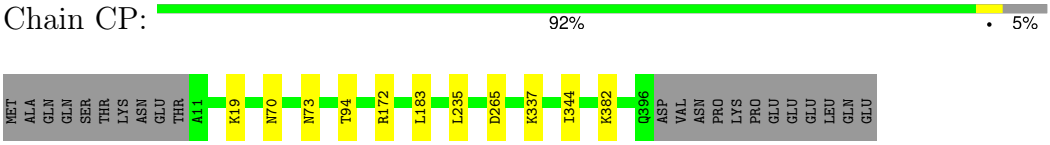
• Molecule 1: Major head protein

Chain BP:



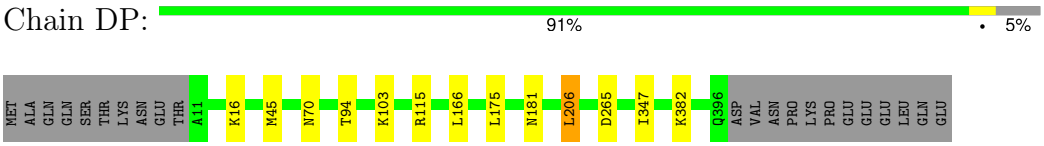
• Molecule 1: Major head protein

Chain CP:



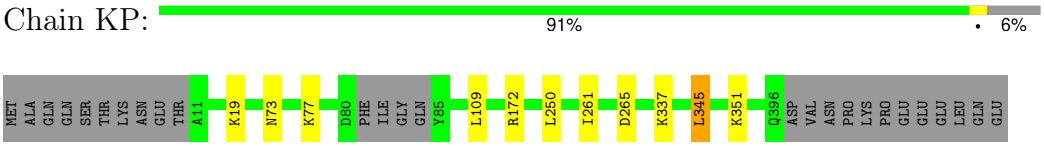
• Molecule 1: Major head protein

Chain DP:



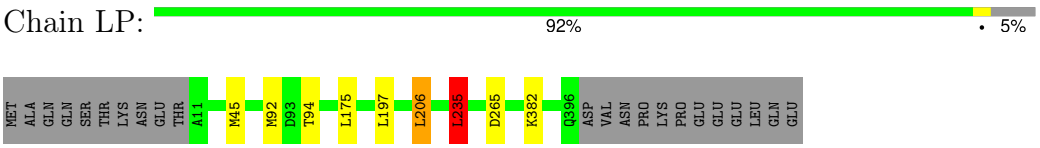
• Molecule 1: Major head protein

Chain KP:



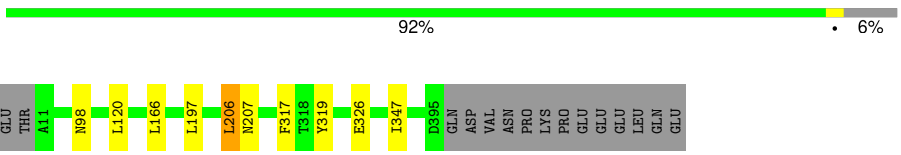
• Molecule 1: Major head protein

Chain LP:



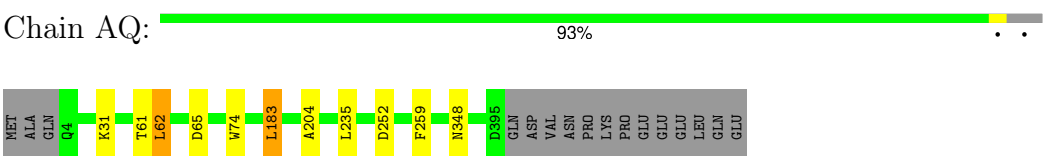
• Molecule 1: Major head protein

Chain CQ:



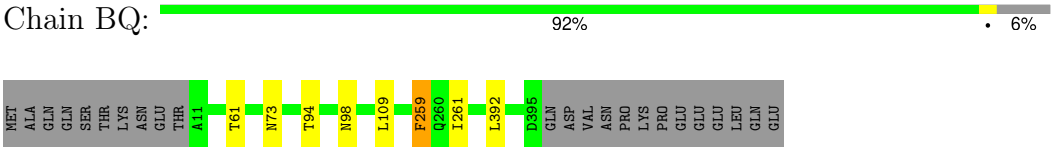
• Molecule 1: Major head protein

Chain AQ:



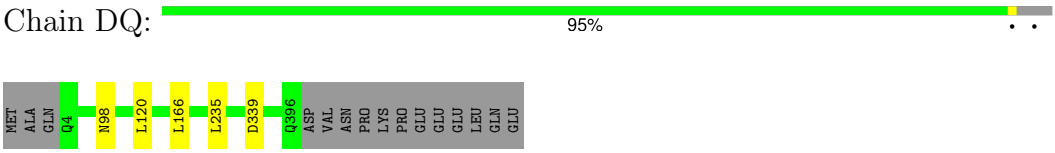
• Molecule 1: Major head protein

Chain BQ:



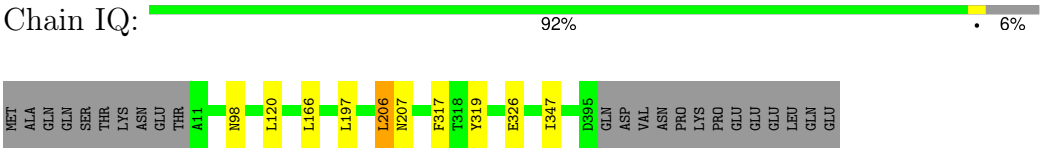
• Molecule 1: Major head protein

Chain DQ:



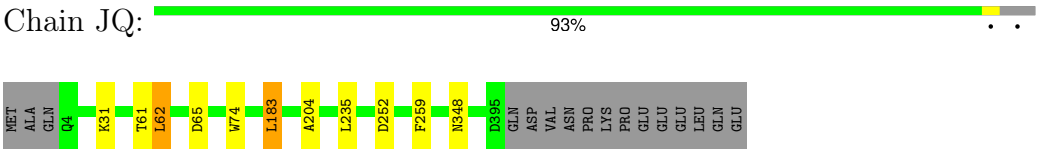
• Molecule 1: Major head protein

Chain IQ:



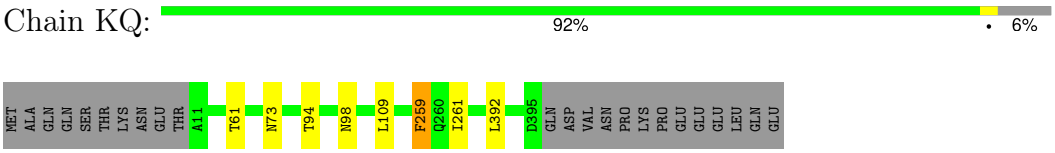
• Molecule 1: Major head protein

Chain JQ:



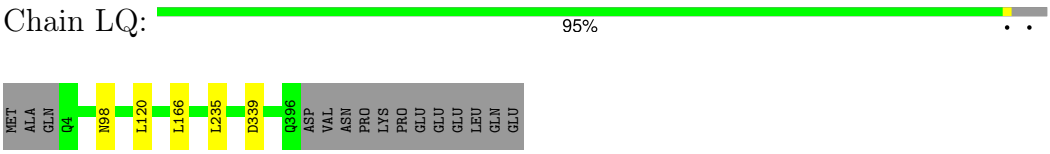
• Molecule 1: Major head protein

Chain KQ:



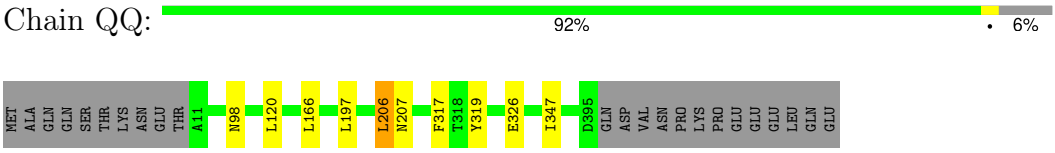
• Molecule 1: Major head protein

Chain LQ:



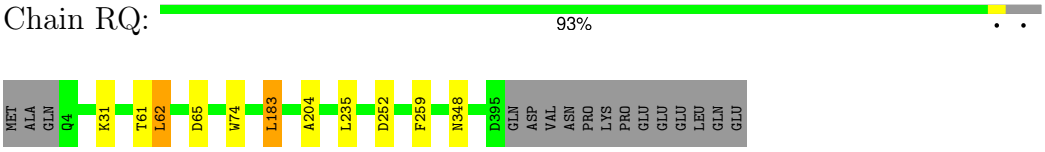
• Molecule 1: Major head protein

Chain QQ:



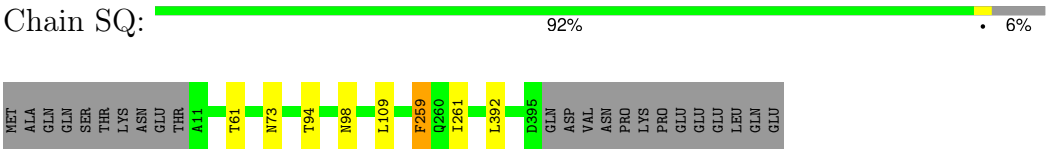
• Molecule 1: Major head protein

Chain RQ:



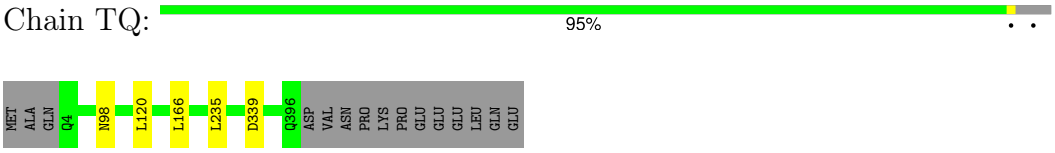
• Molecule 1: Major head protein

Chain SQ:



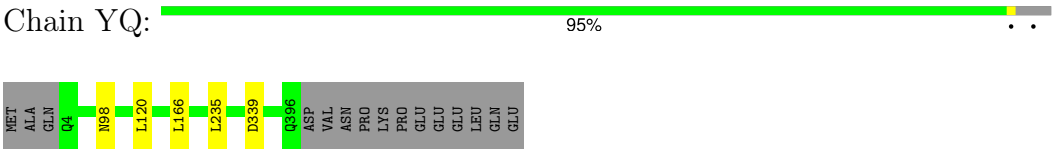
• Molecule 1: Major head protein

Chain TQ:



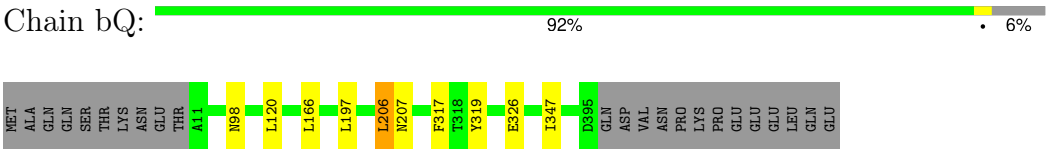
• Molecule 1: Major head protein

Chain YQ:



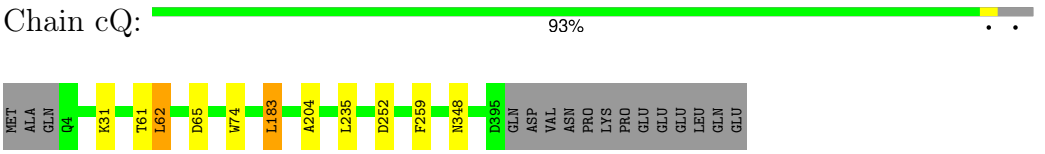
• Molecule 1: Major head protein

Chain bQ:



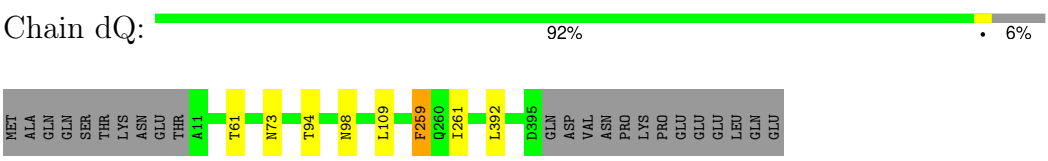
• Molecule 1: Major head protein

Chain cQ:



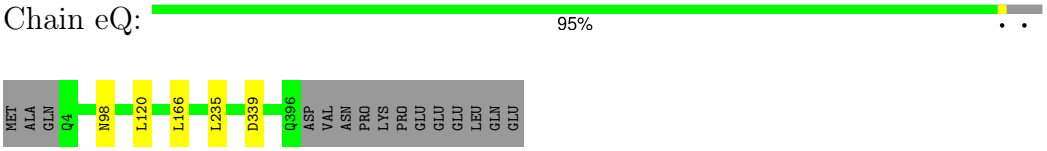
• Molecule 1: Major head protein

Chain dQ:



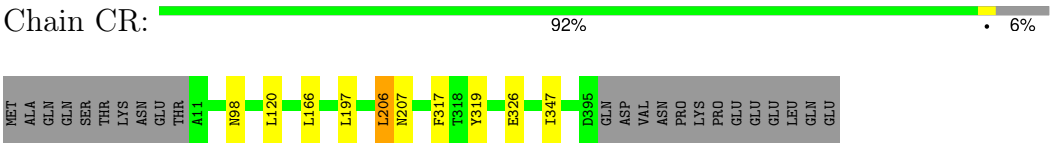
• Molecule 1: Major head protein

Chain eQ:



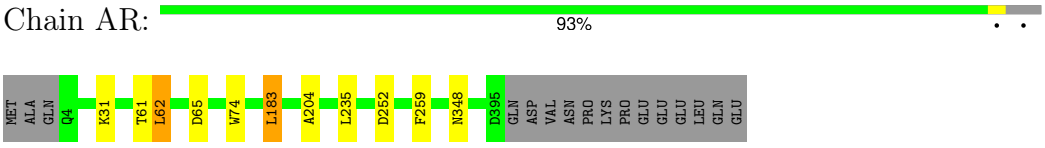
• Molecule 1: Major head protein

Chain CR:



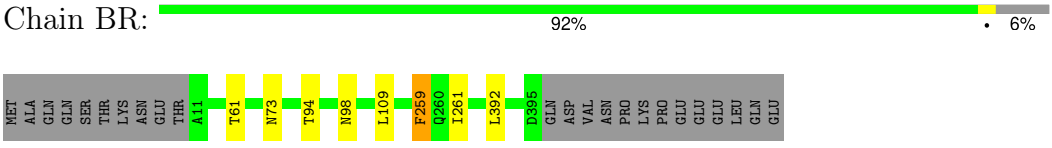
• Molecule 1: Major head protein

Chain AR:



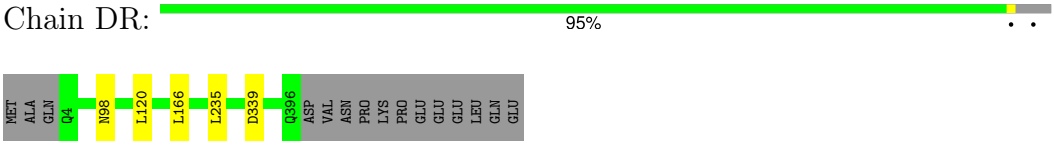
• Molecule 1: Major head protein

Chain BR:



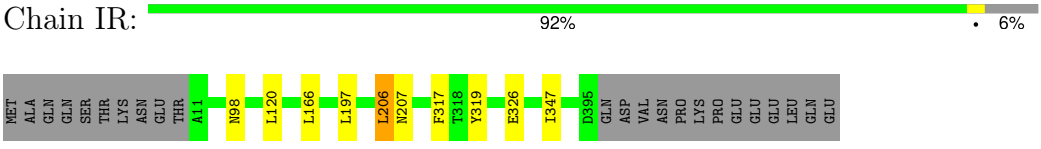
• Molecule 1: Major head protein

Chain DR:



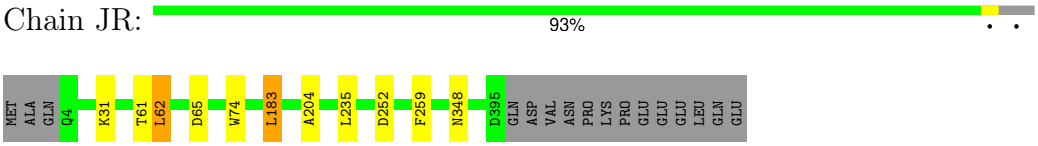
• Molecule 1: Major head protein

Chain IR:



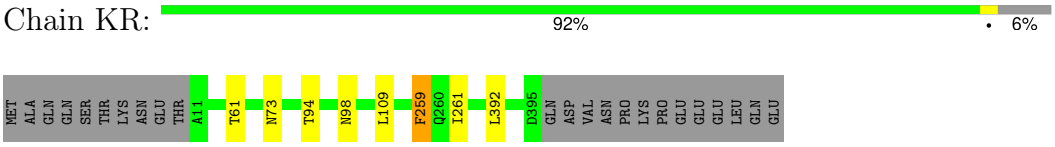
• Molecule 1: Major head protein

Chain JR:



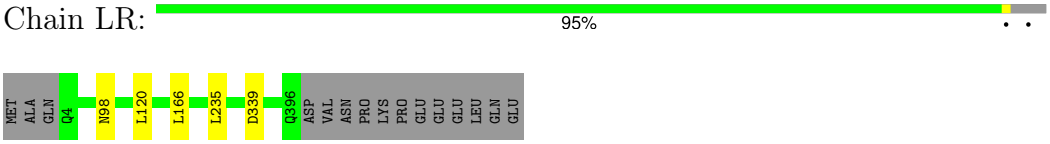
• Molecule 1: Major head protein

Chain KR:



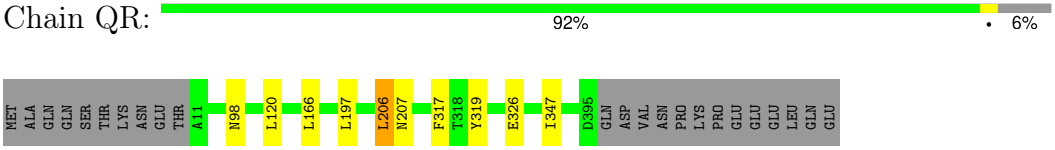
• Molecule 1: Major head protein

Chain LR:



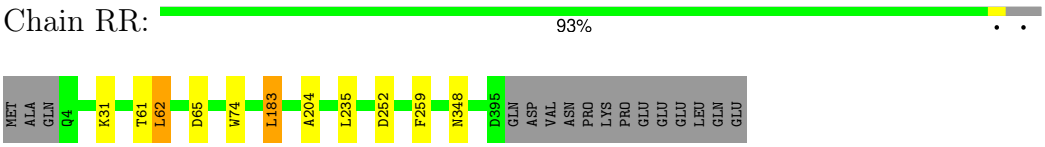
• Molecule 1: Major head protein

Chain QR:



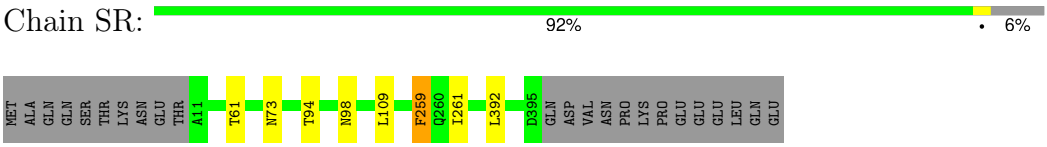
• Molecule 1: Major head protein

Chain RR:



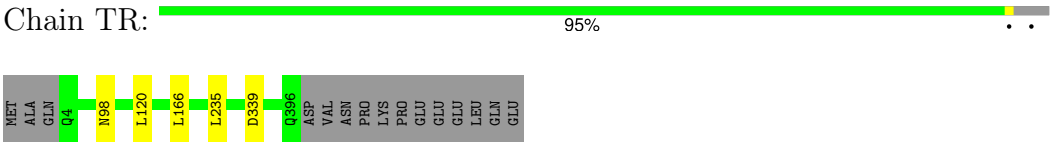
• Molecule 1: Major head protein

Chain SR:



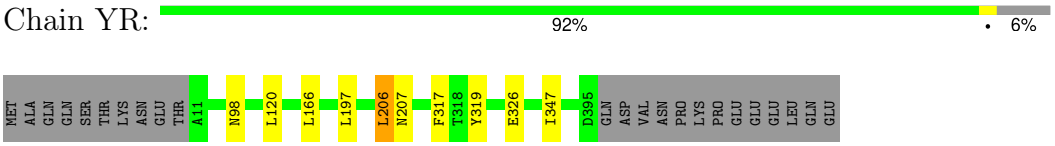
• Molecule 1: Major head protein

Chain TR:



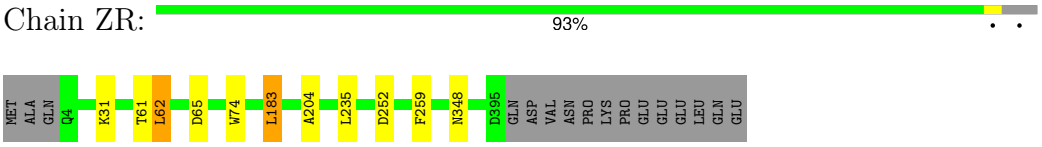
• Molecule 1: Major head protein

Chain YR:



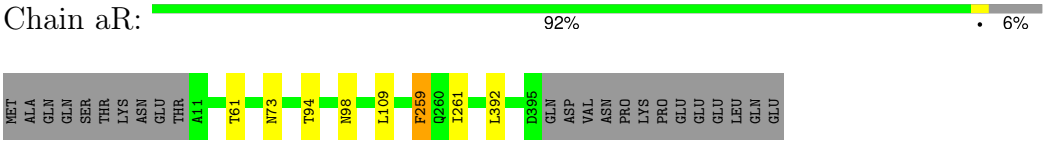
• Molecule 1: Major head protein

Chain ZR:



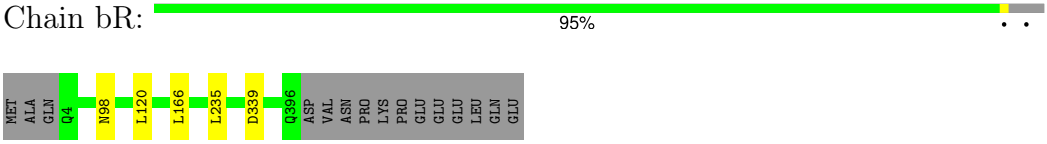
• Molecule 1: Major head protein

Chain aR:



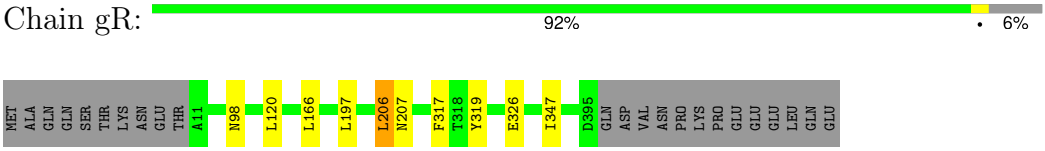
• Molecule 1: Major head protein

Chain bR:



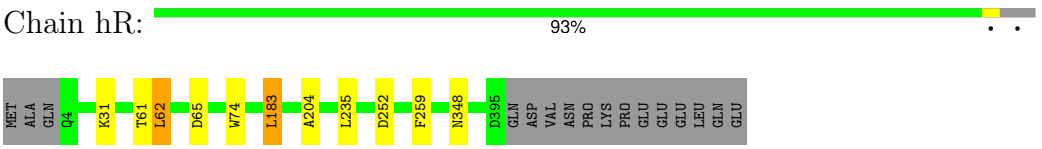
• Molecule 1: Major head protein

Chain gR:



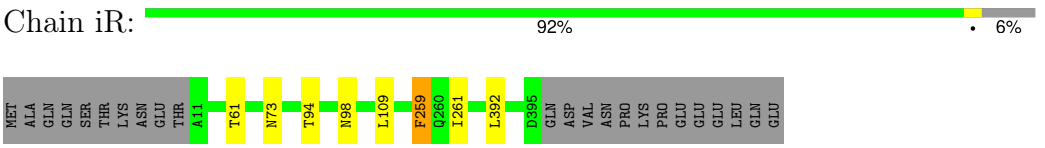
• Molecule 1: Major head protein

Chain hR:



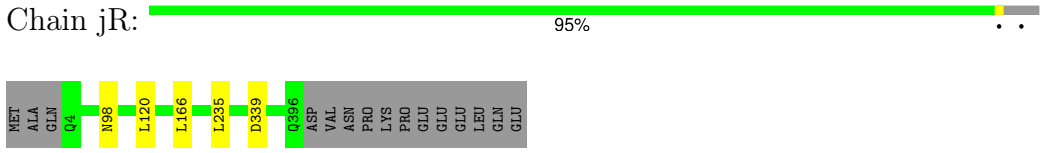
• Molecule 1: Major head protein

Chain iR:



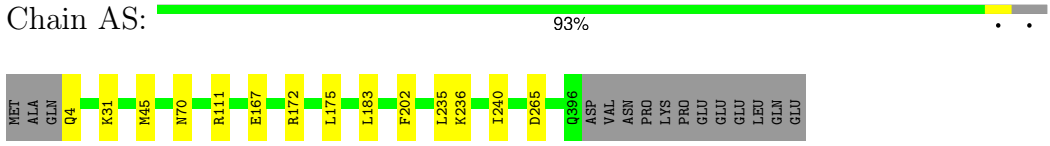
• Molecule 1: Major head protein

Chain jR:



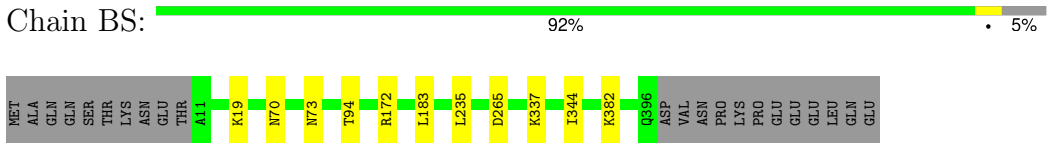
• Molecule 1: Major head protein

Chain AS:



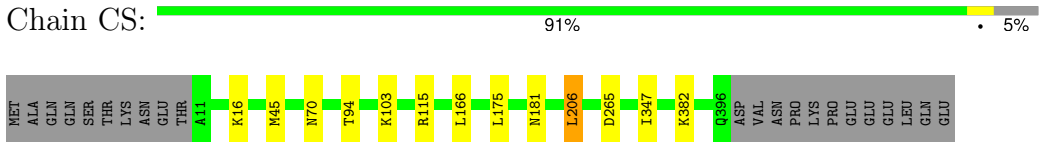
• Molecule 1: Major head protein

Chain BS:



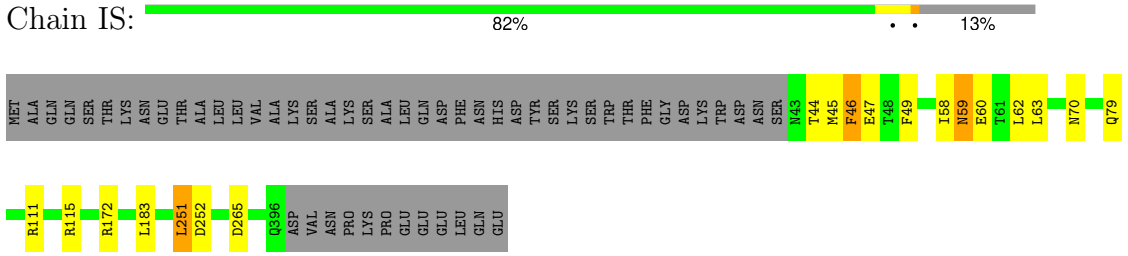
• Molecule 1: Major head protein

Chain CS:



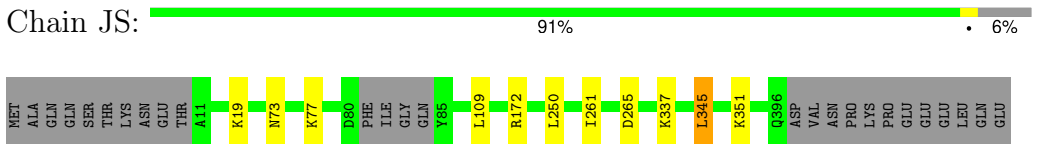
• Molecule 1: Major head protein

Chain IS:



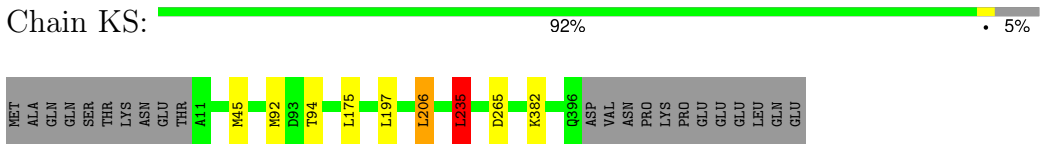
• Molecule 1: Major head protein

Chain JS:



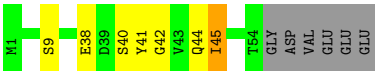
• Molecule 1: Major head protein

Chain KS:



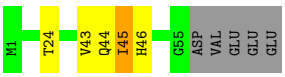
• Molecule 2: Arstotzka protein

Chain E1:



• Molecule 2: Arstotzka protein

Chain F1:

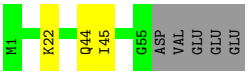


• Molecule 2: Arstotzka protein

Chain G1:

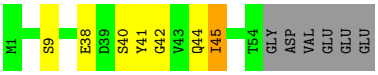
• Molecule 2: Arstotzka protein

Chain H1:



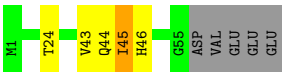
• Molecule 2: Arstotzka protein

Chain M1:



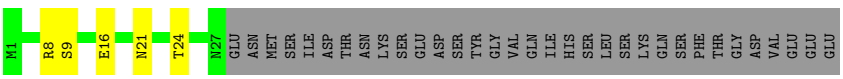
• Molecule 2: Arstotzka protein

Chain N1:



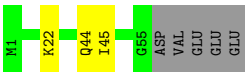
• Molecule 2: Arstotzka protein

Chain O1:



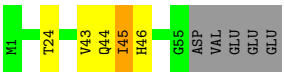
• Molecule 2: Arstotzka protein

Chain P1:



• Molecule 2: Arstotzka protein

Chain U1:

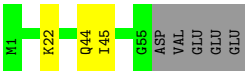


• Molecule 2: Arstotzka protein

Chain V1:

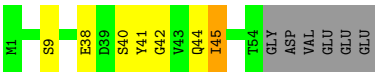
• Molecule 2: Arstotzka protein

Chain W1:



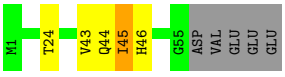
• Molecule 2: Arstotzka protein

Chain b1:



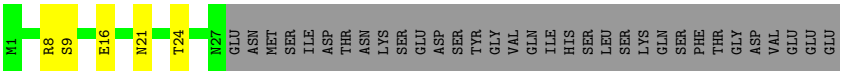
• Molecule 2: Arstotzka protein

Chain c1:



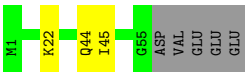
• Molecule 2: Arstotzka protein

Chain d1:



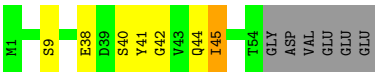
• Molecule 2: Arstotzka protein

Chain e1:



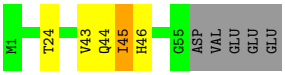
• Molecule 2: Arstotzka protein

Chain j1:



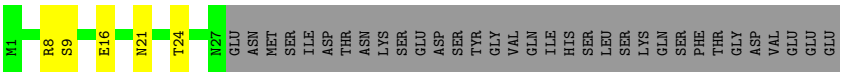
• Molecule 2: Arstotzka protein

Chain k1:



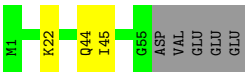
• Molecule 2: Arstotzka protein

Chain l1:



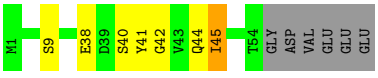
• Molecule 2: Arstotzka protein

Chain m1:



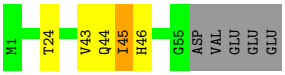
• Molecule 2: Arstotzka protein

Chain E3:



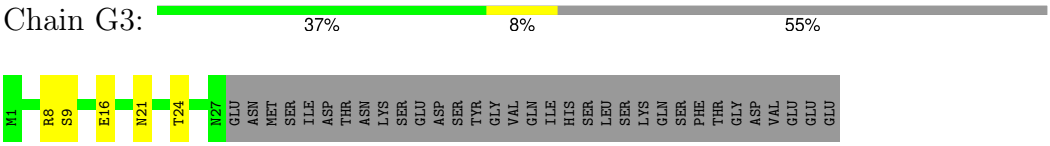
• Molecule 2: Arstotzka protein

Chain F3:



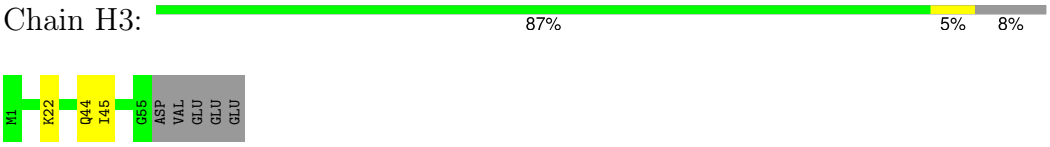
• Molecule 2: Arstotzka protein

Chain G3:



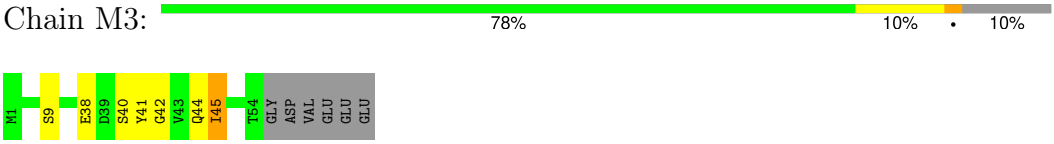
• Molecule 2: Arstotzka protein

Chain H3:



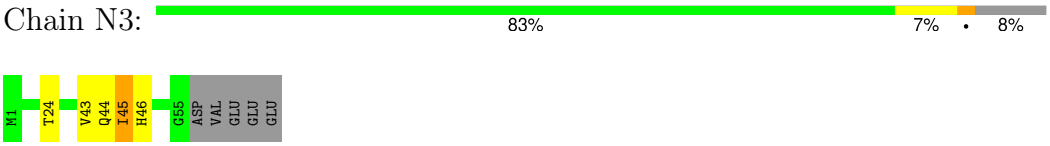
• Molecule 2: Arstotzka protein

Chain M3:



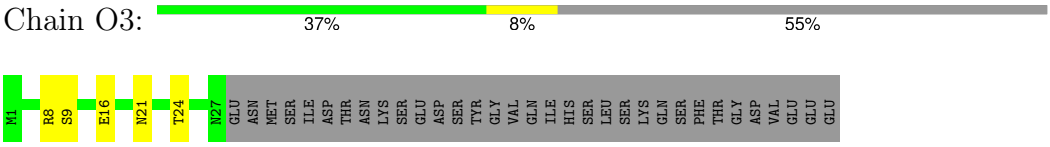
• Molecule 2: Arstotzka protein

Chain N3:



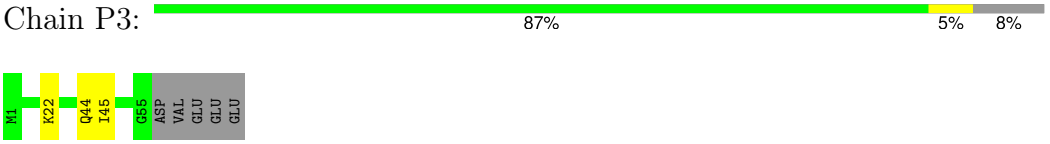
• Molecule 2: Arstotzka protein

Chain O3:



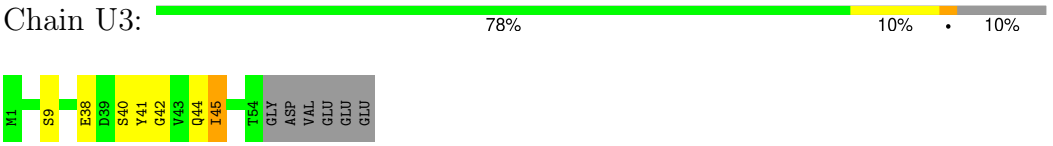
• Molecule 2: Arstotzka protein

Chain P3:



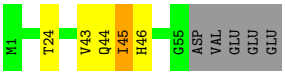
• Molecule 2: Arstotzka protein

Chain U3:



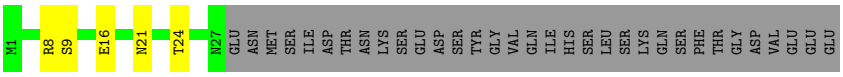
• Molecule 2: Arstotzka protein

Chain V3:



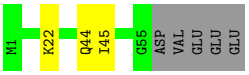
• Molecule 2: Arstotzka protein

Chain W3:



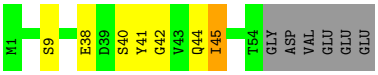
• Molecule 2: Arstotzka protein

Chain X3:



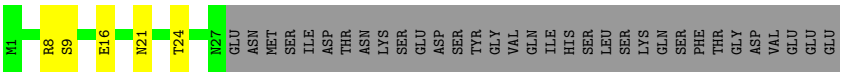
• Molecule 2: Arstotzka protein

Chain Z3:



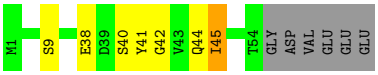
• Molecule 2: Arstotzka protein

Chain a3:



• Molecule 2: Arstotzka protein

Chain c3:

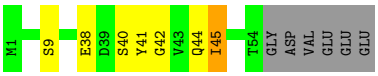


• Molecule 2: Arstotzka protein

Chain d3:

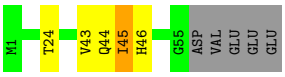
• Molecule 2: Arstotzka protein

Chain E4:



• Molecule 2: Arstotzka protein

Chain F4:

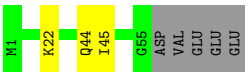


• Molecule 2: Arstotzka protein

Chain G4:

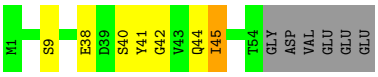
• Molecule 2: Arstotzka protein

Chain H4:



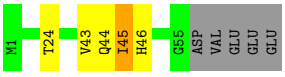
• Molecule 2: Arstotzka protein

Chain M4:



• Molecule 2: Arstotzka protein

Chain N4:

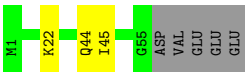


• Molecule 2: Arstotzka protein

Chain O4:

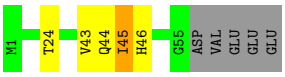
• Molecule 2: Arstotzka protein

Chain P4:



• Molecule 2: Arstotzka protein

Chain U4:

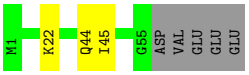


• Molecule 2: Arstotzka protein

Chain V4:

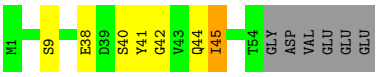
• Molecule 2: Arstotzka protein

Chain W4:



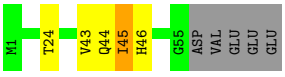
• Molecule 2: Arstotzka protein

Chain b4:



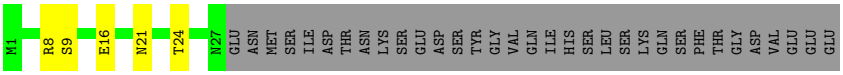
• Molecule 2: Arstotzka protein

Chain c4:



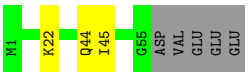
• Molecule 2: Arstotzka protein

Chain d4:



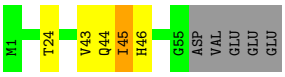
• Molecule 2: Arstotzka protein

Chain e4:



• Molecule 2: Arstotzka protein

Chain j4:

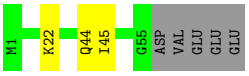


• Molecule 2: Arstotzka protein

Chain k4:

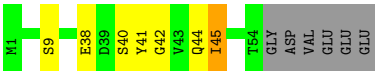
• Molecule 2: Arstotzka protein

Chain l4:



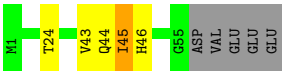
• Molecule 2: Arstotzka protein

Chain E6:



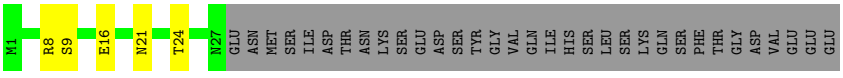
• Molecule 2: Arstotzka protein

Chain F6:



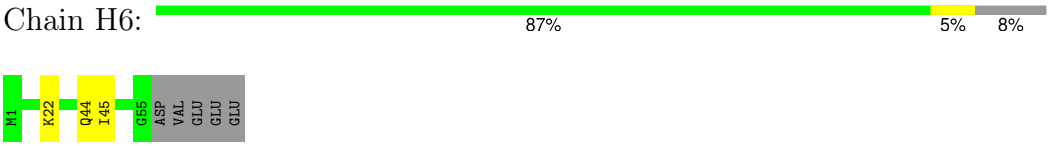
• Molecule 2: Arstotzka protein

Chain G6:



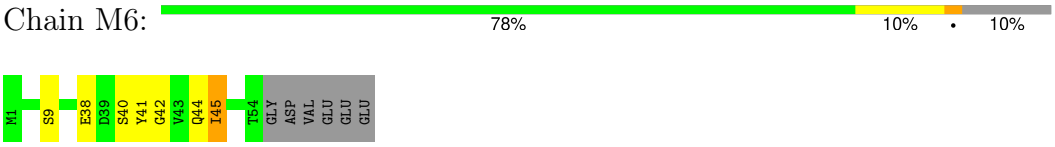
• Molecule 2: Arstotzka protein

Chain H6:



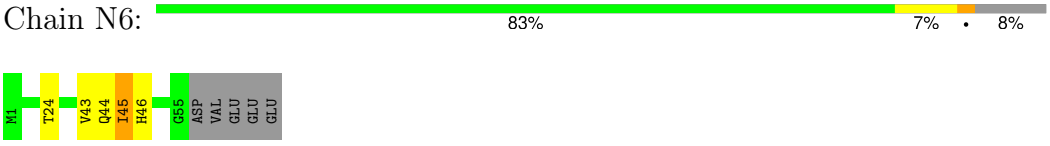
• Molecule 2: Arstotzka protein

Chain M6:



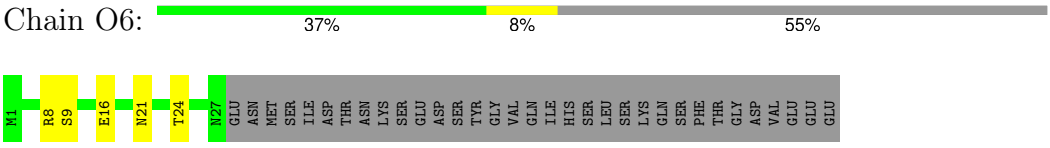
• Molecule 2: Arstotzka protein

Chain N6:



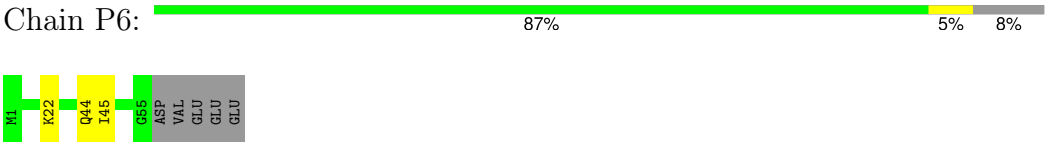
• Molecule 2: Arstotzka protein

Chain O6:



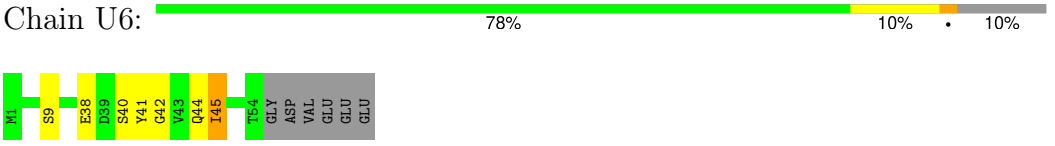
• Molecule 2: Arstotzka protein

Chain P6:



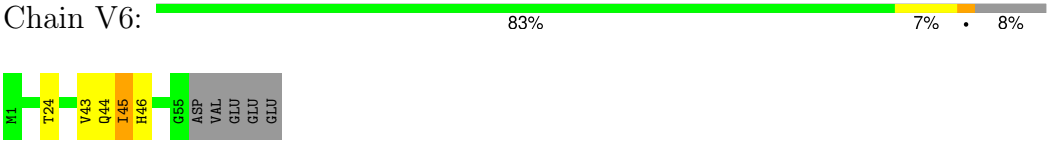
• Molecule 2: Arstotzka protein

Chain U6:



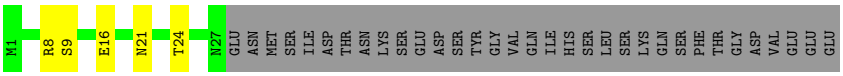
• Molecule 2: Arstotzka protein

Chain V6:



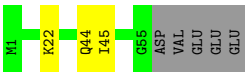
• Molecule 2: Arstotzka protein

Chain W6:



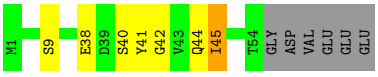
• Molecule 2: Arstotzka protein

Chain X6:



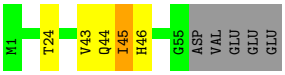
• Molecule 2: Arstotzka protein

Chain c6:



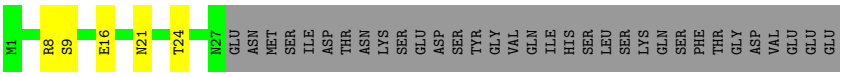
• Molecule 2: Arstotzka protein

Chain d6:



• Molecule 2: Arstotzka protein

Chain e6:

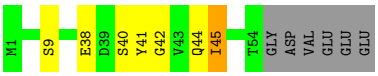


• Molecule 2: Arstotzka protein

Chain f6:

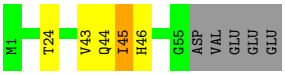
• Molecule 2: Arstotzka protein

Chain k6:



• Molecule 2: Arstotzka protein

Chain l6:

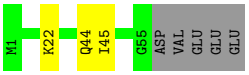


• Molecule 2: Arstotzka protein

Chain m6:

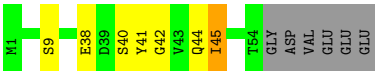
• Molecule 2: Arstotzka protein

Chain n6:



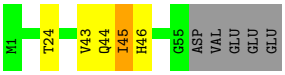
• Molecule 2: Arstotzka protein

Chain E7:



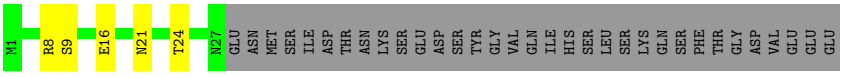
• Molecule 2: Arstotzka protein

Chain F7:



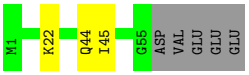
• Molecule 2: Arstotzka protein

Chain G7:



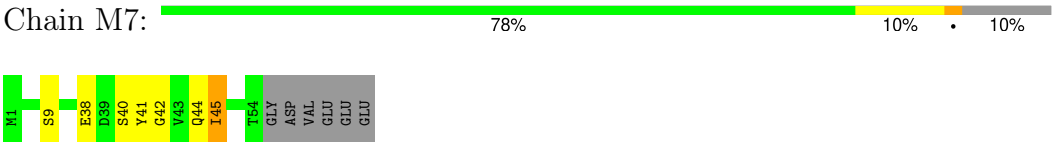
• Molecule 2: Arstotzka protein

Chain H7:



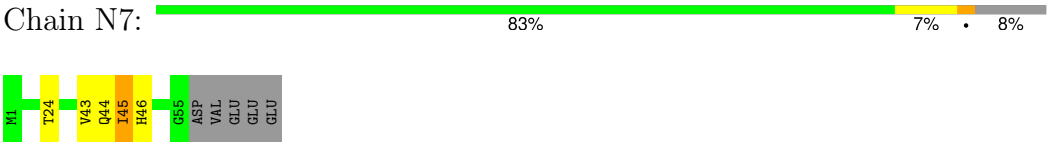
• Molecule 2: Arstotzka protein

Chain M7:



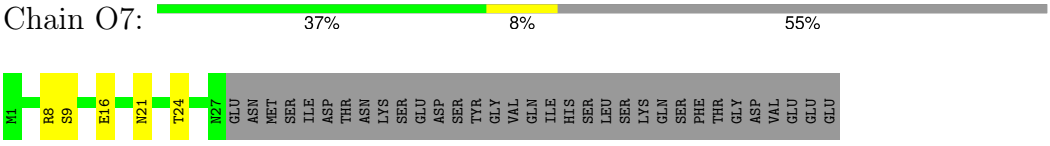
• Molecule 2: Arstotzka protein

Chain N7:



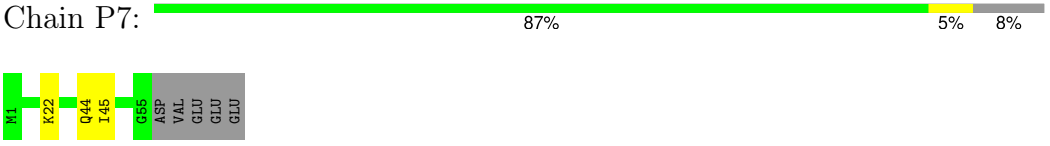
• Molecule 2: Arstotzka protein

Chain O7:



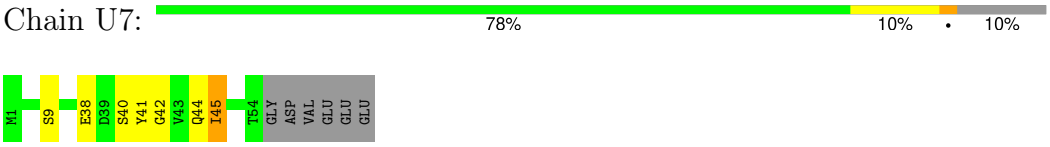
• Molecule 2: Arstotzka protein

Chain P7:



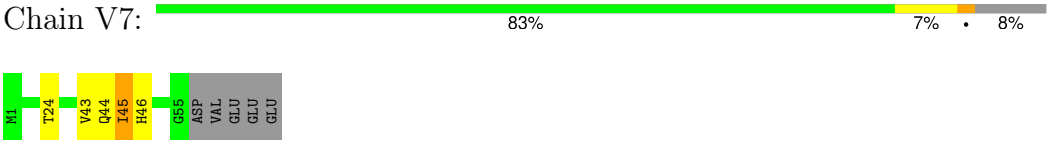
• Molecule 2: Arstotzka protein

Chain U7:



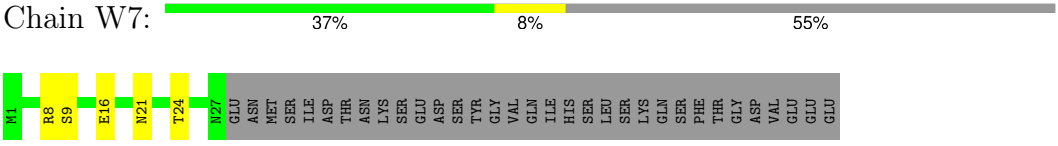
• Molecule 2: Arstotzka protein

Chain V7:



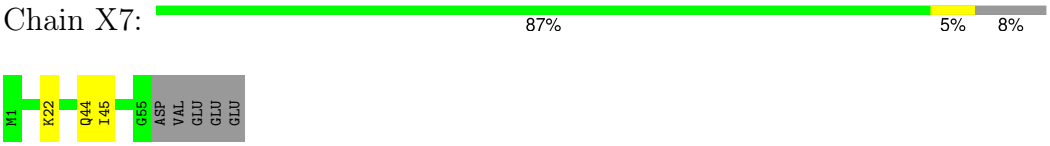
• Molecule 2: Arstotzka protein

Chain W7:



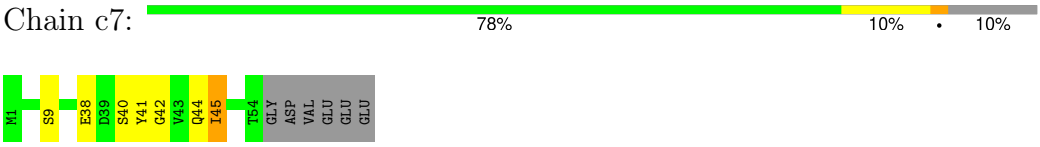
• Molecule 2: Arstotzka protein

Chain X7:



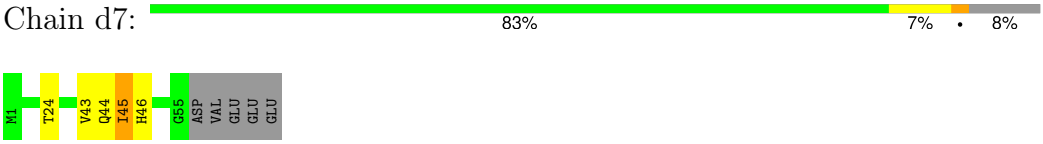
• Molecule 2: Arstotzka protein

Chain c7:



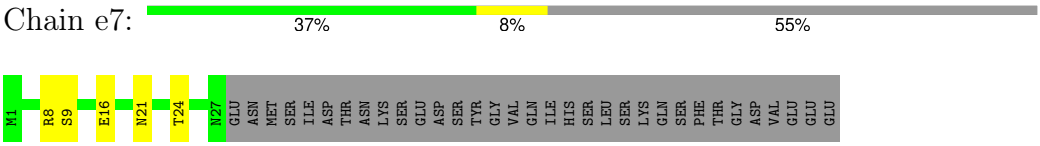
• Molecule 2: Arstotzka protein

Chain d7:



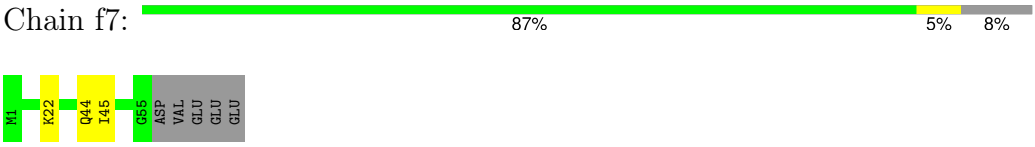
• Molecule 2: Arstotzka protein

Chain e7:



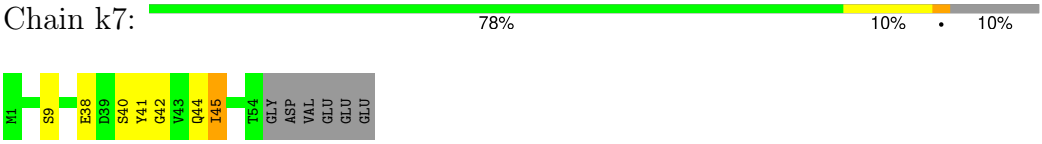
• Molecule 2: Arstotzka protein

Chain f7:



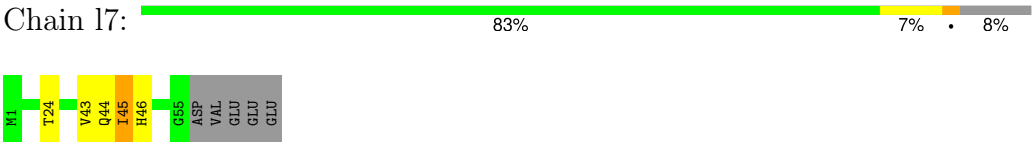
• Molecule 2: Arstotzka protein

Chain k7:



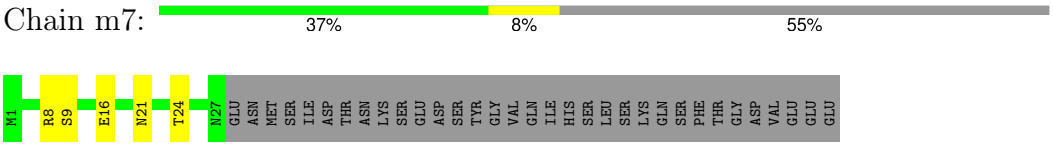
• Molecule 2: Arstotzka protein

Chain l7:



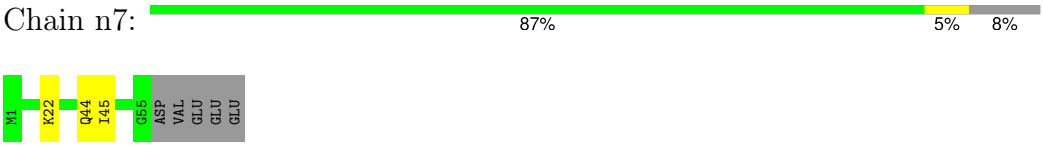
• Molecule 2: Arstotzka protein

Chain m7:



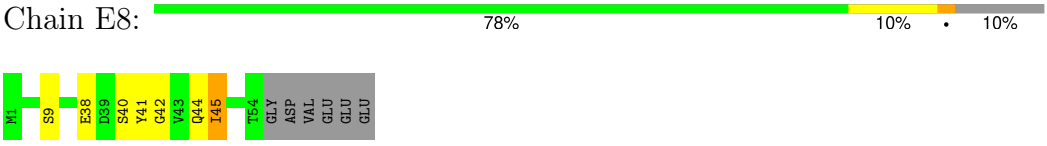
• Molecule 2: Arstotzka protein

Chain n7:



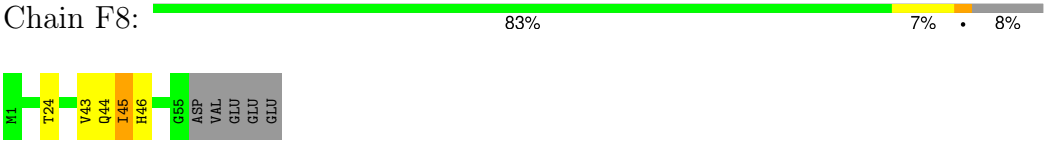
• Molecule 2: Arstotzka protein

Chain E8:



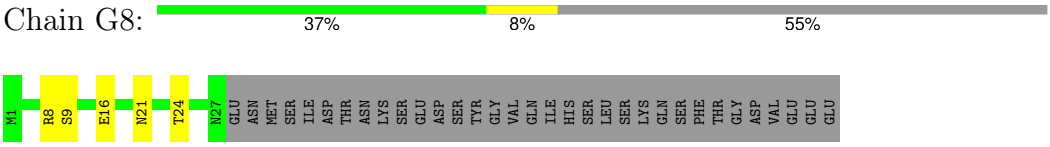
• Molecule 2: Arstotzka protein

Chain F8:



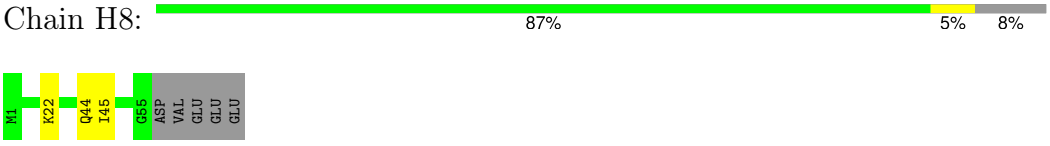
• Molecule 2: Arstotzka protein

Chain G8:



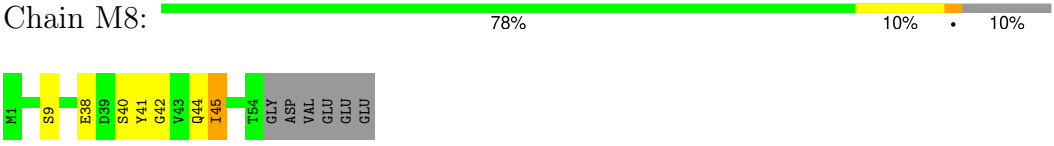
• Molecule 2: Arstotzka protein

Chain H8:



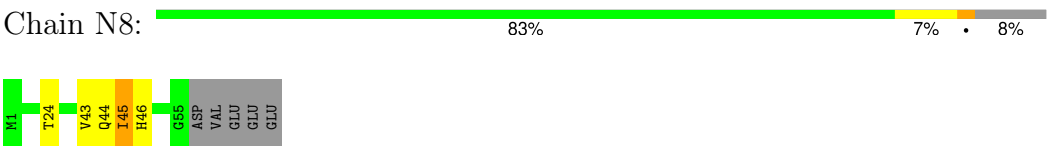
• Molecule 2: Arstotzka protein

Chain M8:



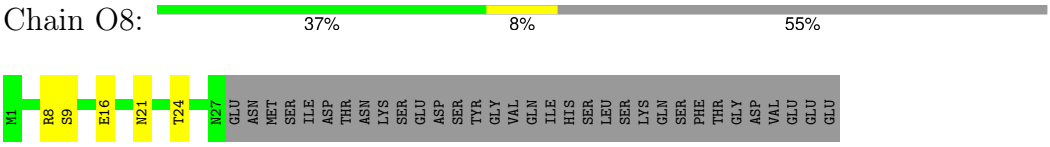
• Molecule 2: Arstotzka protein

Chain N8:



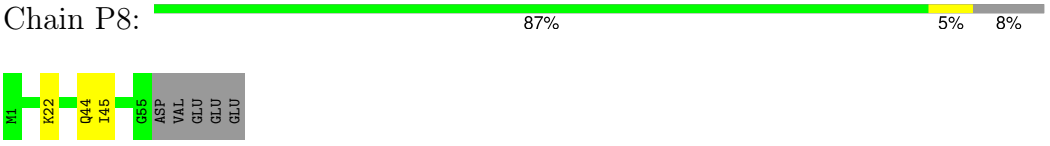
• Molecule 2: Arstotzka protein

Chain O8:



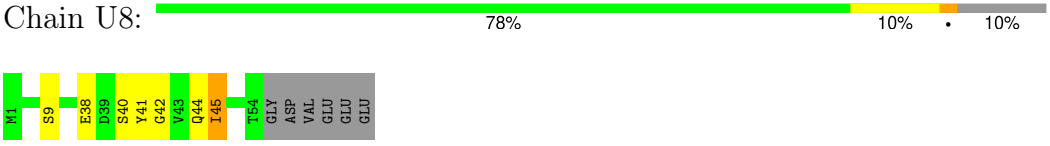
• Molecule 2: Arstotzka protein

Chain P8:



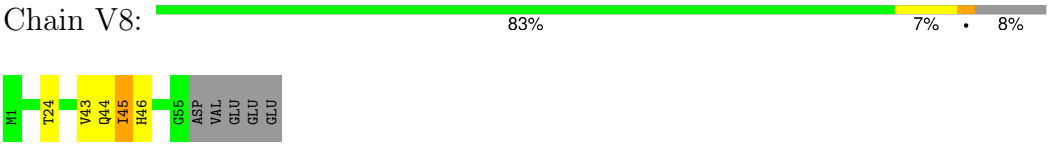
• Molecule 2: Arstotzka protein

Chain U8:



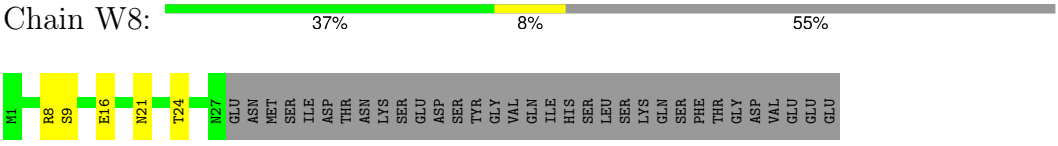
• Molecule 2: Arstotzka protein

Chain V8:



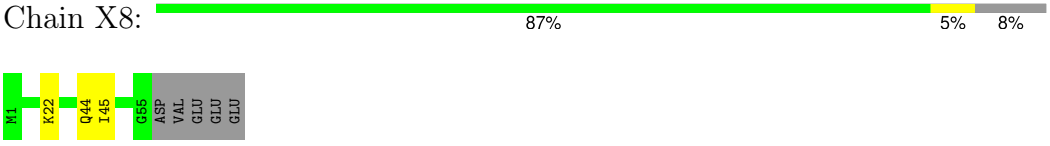
• Molecule 2: Arstotzka protein

Chain W8:



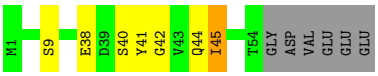
• Molecule 2: Arstotzka protein

Chain X8:



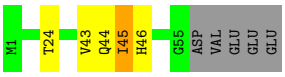
• Molecule 2: Arstotzka protein

Chain c8:



• Molecule 2: Arstotzka protein

Chain d8:

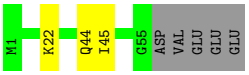


• Molecule 2: Arstotzka protein

Chain e8:

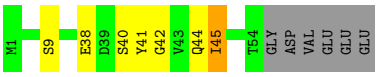
• Molecule 2: Arstotzka protein

Chain f8:



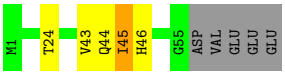
• Molecule 2: Arstotzka protein

Chain k8:



• Molecule 2: Arstotzka protein

Chain l8:

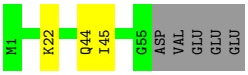


• Molecule 2: Arstotzka protein

Chain m8:

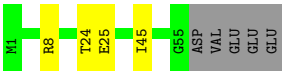
• Molecule 2: Arstotzka protein

Chain n8:



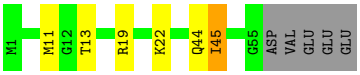
• Molecule 2: Arstotzka protein

Chain ED:



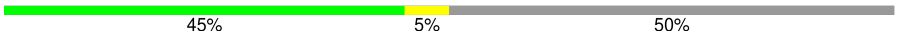
• Molecule 2: Arstotzka protein

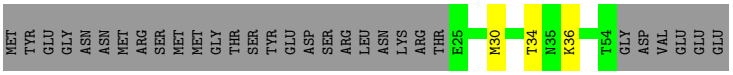
Chain FD:



• Molecule 2: Arstotzka protein

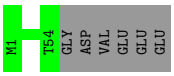
Chain GD:





• Molecule 2: Arstotzka protein

Chain HD:

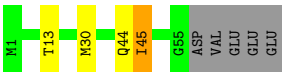


• Molecule 2: Arstotzka protein

Chain MD:

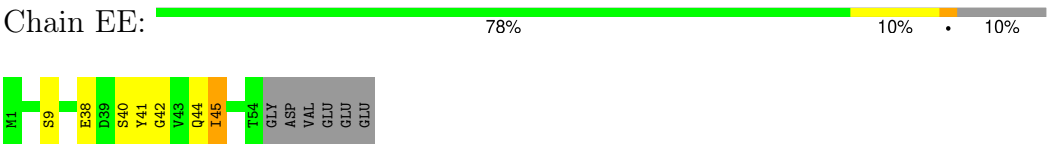
• Molecule 2: Arstotzka protein

Chain ND:



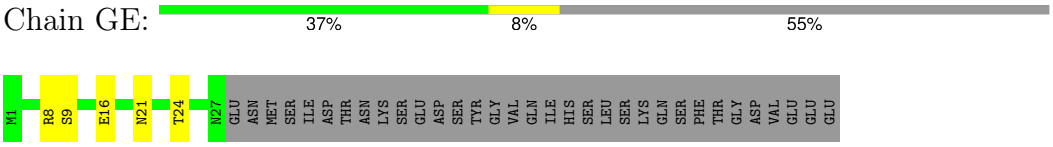
• Molecule 2: Arstotzka protein

Chain EE:



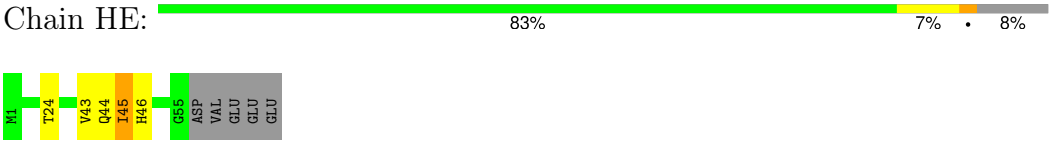
• Molecule 2: Arstotzka protein

Chain GE:



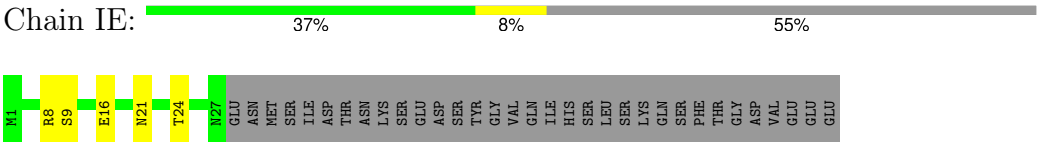
• Molecule 2: Arstotzka protein

Chain HE:



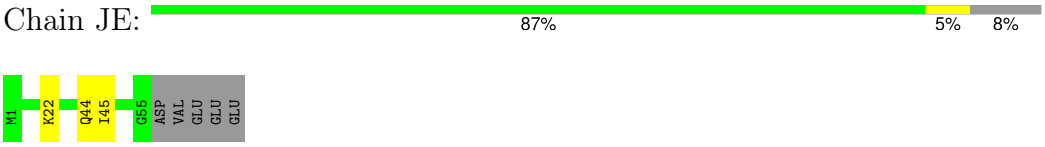
• Molecule 2: Arstotzka protein

Chain IE:



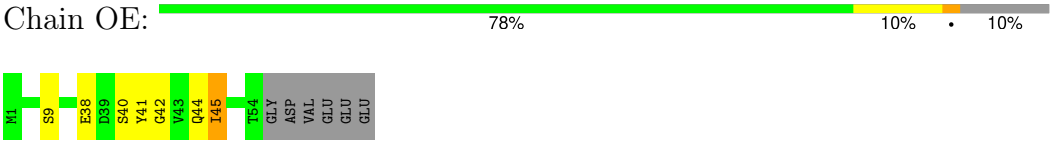
• Molecule 2: Arstotzka protein

Chain JE:



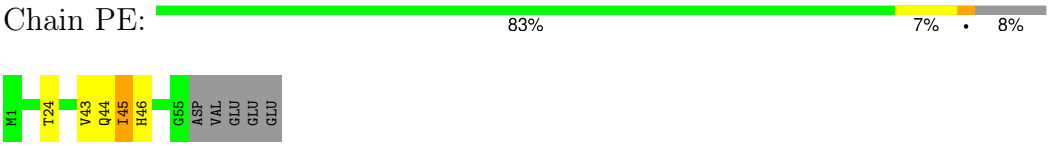
• Molecule 2: Arstotzka protein

Chain OE:



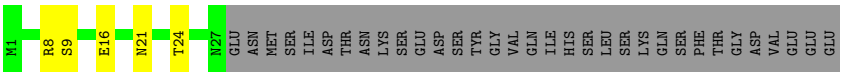
• Molecule 2: Arstotzka protein

Chain PE:



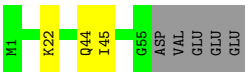
• Molecule 2: Arstotzka protein

Chain QE:



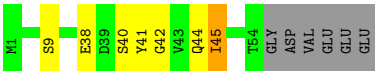
• Molecule 2: Arstotzka protein

Chain RE:



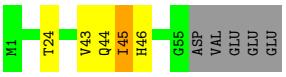
• Molecule 2: Arstotzka protein

Chain WE:



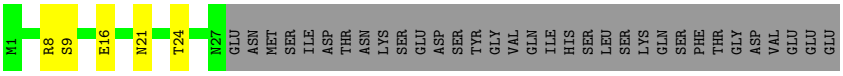
• Molecule 2: Arstotzka protein

Chain XE:



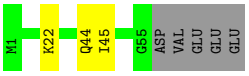
• Molecule 2: Arstotzka protein

Chain YE:



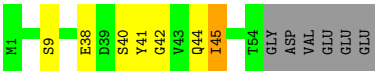
• Molecule 2: Arstotzka protein

Chain ZE:



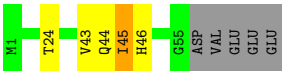
• Molecule 2: Arstotzka protein

Chain eE:



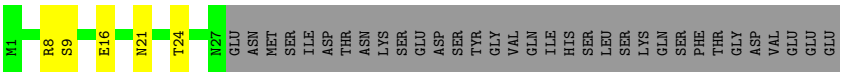
• Molecule 2: Arstotzka protein

Chain fE:



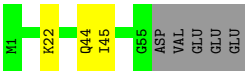
• Molecule 2: Arstotzka protein

Chain gE:



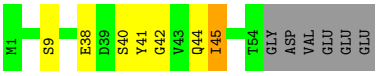
• Molecule 2: Arstotzka protein

Chain hE:



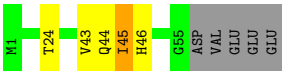
• Molecule 2: Arstotzka protein

Chain EG:



• Molecule 2: Arstotzka protein

Chain FG:

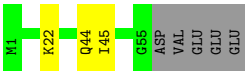


• Molecule 2: Arstotzka protein

Chain GG:

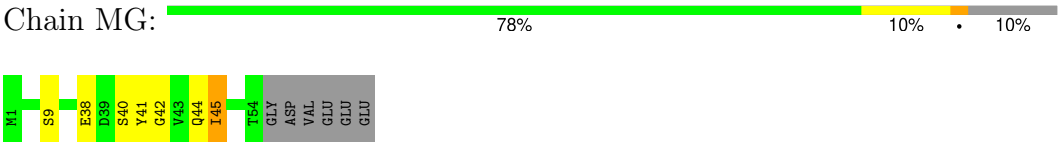
• Molecule 2: Arstotzka protein

Chain HG:



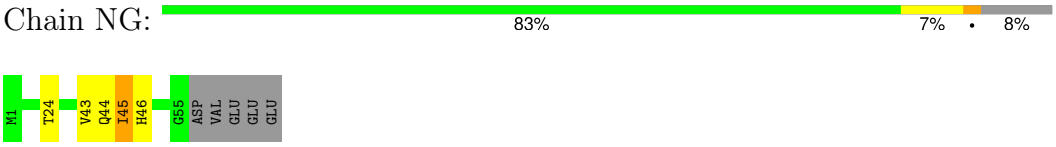
• Molecule 2: Arstotzka protein

Chain MG:



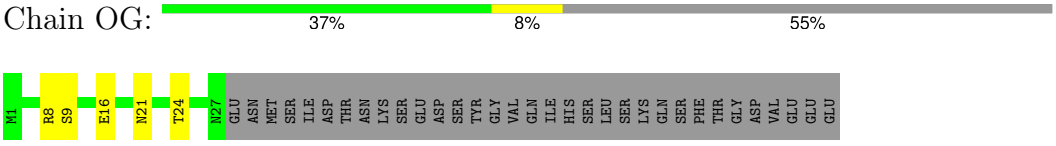
• Molecule 2: Arstotzka protein

Chain NG:



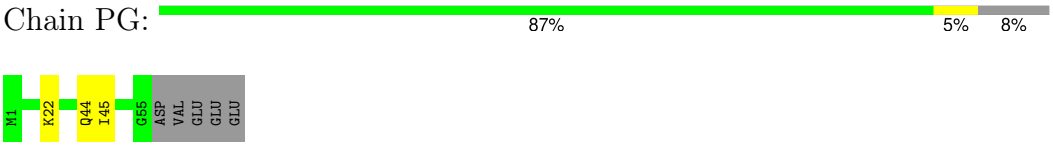
• Molecule 2: Arstotzka protein

Chain OG:



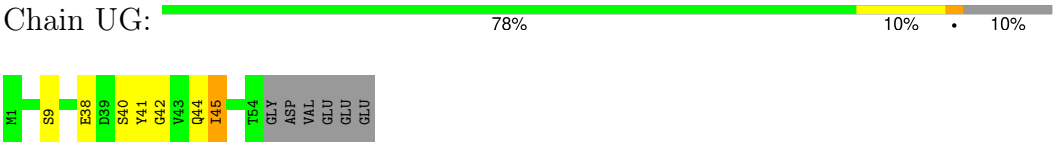
• Molecule 2: Arstotzka protein

Chain PG:



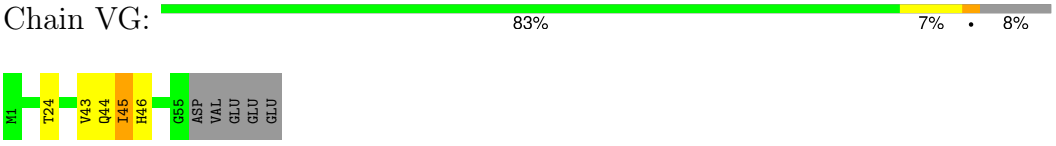
• Molecule 2: Arstotzka protein

Chain UG:



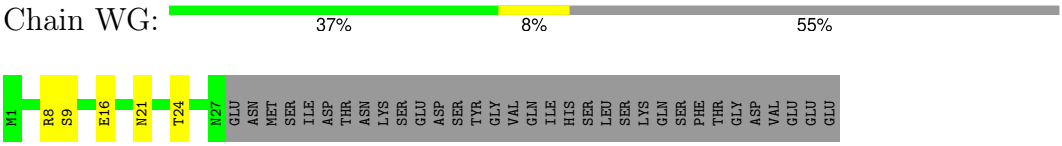
• Molecule 2: Arstotzka protein

Chain VG:



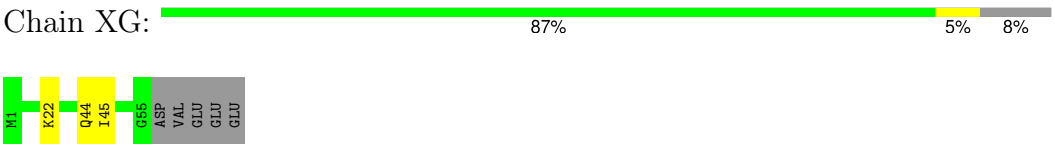
• Molecule 2: Arstotzka protein

Chain WG:



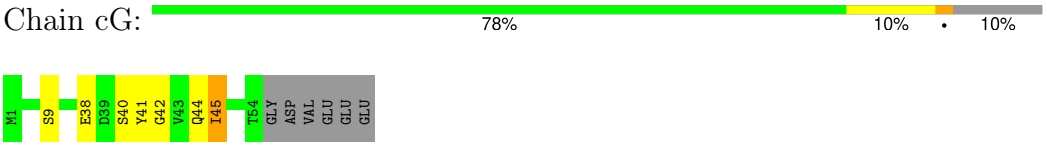
• Molecule 2: Arstotzka protein

Chain XG:



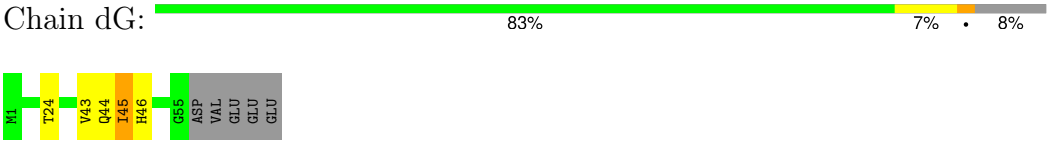
• Molecule 2: Arstotzka protein

Chain cG:



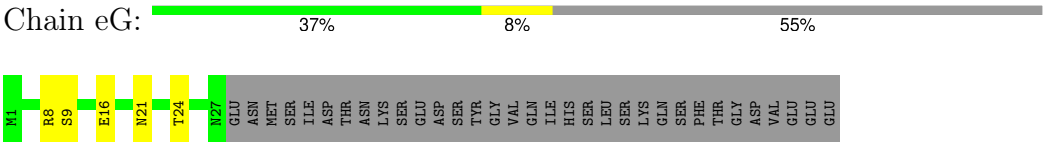
• Molecule 2: Arstotzka protein

Chain dG:



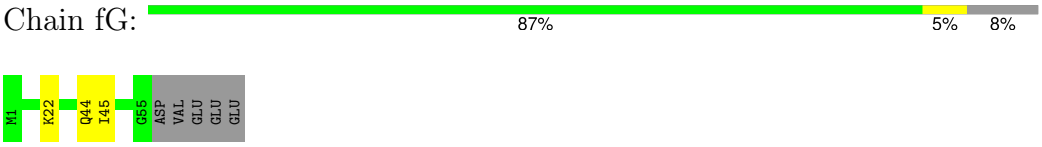
• Molecule 2: Arstotzka protein

Chain eG:



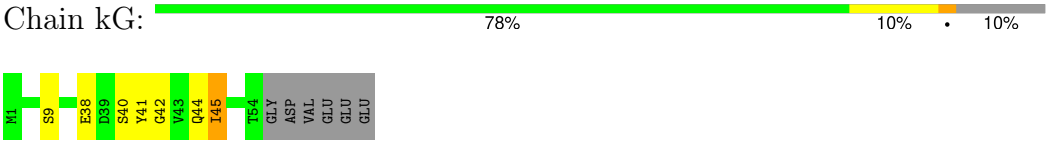
• Molecule 2: Arstotzka protein

Chain fG:



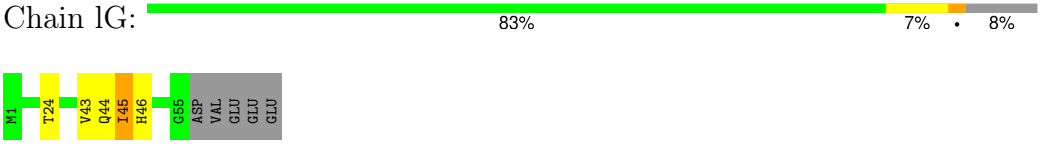
• Molecule 2: Arstotzka protein

Chain kG:



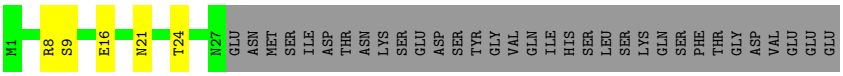
• Molecule 2: Arstotzka protein

Chain lG:



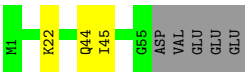
• Molecule 2: Arstotzka protein

Chain mG:



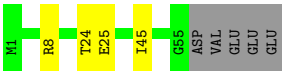
• Molecule 2: Arstotzka protein

Chain nG:



• Molecule 2: Arstotzka protein

Chain EJ:

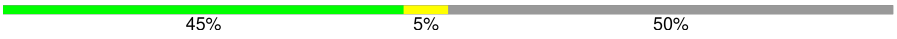


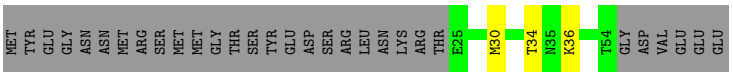
• Molecule 2: Arstotzka protein

Chain FJ:

• Molecule 2: Arstotzka protein

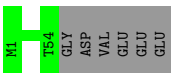
Chain GJ:





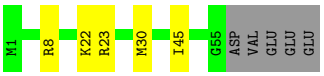
• Molecule 2: Arstotzka protein

Chain HJ:



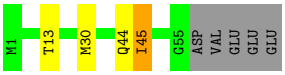
• Molecule 2: Arstotzka protein

Chain MJ:



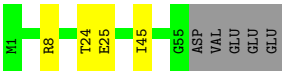
• Molecule 2: Arstotzka protein

Chain NJ:



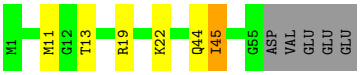
• Molecule 2: Arstotzka protein

Chain EK:



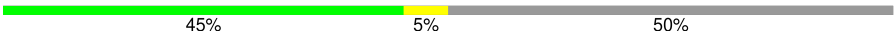
• Molecule 2: Arstotzka protein

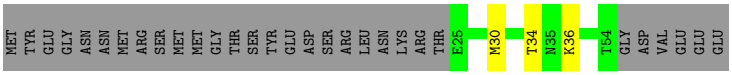
Chain FK:



• Molecule 2: Arstotzka protein

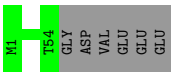
Chain GK:





• Molecule 2: Arstotzka protein

Chain HK:

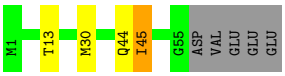


• Molecule 2: Arstotzka protein

Chain MK:

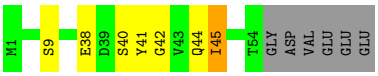
• Molecule 2: Arstotzka protein

Chain NK:



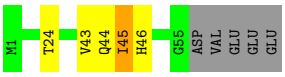
• Molecule 2: Arstotzka protein

Chain EL:



• Molecule 2: Arstotzka protein

Chain FL:

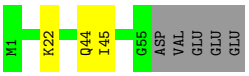


• Molecule 2: Arstotzka protein

Chain GL:

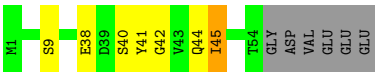
• Molecule 2: Arstotzka protein

Chain HL:



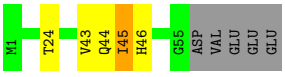
• Molecule 2: Arstotzka protein

Chain ML:



• Molecule 2: Arstotzka protein

Chain NL:

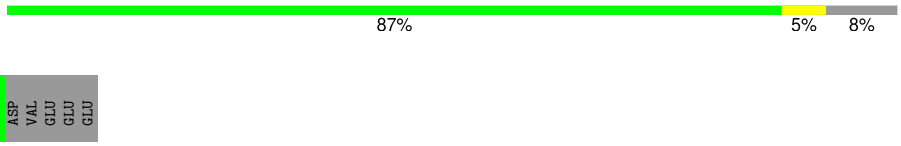


• Molecule 2: Arstotzka protein

Chain OL:

• Molecule 2: Arstotzka protein

Chain PL:

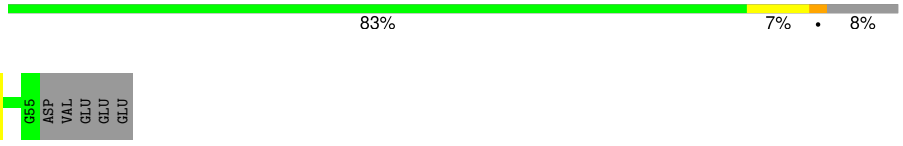


• Molecule 2: Arstotzka protein

Chain UL:

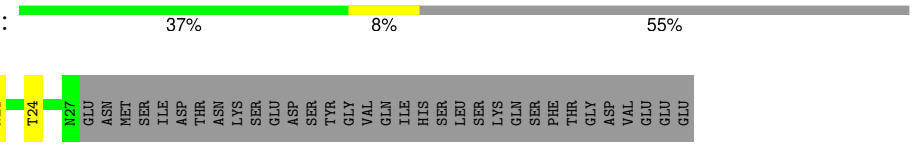
• Molecule 2: Arstotzka protein

Chain VL:



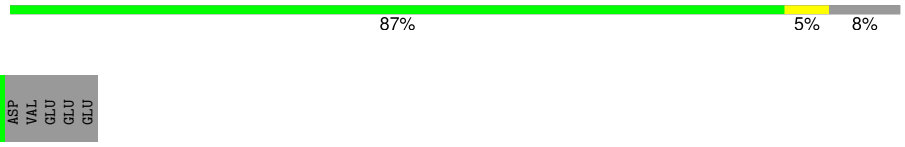
• Molecule 2: Arstotzka protein

Chain WL:



• Molecule 2: Arstotzka protein

Chain XL:

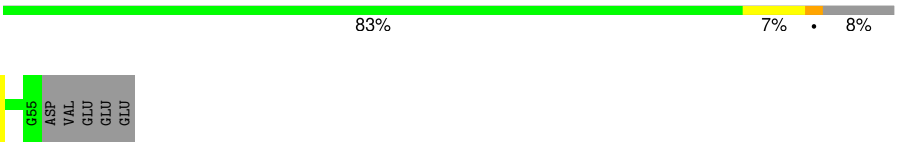


• Molecule 2: Arstotzka protein

Chain cL:

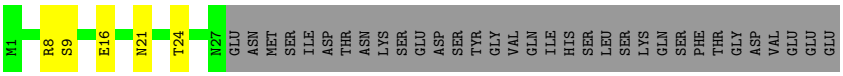
• Molecule 2: Arstotzka protein

Chain dL:



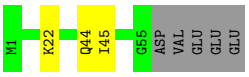
• Molecule 2: Arstotzka protein

Chain eL:



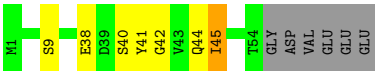
• Molecule 2: Arstotzka protein

Chain fL:



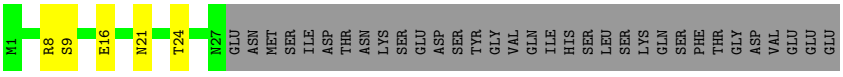
• Molecule 2: Arstotzka protein

Chain hL:



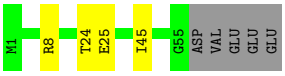
• Molecule 2: Arstotzka protein

Chain iL:



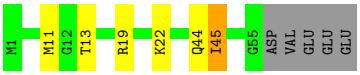
• Molecule 2: Arstotzka protein

Chain EP:



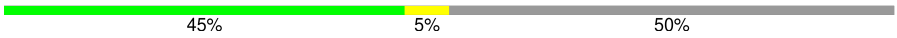
• Molecule 2: Arstotzka protein

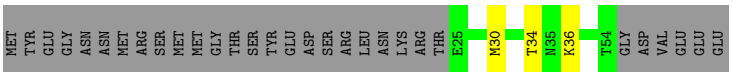
Chain FP:



• Molecule 2: Arstotzka protein

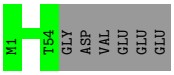
Chain GP:





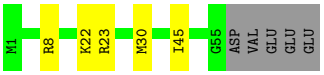
• Molecule 2: Arstotzka protein

Chain HP:



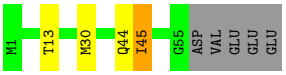
• Molecule 2: Arstotzka protein

Chain MP:



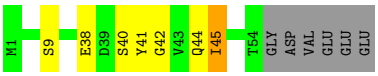
• Molecule 2: Arstotzka protein

Chain NP:



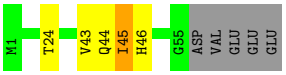
• Molecule 2: Arstotzka protein

Chain EQ:



• Molecule 2: Arstotzka protein

Chain FQ:

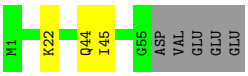


• Molecule 2: Arstotzka protein

Chain GQ:

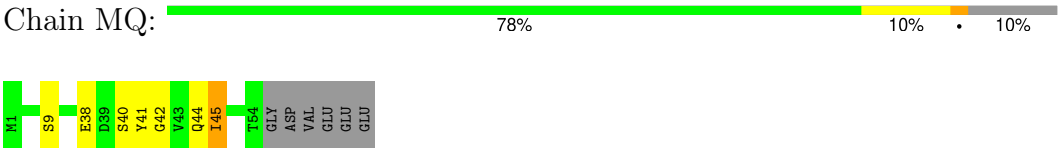
• Molecule 2: Arstotzka protein

Chain HQ:



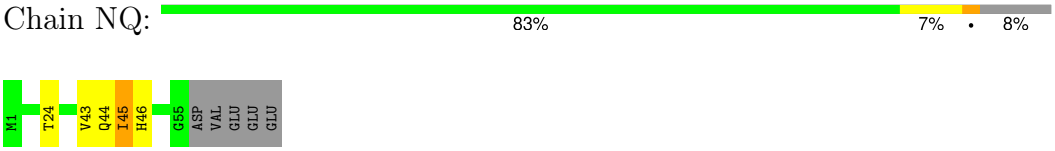
• Molecule 2: Arstotzka protein

Chain MQ:



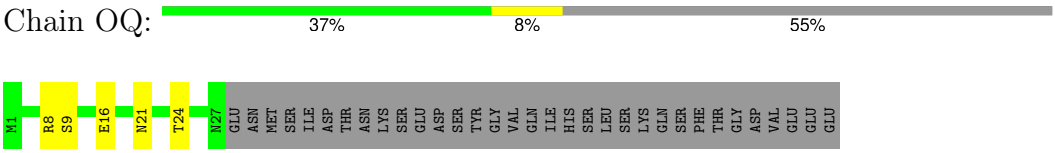
• Molecule 2: Arstotzka protein

Chain NQ:



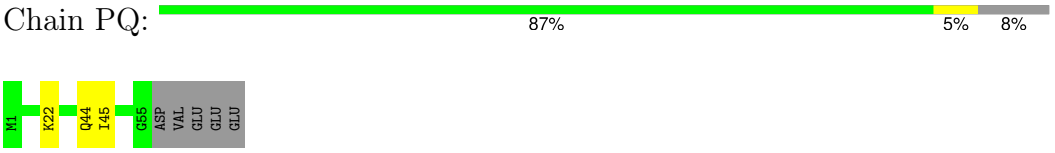
• Molecule 2: Arstotzka protein

Chain OQ:



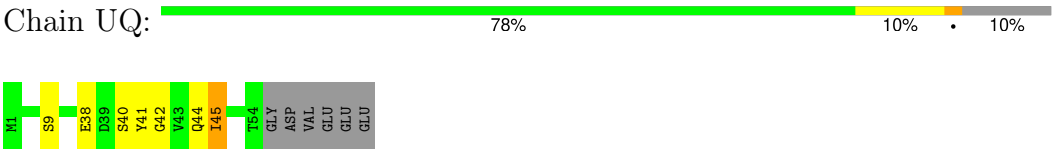
• Molecule 2: Arstotzka protein

Chain PQ:



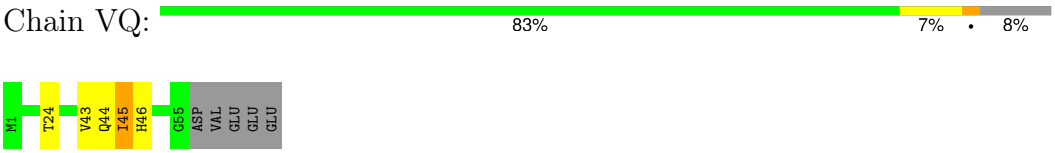
• Molecule 2: Arstotzka protein

Chain UQ:



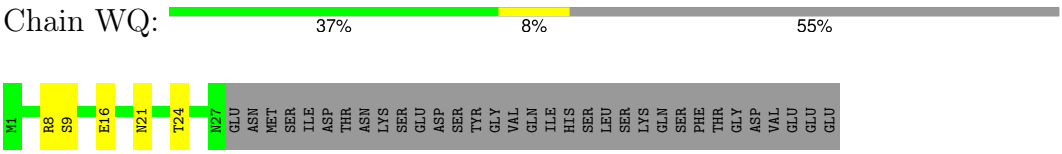
• Molecule 2: Arstotzka protein

Chain VQ:



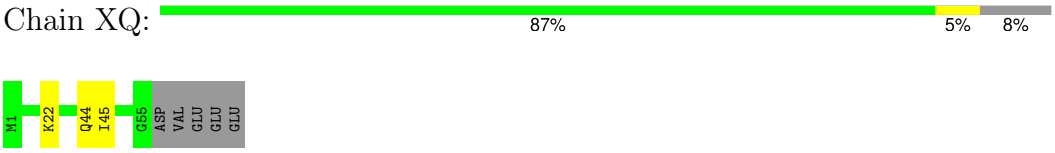
• Molecule 2: Arstotzka protein

Chain WQ:



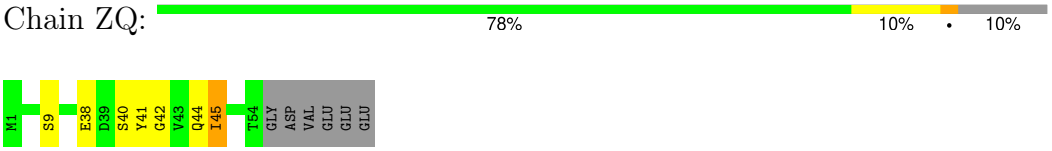
• Molecule 2: Arstotzka protein

Chain XQ:



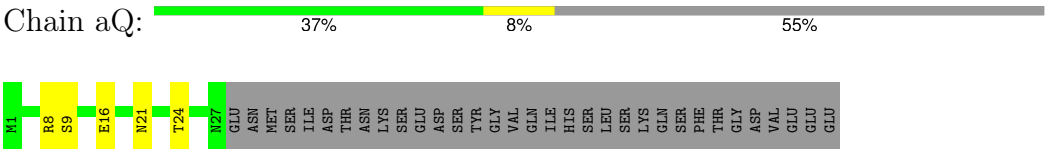
• Molecule 2: Arstotzka protein

Chain ZQ:



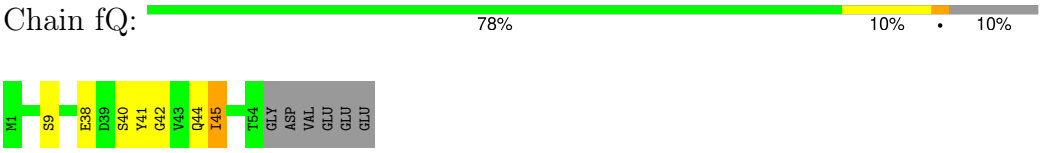
• Molecule 2: Arstotzka protein

Chain aQ:



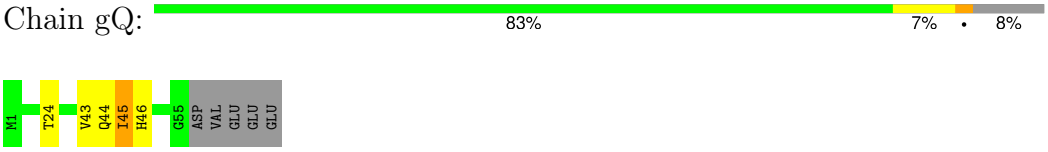
• Molecule 2: Arstotzka protein

Chain fQ:



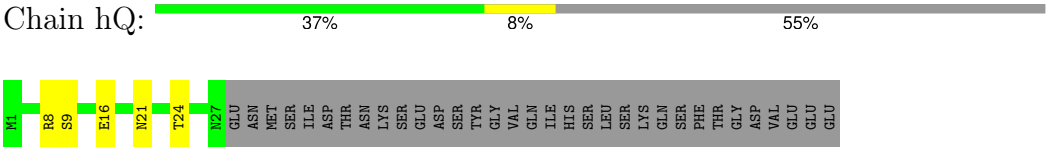
• Molecule 2: Arstotzka protein

Chain gQ:



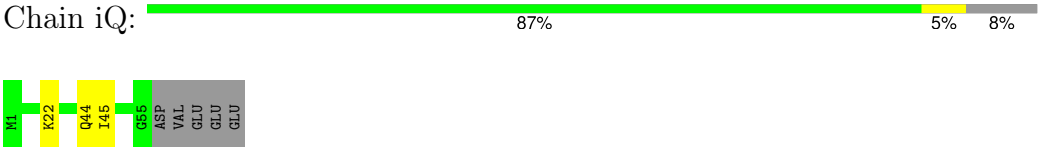
• Molecule 2: Arstotzka protein

Chain hQ:



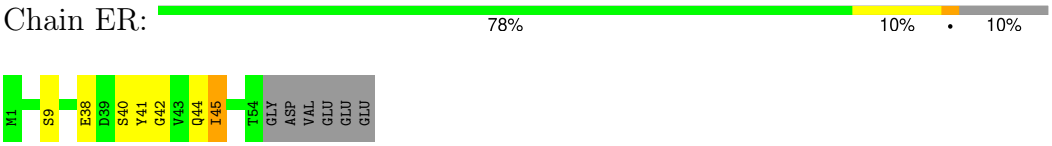
• Molecule 2: Arstotzka protein

Chain iQ:



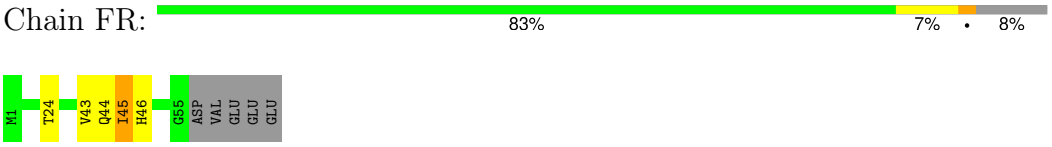
• Molecule 2: Arstotzka protein

Chain ER:



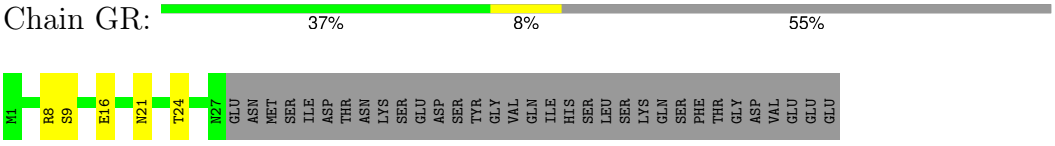
• Molecule 2: Arstotzka protein

Chain FR:



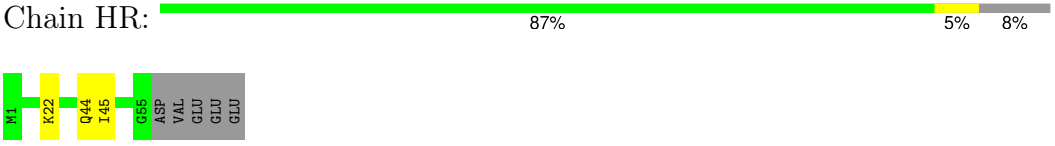
• Molecule 2: Arstotzka protein

Chain GR:



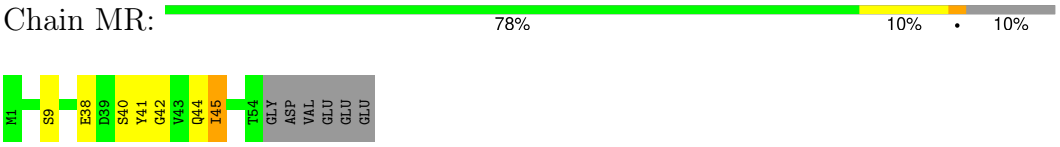
• Molecule 2: Arstotzka protein

Chain HR:



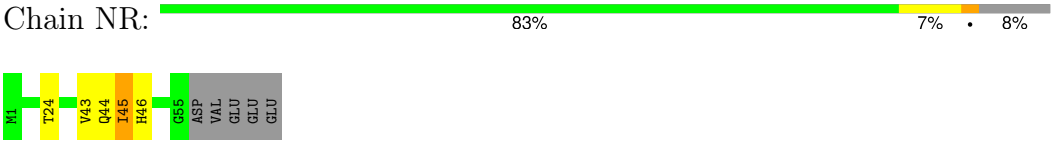
• Molecule 2: Arstotzka protein

Chain MR:



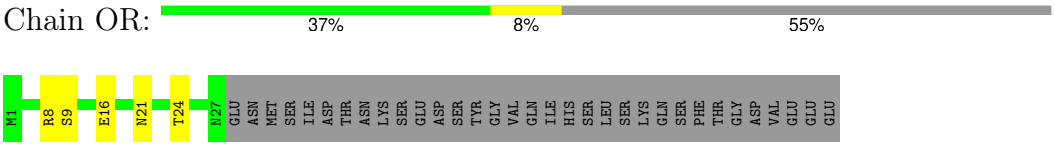
• Molecule 2: Arstotzka protein

Chain NR:



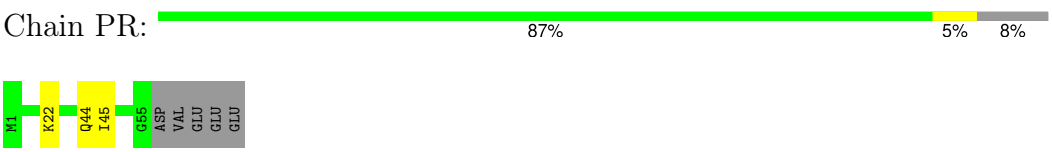
• Molecule 2: Arstotzka protein

Chain OR:



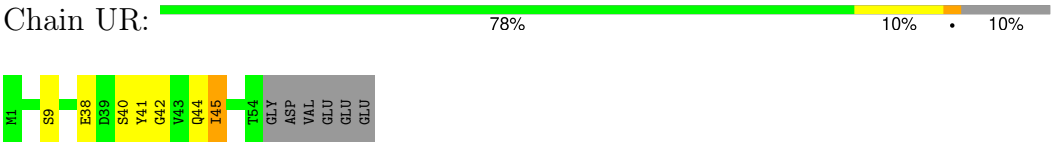
• Molecule 2: Arstotzka protein

Chain PR:



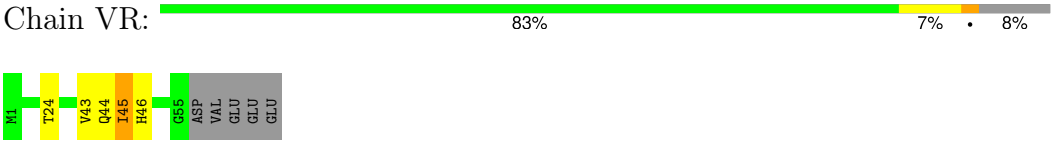
• Molecule 2: Arstotzka protein

Chain UR:



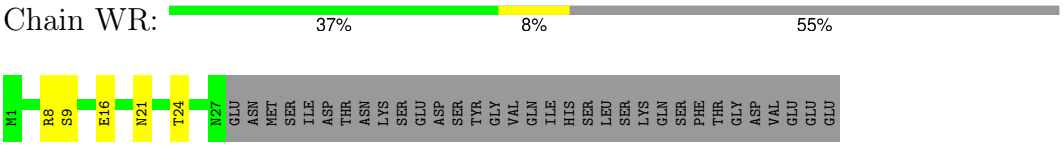
• Molecule 2: Arstotzka protein

Chain VR:



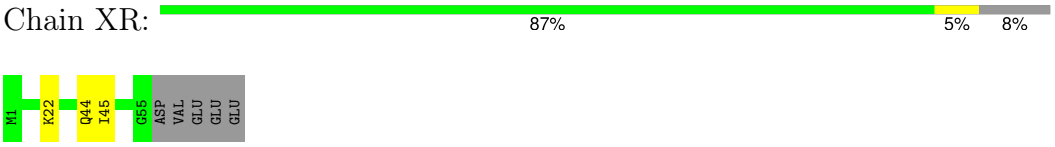
• Molecule 2: Arstotzka protein

Chain WR:



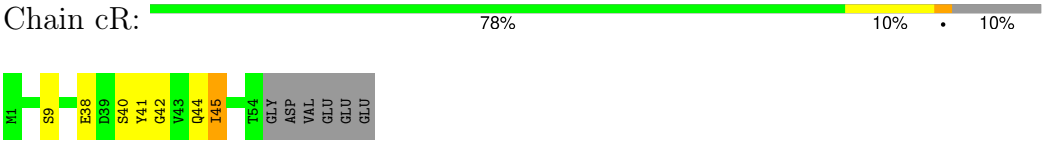
• Molecule 2: Arstotzka protein

Chain XR:



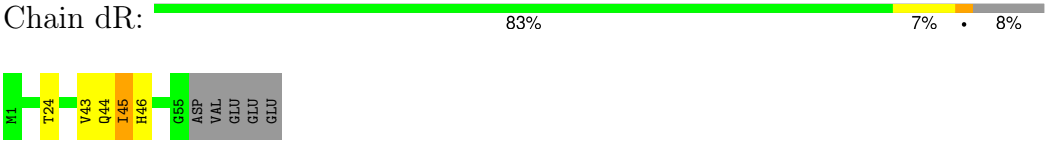
• Molecule 2: Arstotzka protein

Chain cR:



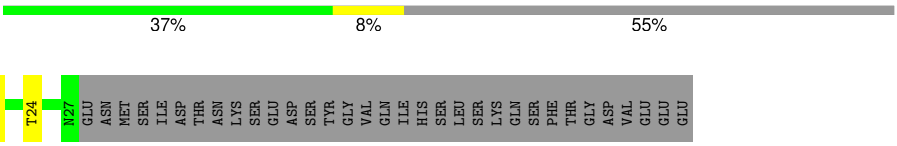
• Molecule 2: Arstotzka protein

Chain dR:



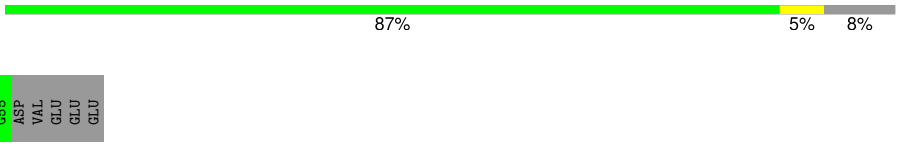
• Molecule 2: Arstotzka protein

Chain eR:



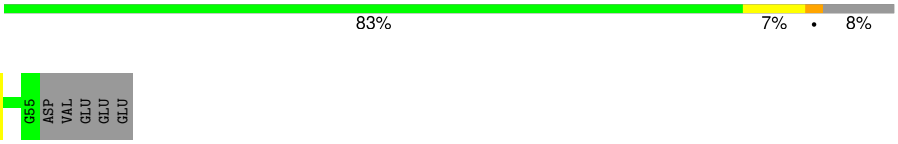
• Molecule 2: Arstotzka protein

Chain fR:



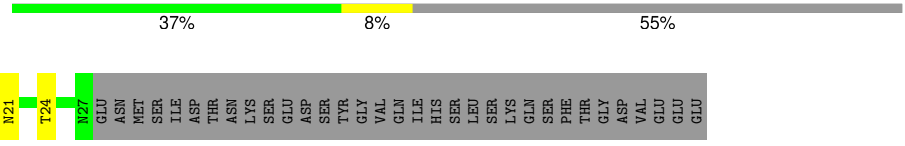
• Molecule 2: Arstotzka protein

Chain kR:



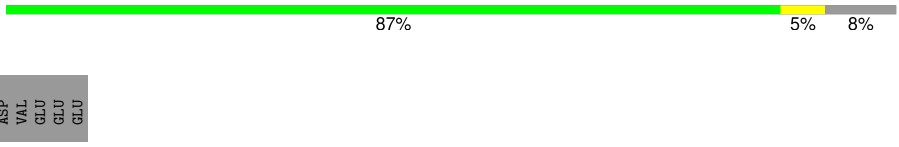
• Molecule 2: Arstotzka protein

Chain lR:



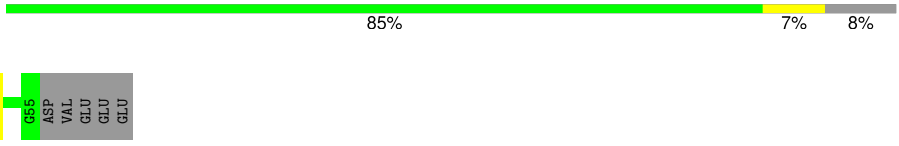
• Molecule 2: Arstotzka protein

Chain mR:



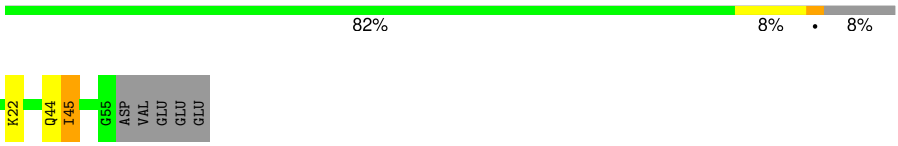
• Molecule 2: Arstotzka protein

Chain DS:



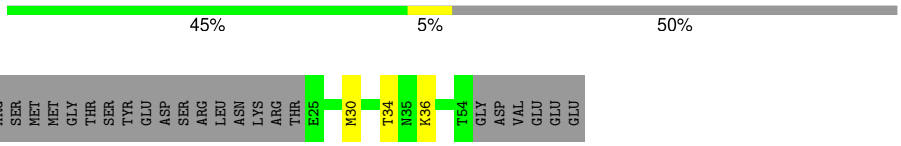
• Molecule 2: Arstotzka protein

Chain ES:



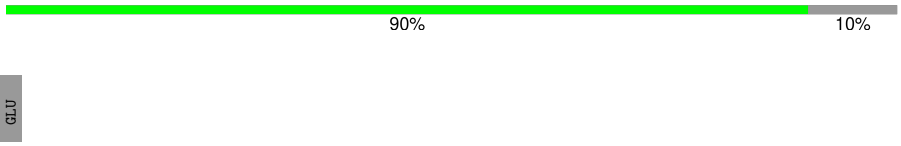
• Molecule 2: Arstotzka protein

Chain FS:



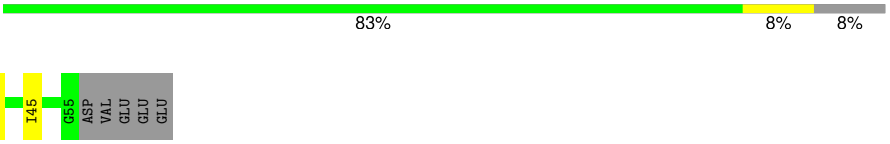
• Molecule 2: Arstotzka protein

Chain GS:



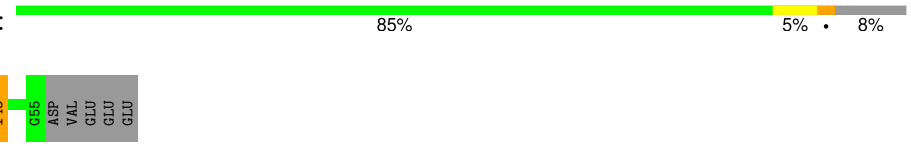
• Molecule 2: Arstotzka protein

Chain LS:



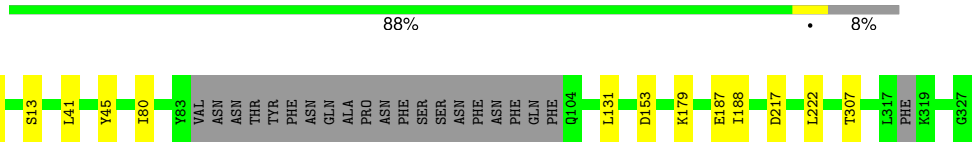
• Molecule 2: Arstotzka protein

Chain MS:



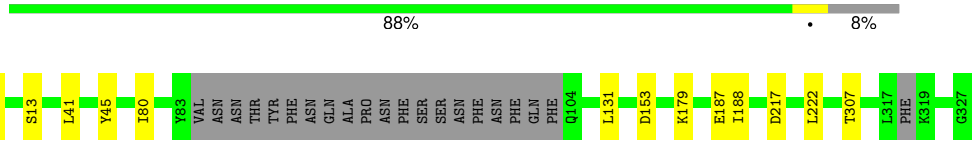
• Molecule 3: Portal protein

Chain A2:



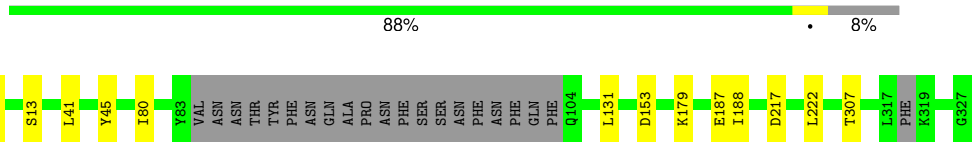
• Molecule 3: Portal protein

Chain A5:



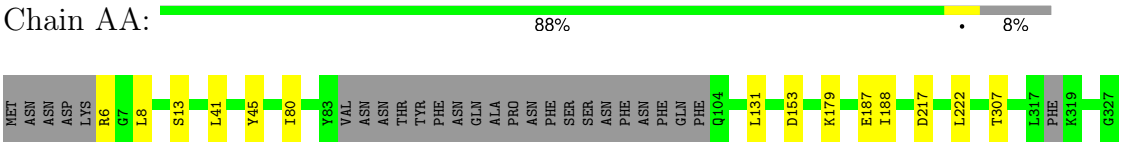
• Molecule 3: Portal protein

Chain A9:



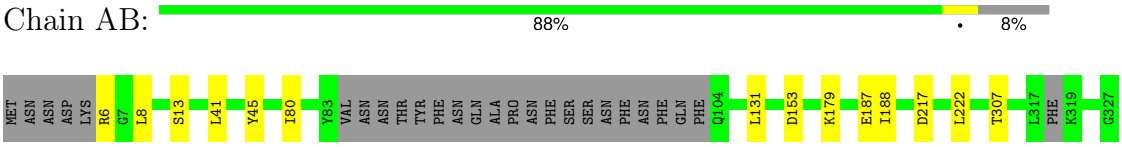
• Molecule 3: Portal protein

Chain AA:



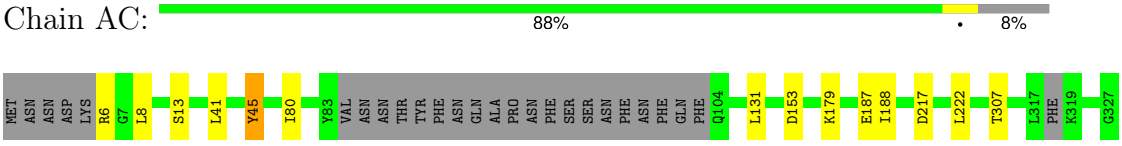
• Molecule 3: Portal protein

Chain AB:



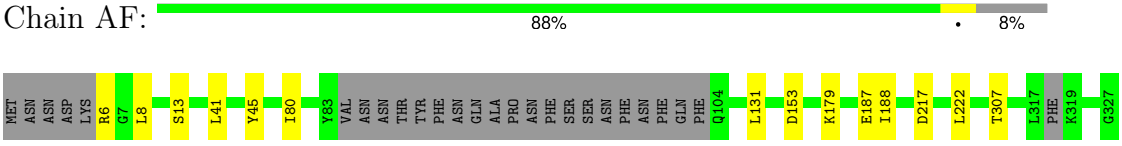
• Molecule 3: Portal protein

Chain AC:



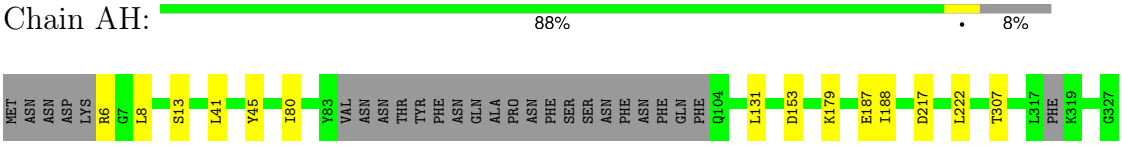
• Molecule 3: Portal protein

Chain AF:



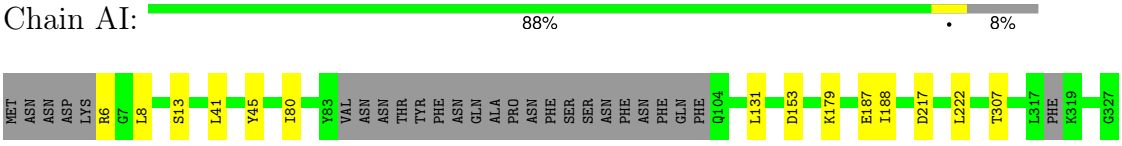
• Molecule 3: Portal protein

Chain AH:



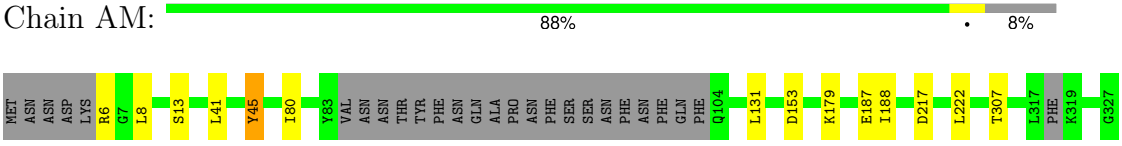
• Molecule 3: Portal protein

Chain AI:



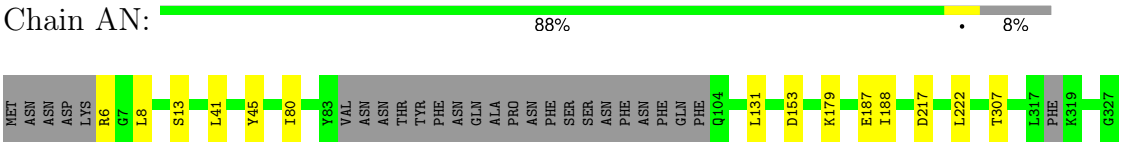
• Molecule 3: Portal protein

Chain AM:



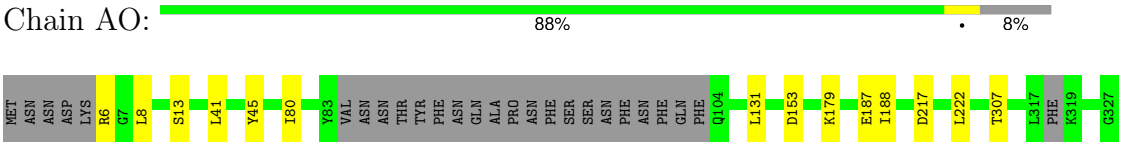
• Molecule 3: Portal protein

Chain AN:



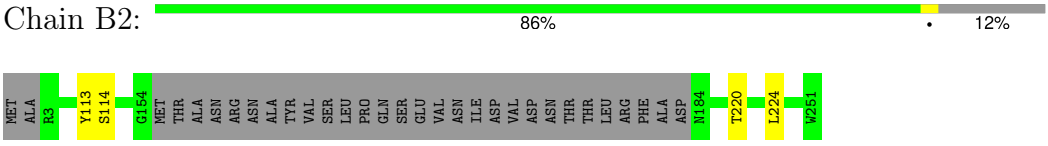
• Molecule 3: Portal protein

Chain AO:



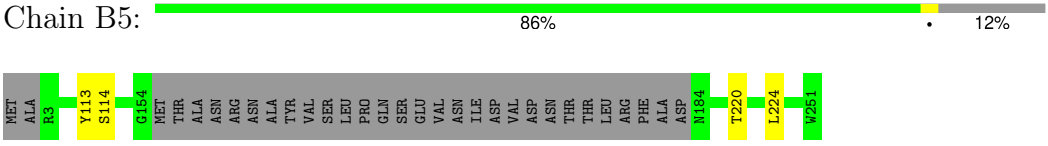
• Molecule 4: Lower collar protein

Chain B2:



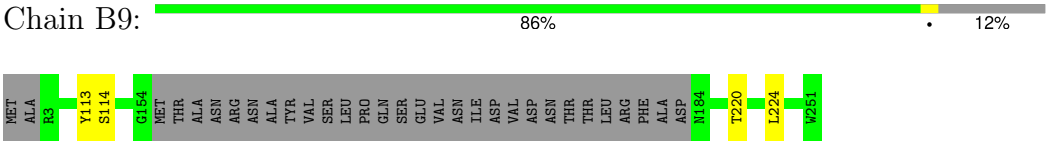
• Molecule 4: Lower collar protein

Chain B5:



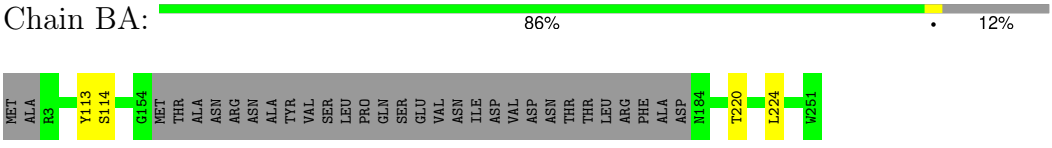
• Molecule 4: Lower collar protein

Chain B9:



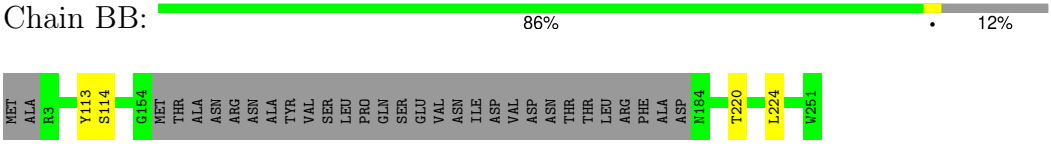
• Molecule 4: Lower collar protein

Chain BA:



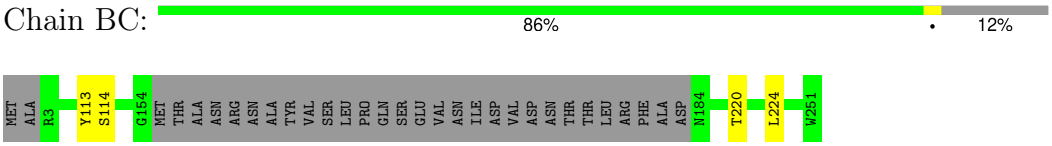
• Molecule 4: Lower collar protein

Chain BB:



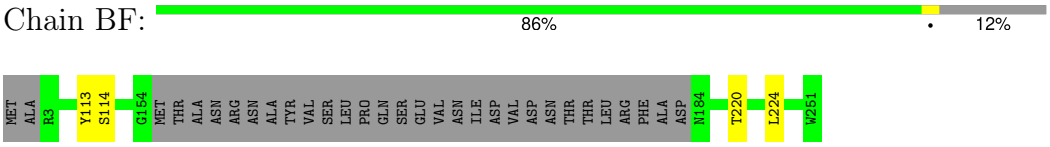
• Molecule 4: Lower collar protein

Chain BC:



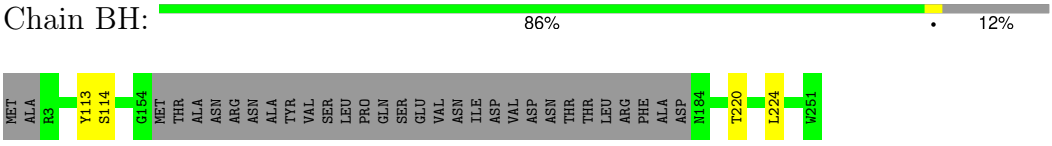
• Molecule 4: Lower collar protein

Chain BF:



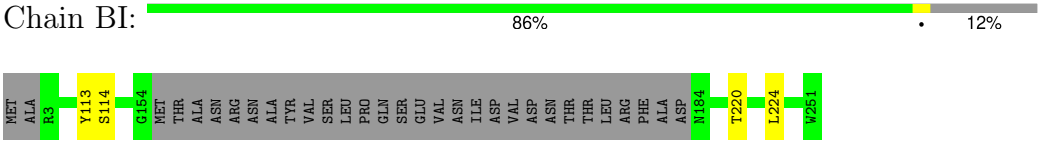
• Molecule 4: Lower collar protein

Chain BH:



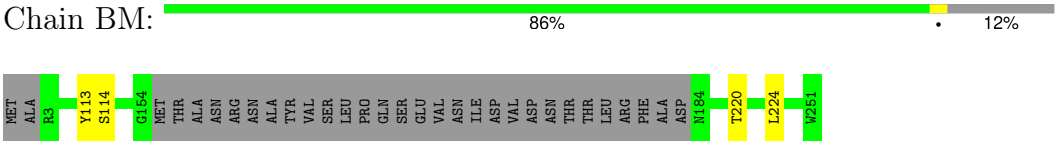
• Molecule 4: Lower collar protein

Chain BI:



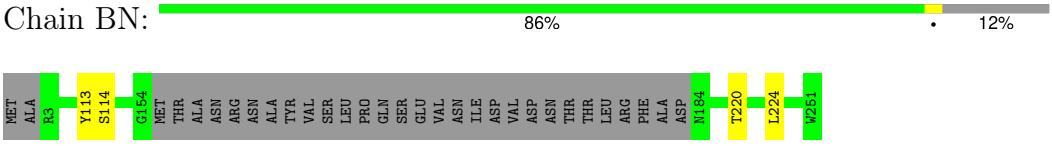
• Molecule 4: Lower collar protein

Chain BM:



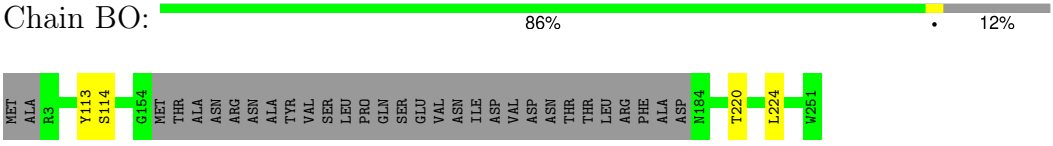
• Molecule 4: Lower collar protein

Chain BN:



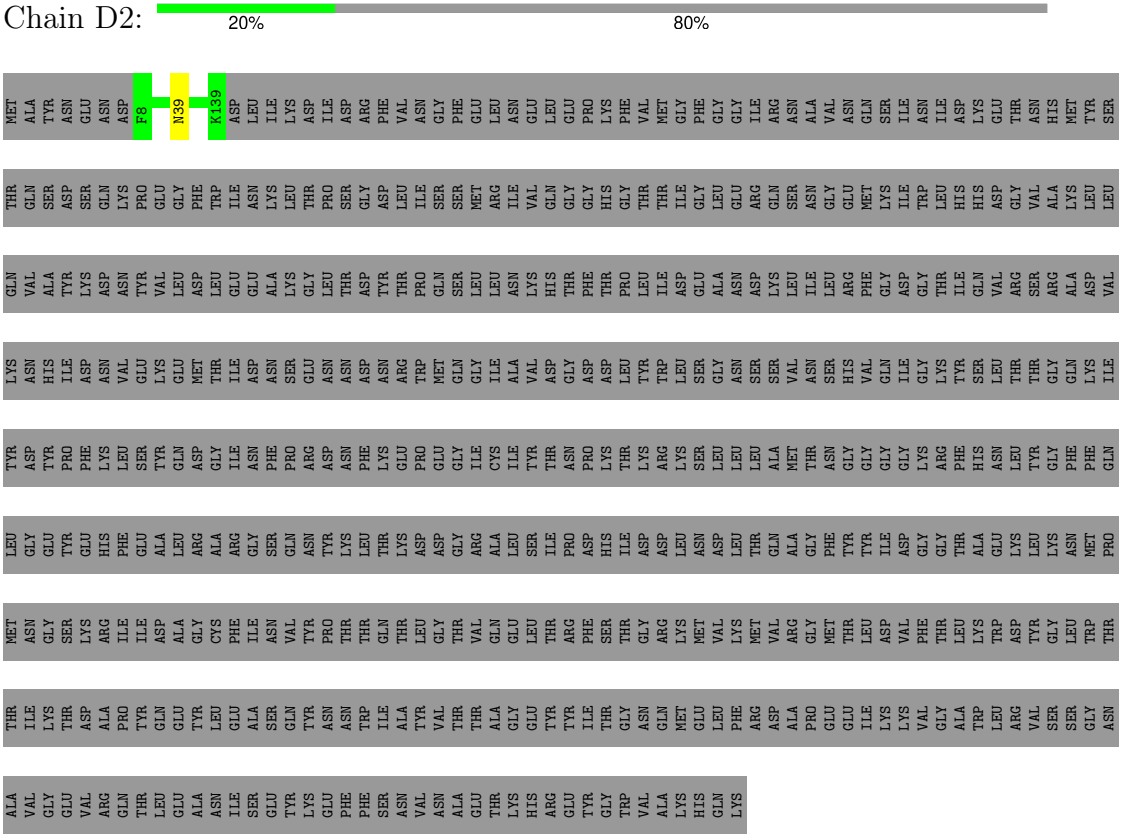
• Molecule 4: Lower collar protein

Chain BO:



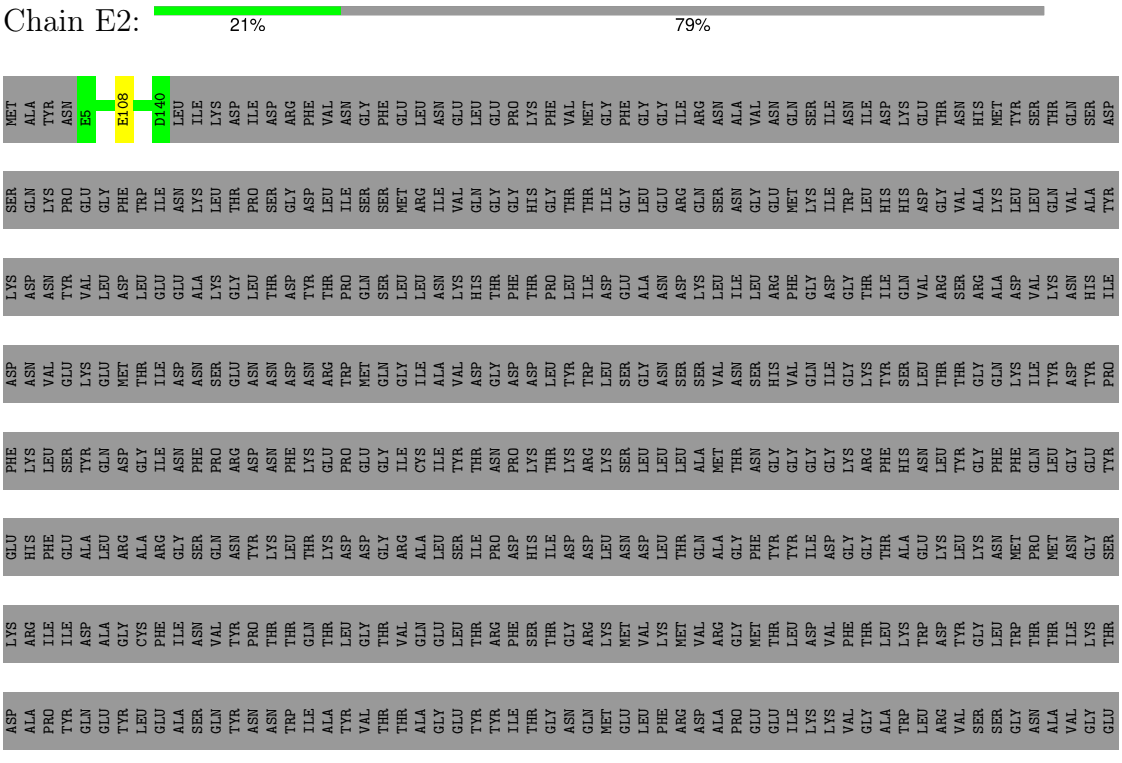
• Molecule 5: Minor structural protein

Chain D2:



• Molecule 5: Minor structural protein

Chain E2:

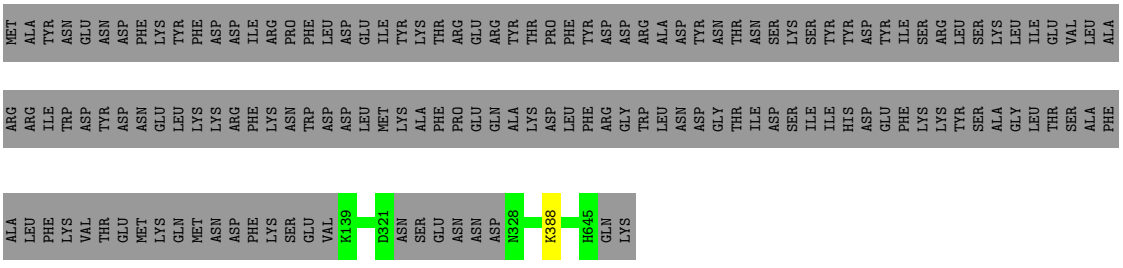


• Molecule 5: Minor structural protein

Chain F2:

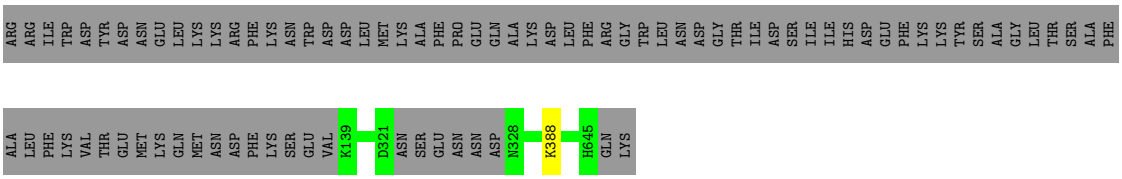
• Molecule 5: Minor structural protein

Chain C2:



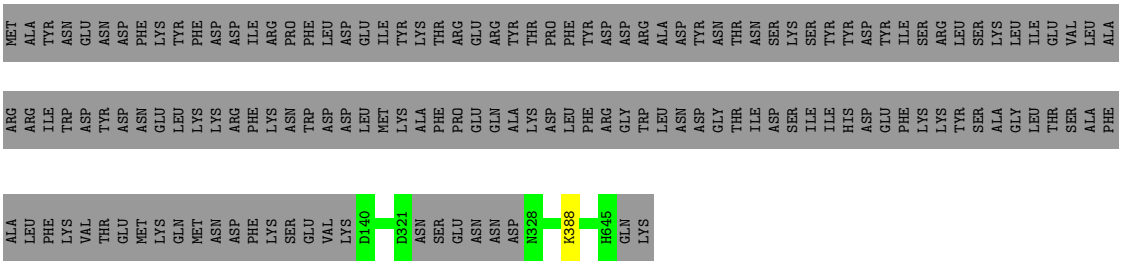
• Molecule 5: Minor structural protein

Chain N2:



• Molecule 5: Minor structural protein

Chain O2:

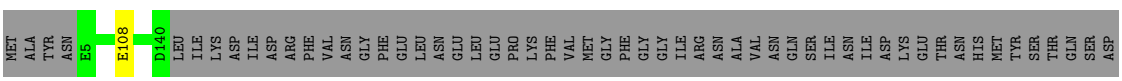


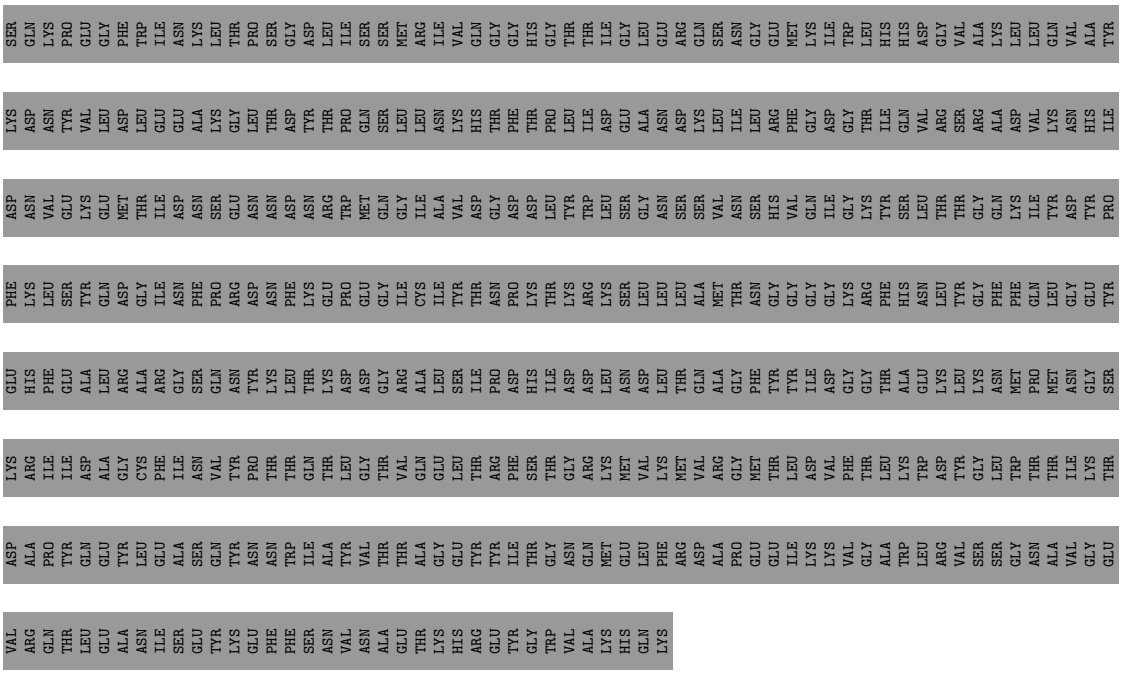
• Molecule 5: Minor structural protein

Chain D5:

• Molecule 5: Minor structural protein

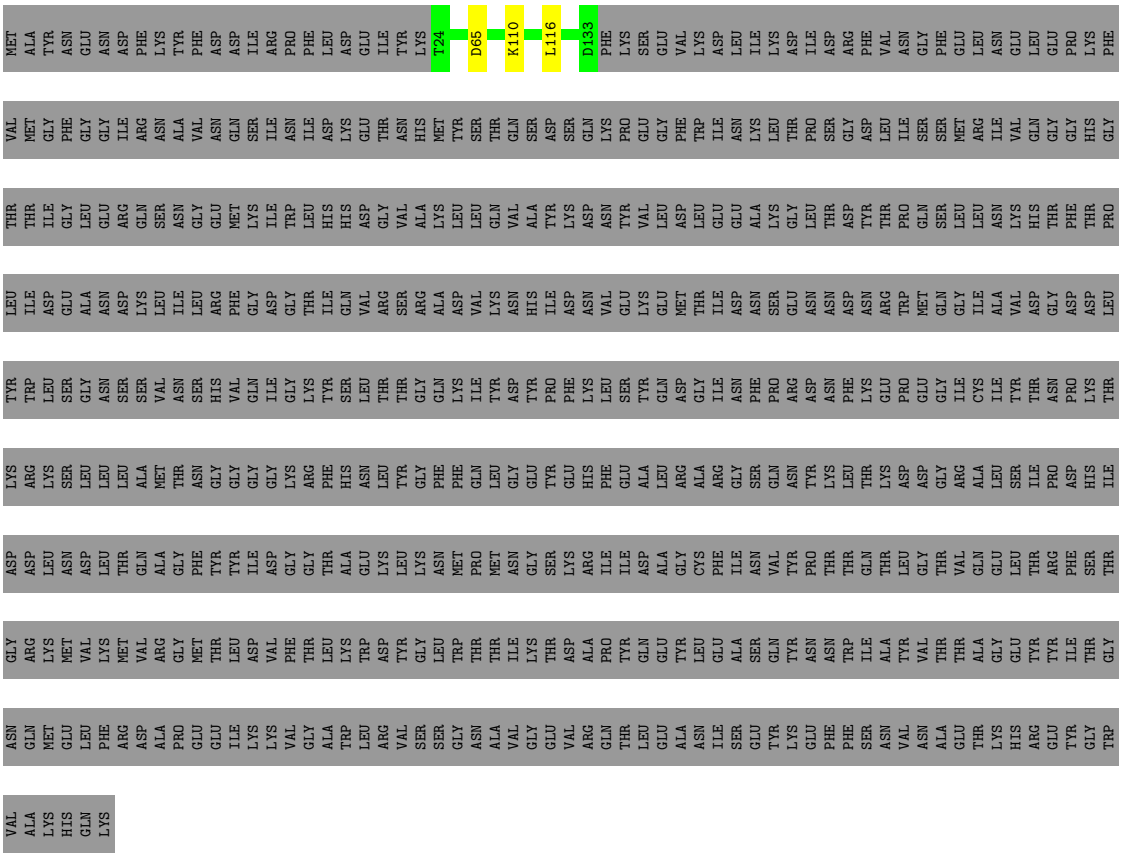
Chain E5:





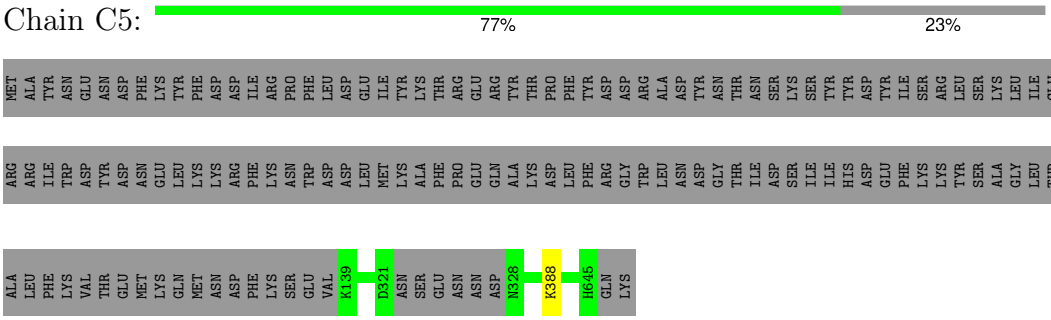
- Molecule 5: Minor structural protein

Chain F5:



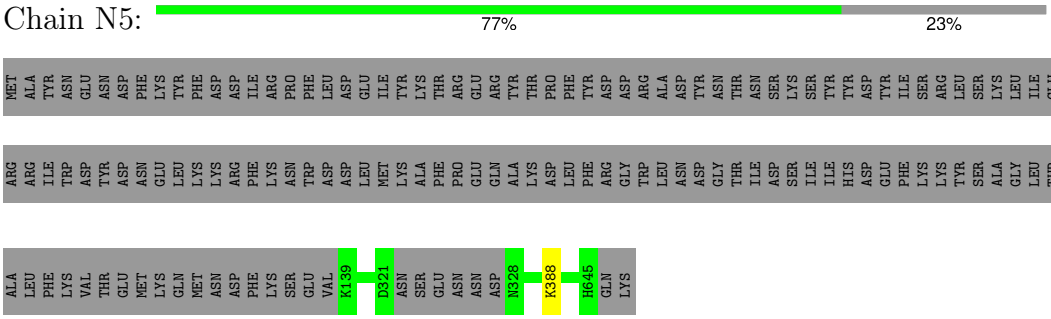
- Molecule 5: Minor structural protein

Chain C5:



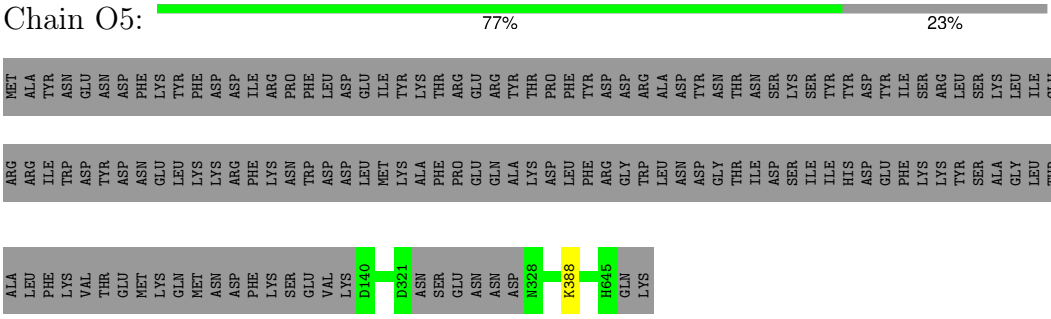
• Molecule 5: Minor structural protein

Chain N5:



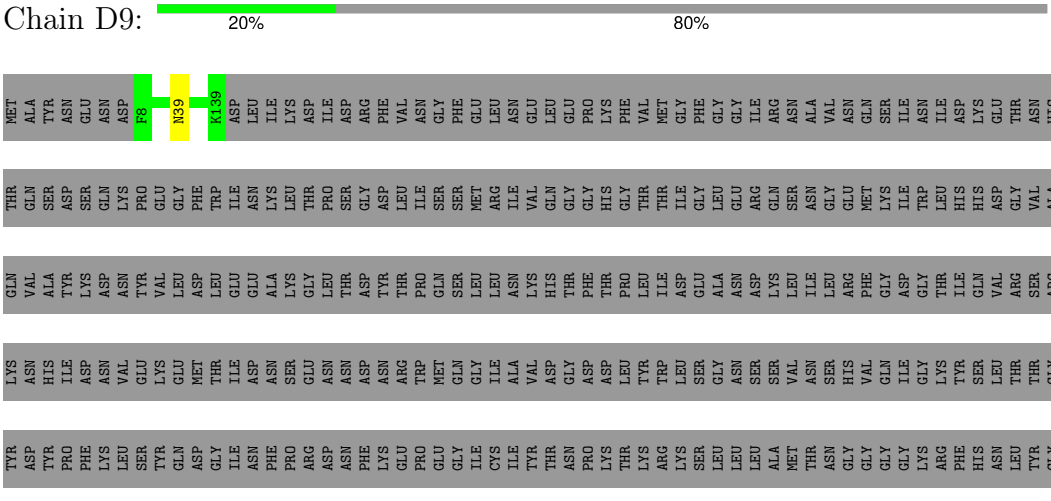
• Molecule 5: Minor structural protein

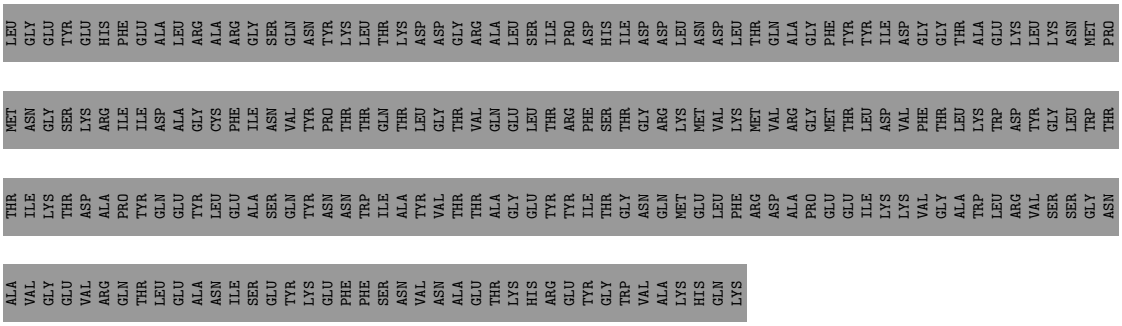
Chain O5:



• Molecule 5: Minor structural protein

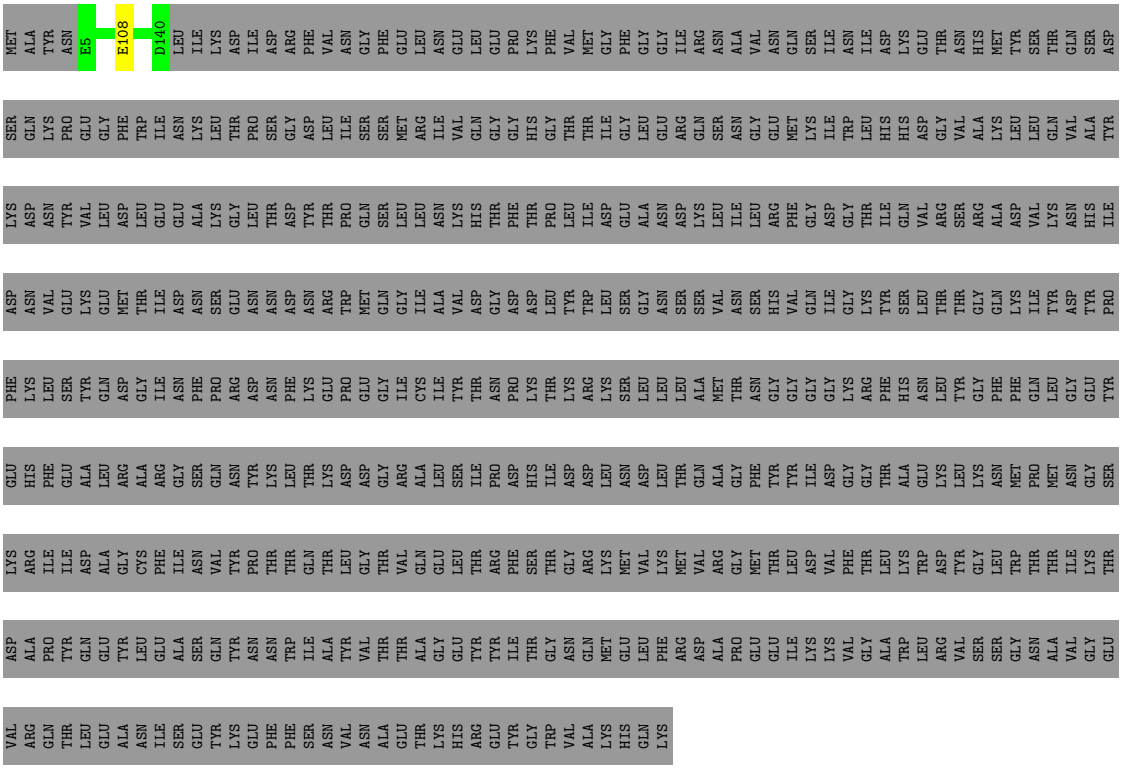
Chain D9:





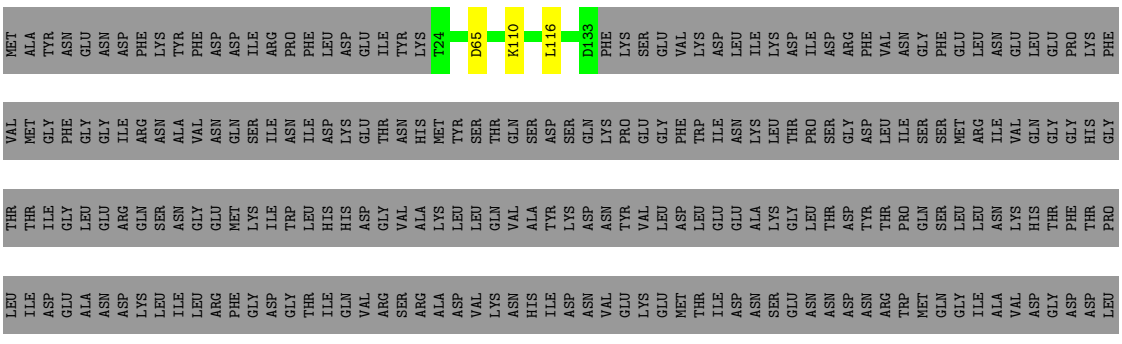
• Molecule 5: Minor structural protein

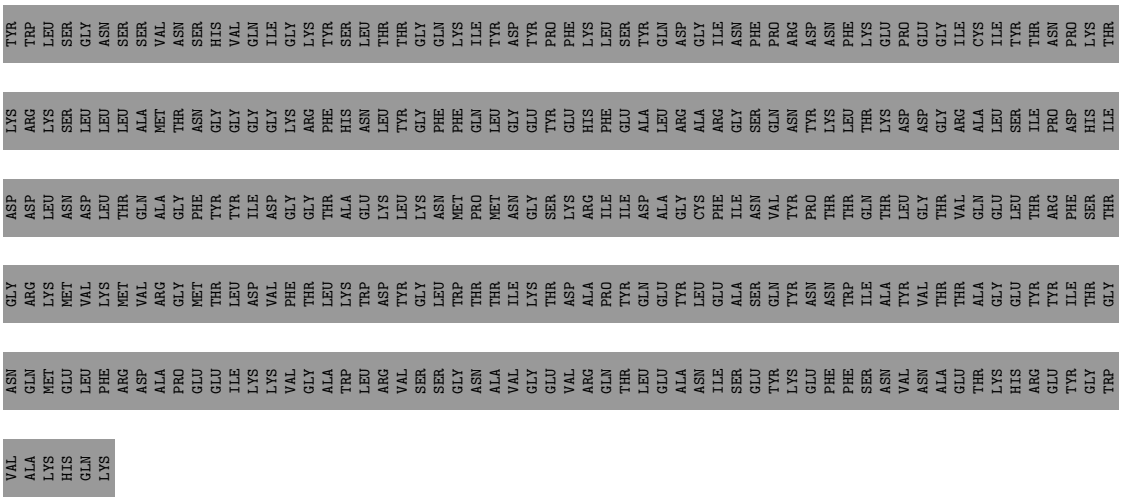
Chain E9:



• Molecule 5: Minor structural protein

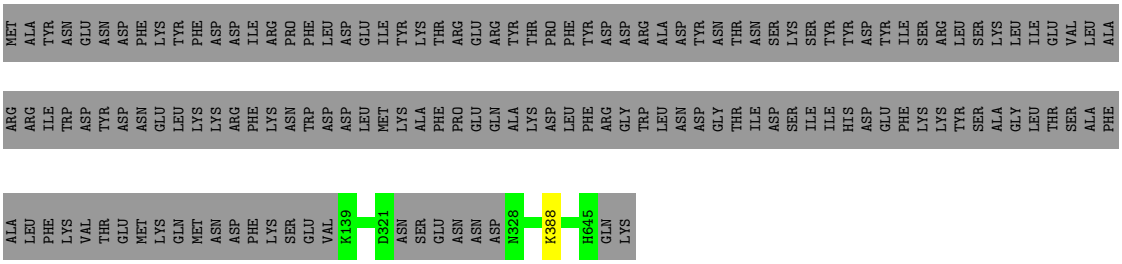
Chain F9:





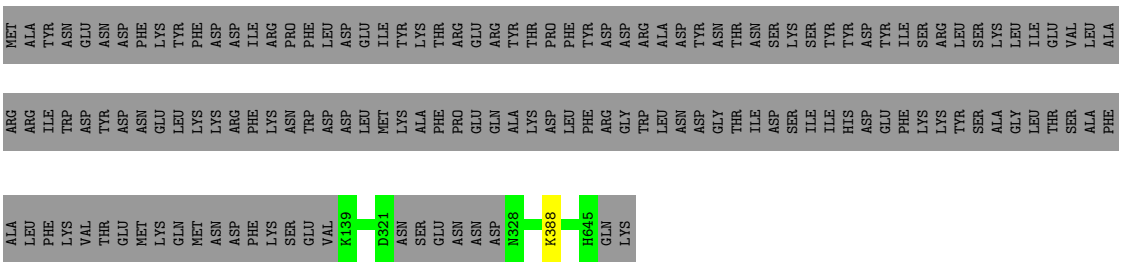
• Molecule 5: Minor structural protein

Chain C9:



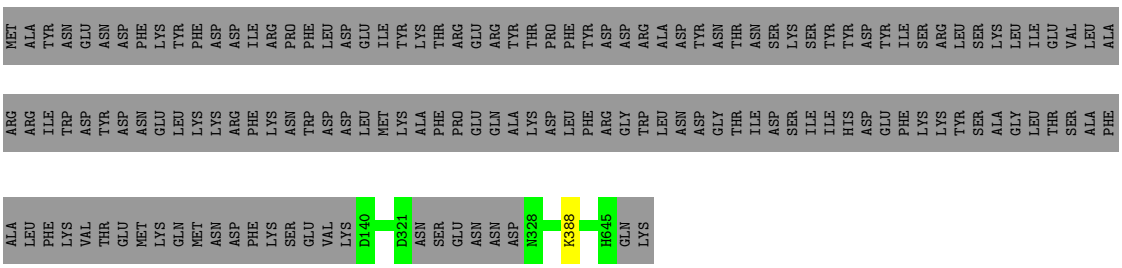
• Molecule 5: Minor structural protein

Chain N9:



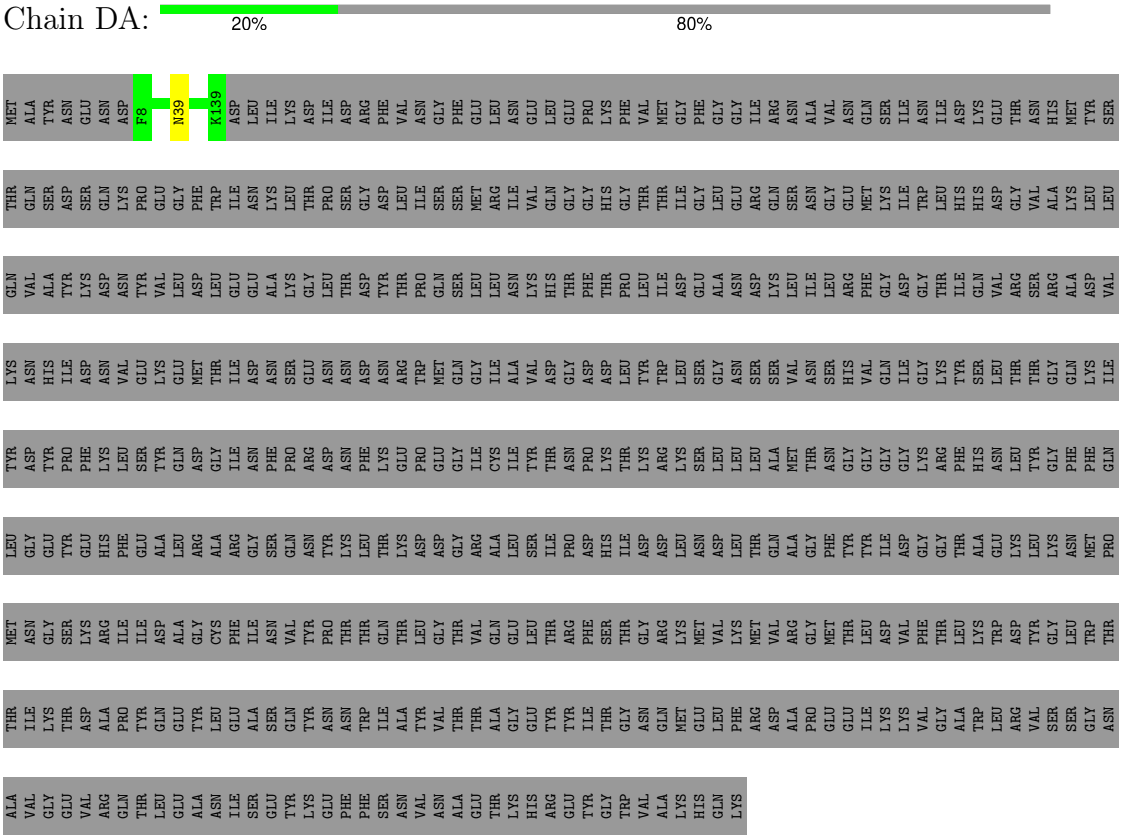
• Molecule 5: Minor structural protein

Chain O9:



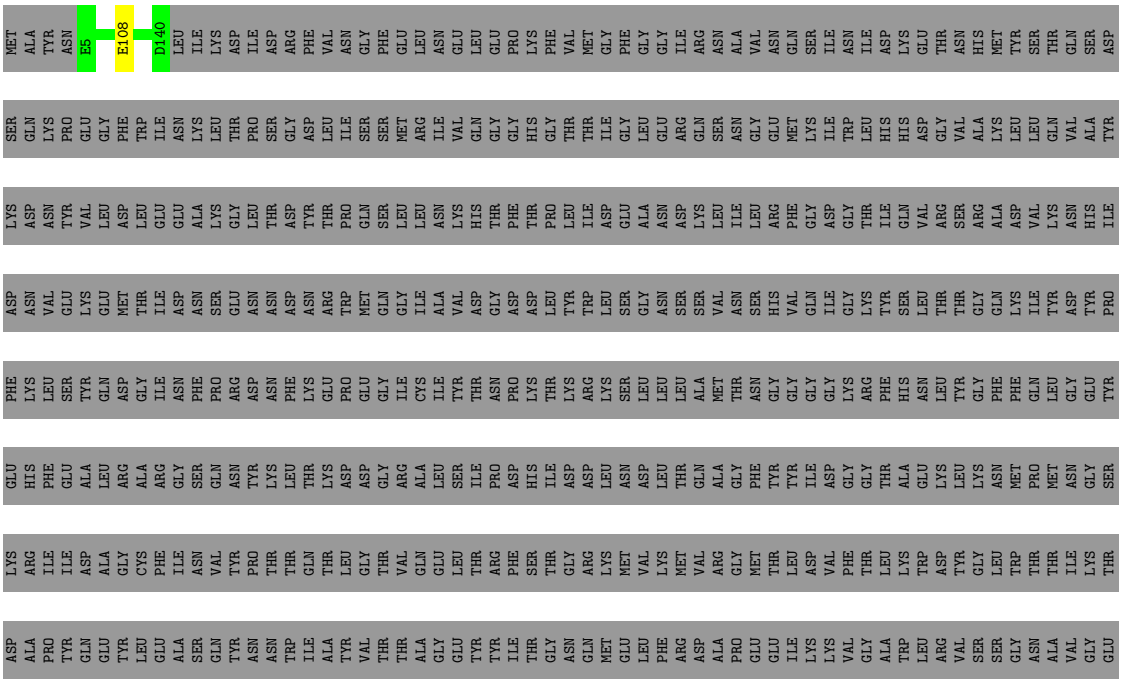
• Molecule 5: Minor structural protein

Chain DA:



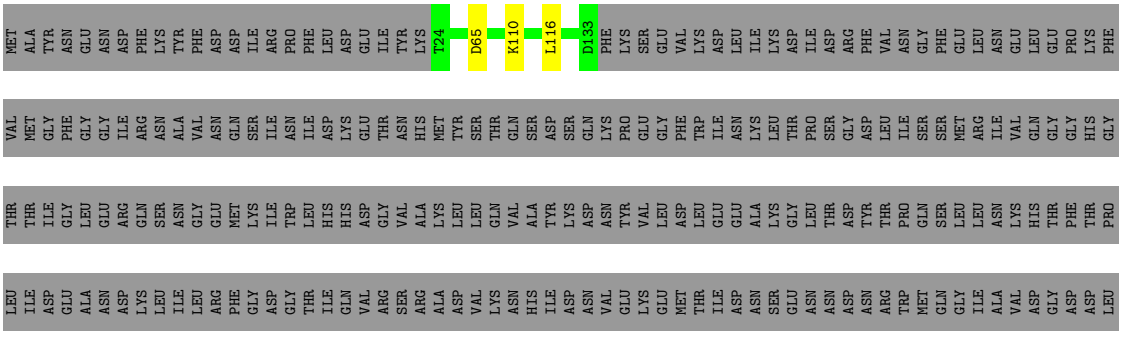
• Molecule 5: Minor structural protein

Chain EA:



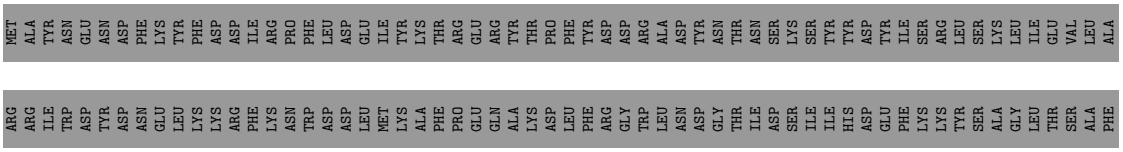
• Molecule 5: Minor structural protein

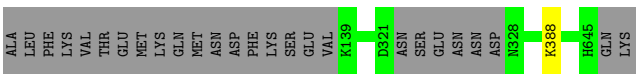
Chain FA:



• Molecule 5: Minor structural protein

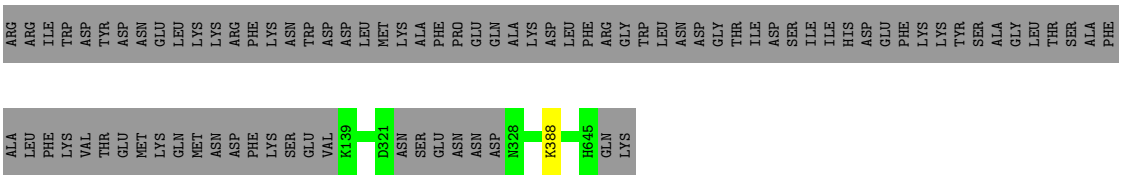
Chain CA:





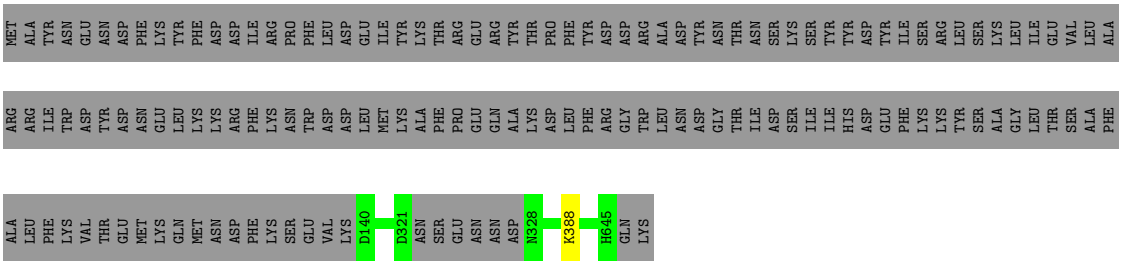
• Molecule 5: Minor structural protein

Chain NA:



• Molecule 5: Minor structural protein

Chain OA:

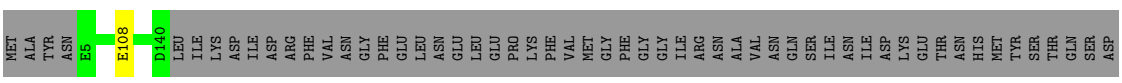


• Molecule 5: Minor structural protein

Chain DB:

• Molecule 5: Minor structural protein

Chain EB:



SER GLN LYS PRO GLU GLY PHE TRP ILE ASN LYS LEU THR PRO SER GLY ASP LEU ILE SER SER MET ARG ILE VAL GLN GLY GLY HIS GLY THR THR ILE GLY LEU GLU ARG GLN SER ASN GLY GLU MET LYS ILE TRP LEU HIS HIS ASP GLY VAL ALA LYS LEU LEU GLN VAL ALA TYR

LYS ASP ASN TYR VAL LEU ASP LEU GLU GLU ALA LYS GLY LEU THR ASP TYR THR PRO GLN SER LEU LEU ASN LYS HIS THR PHE THR PRO LEU ILE ASP GLU ALA ASN ASP LYS LEU ILE LEU ARG PHE GLY ASP GLY THR ILE GLN VAL ARG SER ARG ALA ASP VAL LYS ASN HIS ILE

ASP ASN VAL GLU LYS GLU MET THR ILE ASP ASN SER GLU ASN ASN ASP ASN ARG TRP MET GLN GLY ILE ALA VAL ASP GLY ASP ASP LEU TYR TRP LEU SER GLY ASN SER SER VAL ASN SER HIS VAL GLN ILE GLY LYS TYR SER LEU THR THR GLY GLN LYS ILE TYR ASP TYR PRO

PHE LYS LEU SER TYR GLN ASP GLY ILE ASN PHE PRO ARG ASP ASN PHE LYS GLU PRO GLU GLY ILE CYS ILE TYR THR ASN PRO LYS THR LYS ARG LYS SER LEU LEU LEU ALA MET THR ASN GLY GLY GLY GLY LYS ARG PHE HIS ASN LEU TYR GLY PHE PHE GLN LEU GLY GLU TYR

GLU HIS PHE GLU ALA LEU ARG ALA ARG GLY SER GLN ASN TYR LYS LEU THR LYS ASP ASP GLY ARG ALA LEU SER ILE PRO ASP HIS ILE ASP ASP LEU ASN ASP LEU THR GLN ALA GLY PHE TYR TYR ILE ASP GLY GLY THR ALA GLU LYS LEU LYS ASN MET PRO MET ASN GLY SER

LYS ARG ILE ILE ASP ALA GLY CYS PHE ILE ASN VAL TYR PRO THR THR GLN THR LEU GLY THR VAL GLN GLU LEU THR ARG PHE SER THR GLY ARG LYS MET VAL LYS MET VAL ARG GLY MET THR LEU ASP VAL PHE THR LEU LYS TRP ASP TYR GLY LEU TRP THR THR ILE LYS THR

ASP ALA PRO TYR GLN GLU TYR LEU GLU ALA SER GLN TYR ASN ASN TRP ILE ALA TYR VAL THR THR ALA GLY GLU TYR TYR ILE THR GLY ASN GLN MET GLU LEU PHE ARG ASP ALA PRO GLU GLU ILE LYS LYS VAL GLY ALA TRP LEU ARG VAL SER SER GLY ASN ALA VAL GLY GLU

VAL ARG GLN THR LEU GLU ALA ASN ILE SER GLU TYR LYS GLU PHE PHE SER ASN VAL ASN ALA GLU THR LYS HIS ARG GLU TYR GLY TRP VAL ALA LYS HIS GLN LYS

- Molecule 5: Minor structural protein

Chain FB: 17% 83%

MET ALA TYR ASN GLU ASN ASP PHE LYS TYR PHE ASP ASP ILE ARG PRO PHE LEU ASP GLU ILE LYS T24 D65 K110 L116 D133 PHE LYS SER GLU VAL LYS ASP LEU ILE LYS ASP ILE ASP ARG PHE VAL ASN GLY PHE GLU LEU ASN GLU LEU GLU PRO LYS PHE

VAL MET GLY PHE GLY GLY ILE ARG ASN ALA VAL ASN GLN SER ILE ASN ILE ASP LYS GLU THR ASN HIS MET TYR SER THR GLN SER ASP SER GLN LYS PRO GLU GLY PHE TRP ILE ASN LYS LEU THR PRO SER GLY ASP LEU ILE SER SER MET ARG ILE VAL GLN GLY GLY HIS GLY

THR THR ILE GLY LEU GLU ARG GLN SER ASN GLY GLU MET LYS ILE TRP LEU HIS HIS ASP GLY VAL ALA LYS LEU LEU GLN VAL ALA TYR LYS ASP ASN TYR VAL LEU ASP LEU GLU GLU ALA LYS GLY LEU THR ASP TYR THR PRO GLN SER LEU LEU ASN LYS HIS THR PHE THR PRO

LEU ILE ASP GLU ALA ASN ASP LYS LEU ILE LEU ARG PHE GLY ASP GLY THR ILE GLN VAL ARG SER ARG ALA ASP VAL LYS ASN HIS ILE ASP ASN VAL GLU LYS GLU MET THR ILE ASP ASN SER GLU ASN ASN ASP ASN ARG TRP MET GLN GLY ILE ALA VAL ASP GLY ASP ASP LEU

TYR TRP LEU SER GLY ASN SER SER VAL ASN SER HIS VAL GLN ILE GLY LYS TYR SER LEU THR THR GLY GLN LYS ILE TYR ASP TYR PRO PHE LYS LEU SER TYR GLN ASP GLY ILE ASN PHE PRO ARG ASP ASN PHE LYS GLU PRO GLU GLY ILE CYS ILE TYR THR ASN PRO LYS THR

LYS ARG LYS SER LEU LEU LEU ALA MET THR ASN GLY GLY GLY GLY LYS ARG PHE HIS ASN LEU TYR GLY PHE PHE GLN LEU GLY GLU TYR GLU HIS PHE GLU ALA LEU ARG ALA ARG GLY SER GLN ASN TYR LYS LEU THR LYS ASP ASP GLY ARG ALA LEU SER ILE PRO ASP HIS ILE

ASP ASP LEU ASN ASP LEU THR GLN ALA GLY PHE TYR TYR ILE ASP GLY GLY THR ALA GLU LYS LEU LYS ASN MET PRO MET ASN GLY SER LYS ARG ILE ILE ASP ALA GLY CYS PHE ILE ASN VAL TYR PRO THR THR GLN THR LEU GLY THR VAL GLN GLU LEU THR ARG PHE SER THR

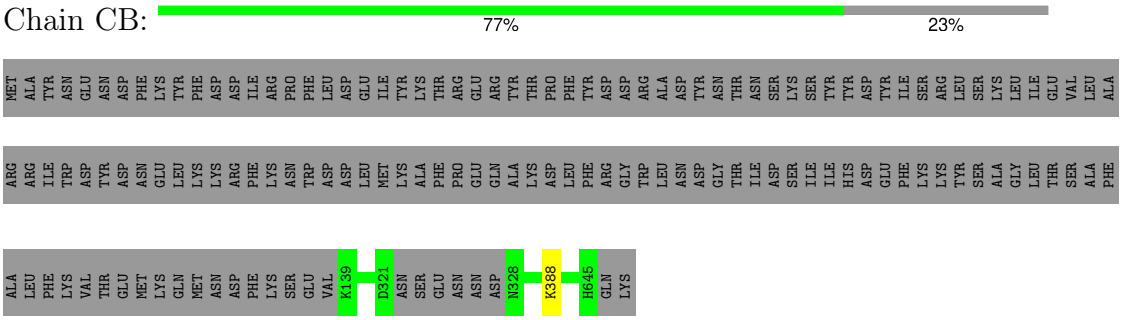
GLY ARG LYS MET VAL LYS MET VAL ARG GLY MET THR LEU ASP VAL PHE THR LEU LYS TRP ASP TYR GLY LEU TRP THR THR ILE LYS THR ASP ALA PRO TYR GLN GLU TYR LEU GLU ALA SER GLN TYR ASN ASN TRP ILE ALA TYR VAL THR THR ALA GLY GLU TYR TYR ILE THR GLY

ASN GLN MET GLU LEU PHE ARG ASP ALA PRO GLU GLU ILE LYS LYS VAL GLY ALA TRP LEU ARG VAL SER SER GLY ASN ALA VAL GLY GLU VAL ARG GLN THR LEU GLU ALA ASN ILE SER GLU TYR LYS GLU PHE PHE SER ASN VAL ASN ALA GLU THR LYS HIS ARG GLU TYR GLY TRP

VAL ALA LYS HIS GLN LYS

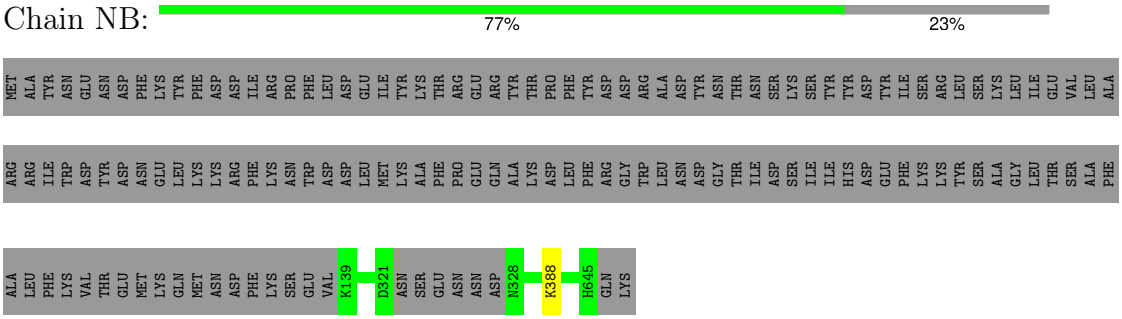
- Molecule 5: Minor structural protein

Chain CB:



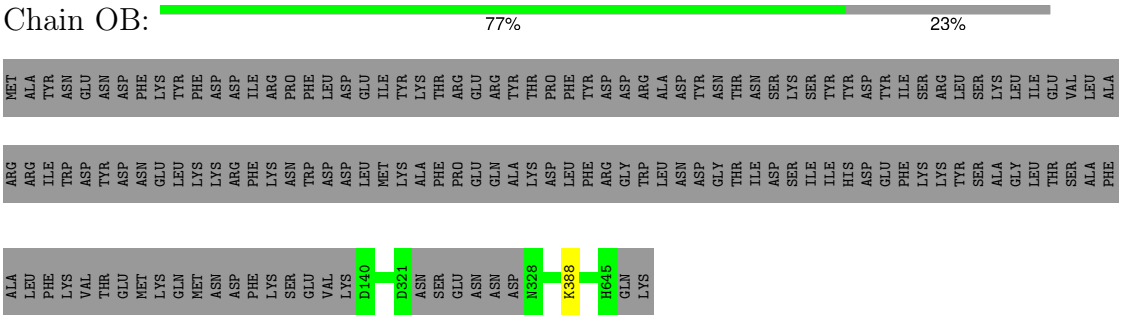
• Molecule 5: Minor structural protein

Chain NB:



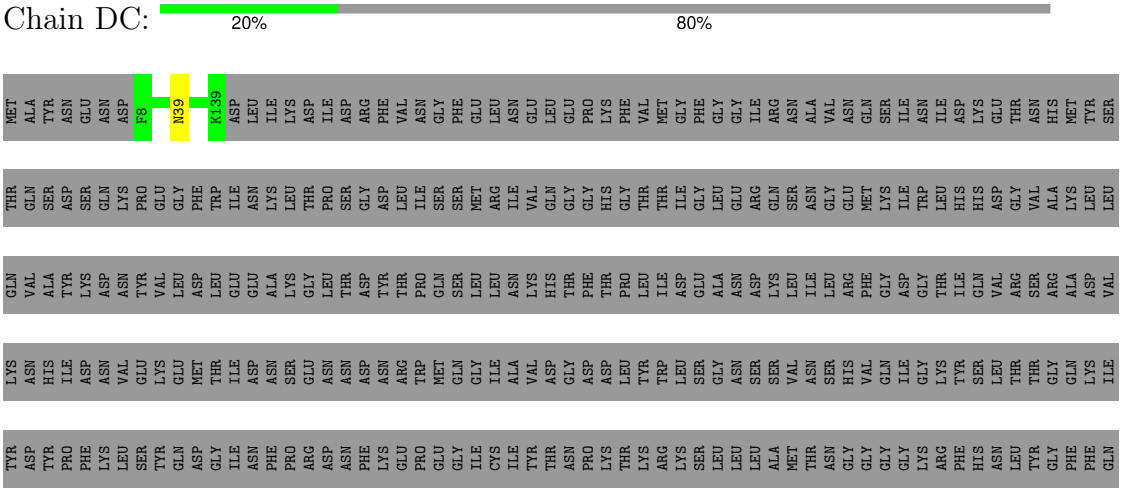
• Molecule 5: Minor structural protein

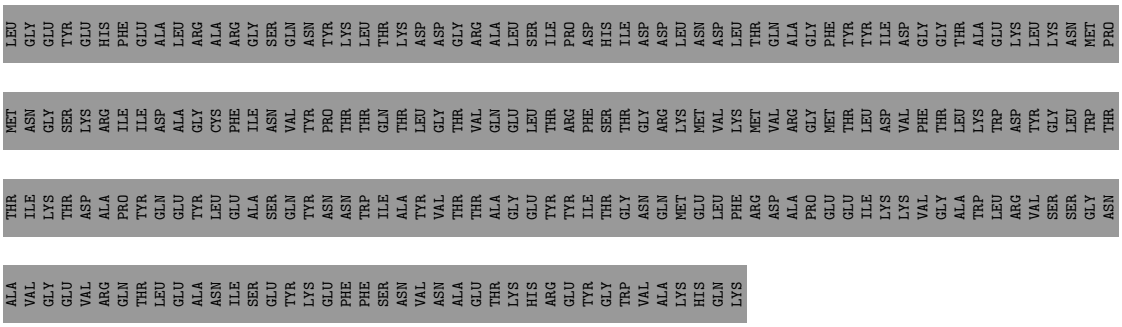
Chain OB:



• Molecule 5: Minor structural protein

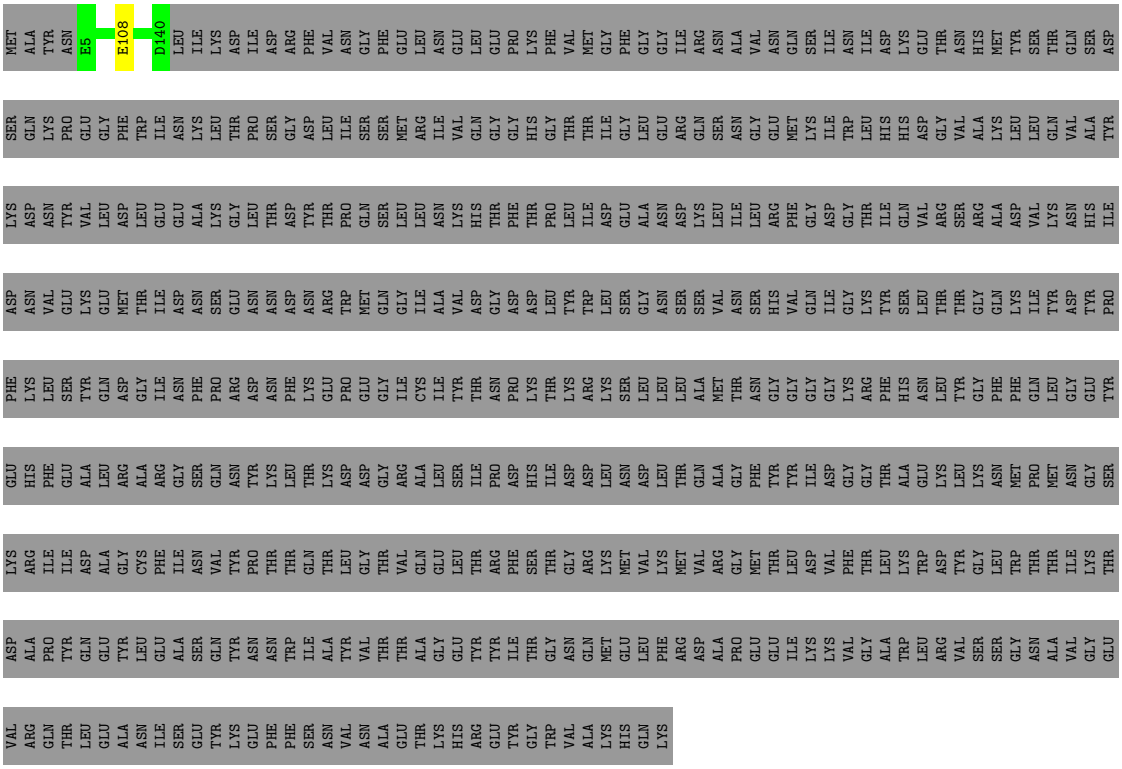
Chain DC:





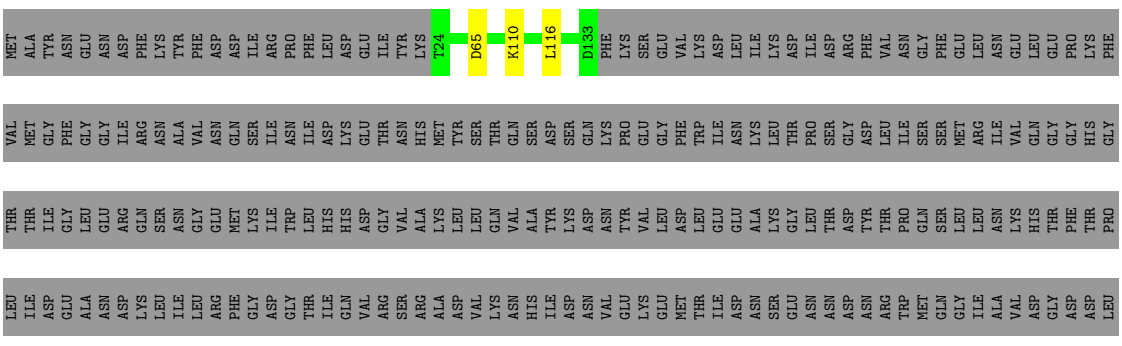
• Molecule 5: Minor structural protein

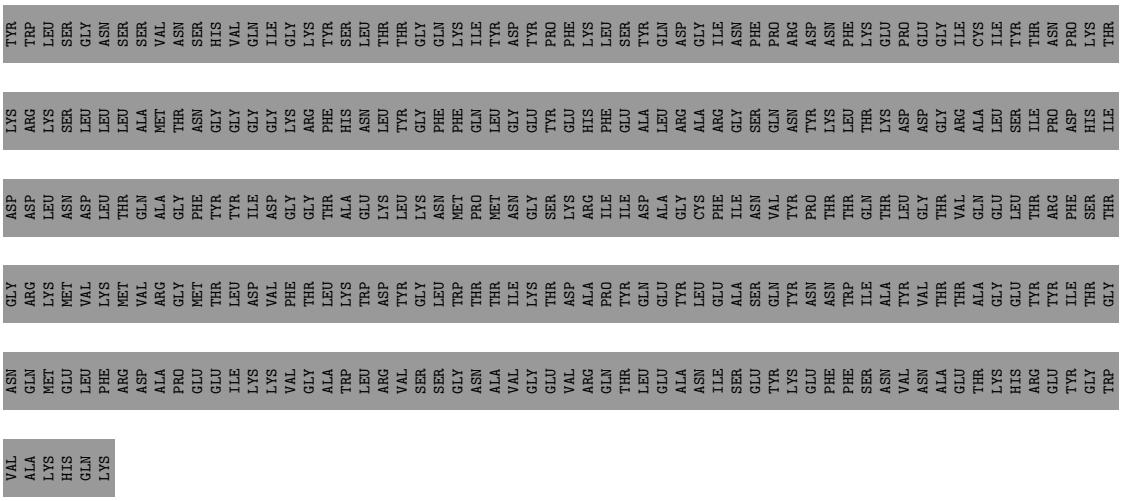
Chain EC:



• Molecule 5: Minor structural protein

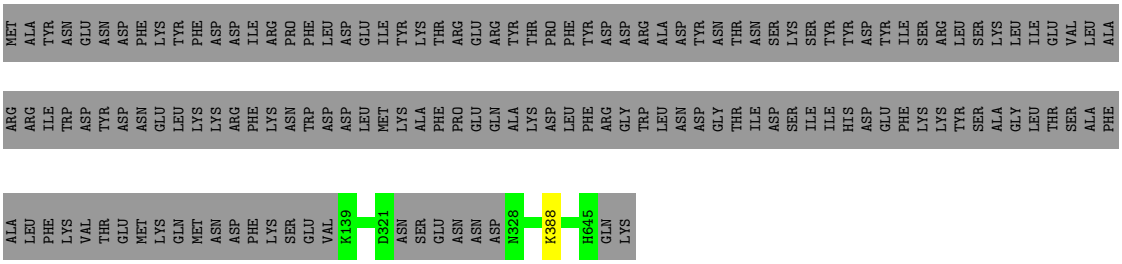
Chain FC:





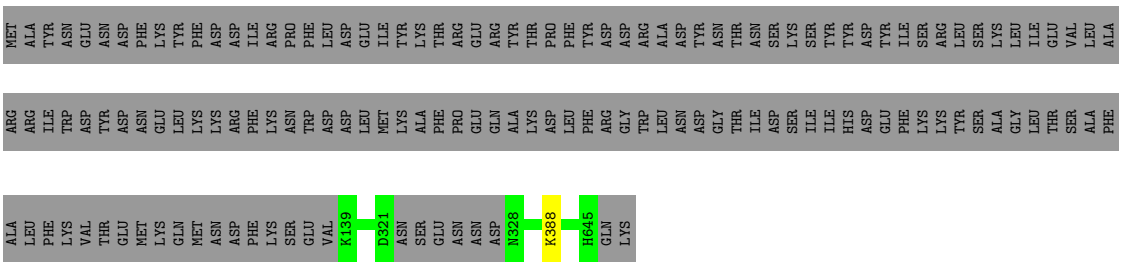
• Molecule 5: Minor structural protein

Chain CC:



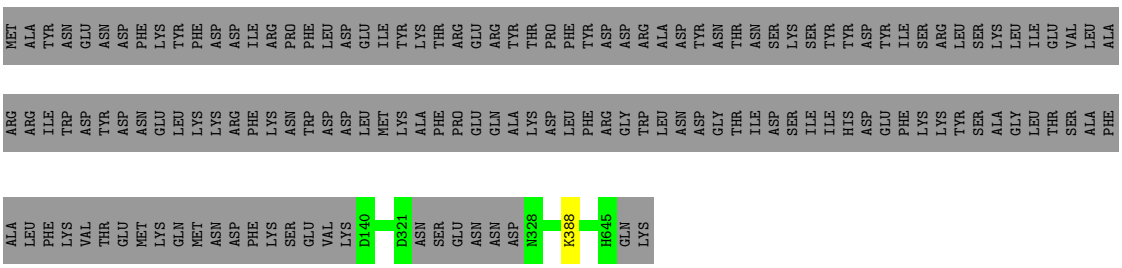
• Molecule 5: Minor structural protein

Chain NC:



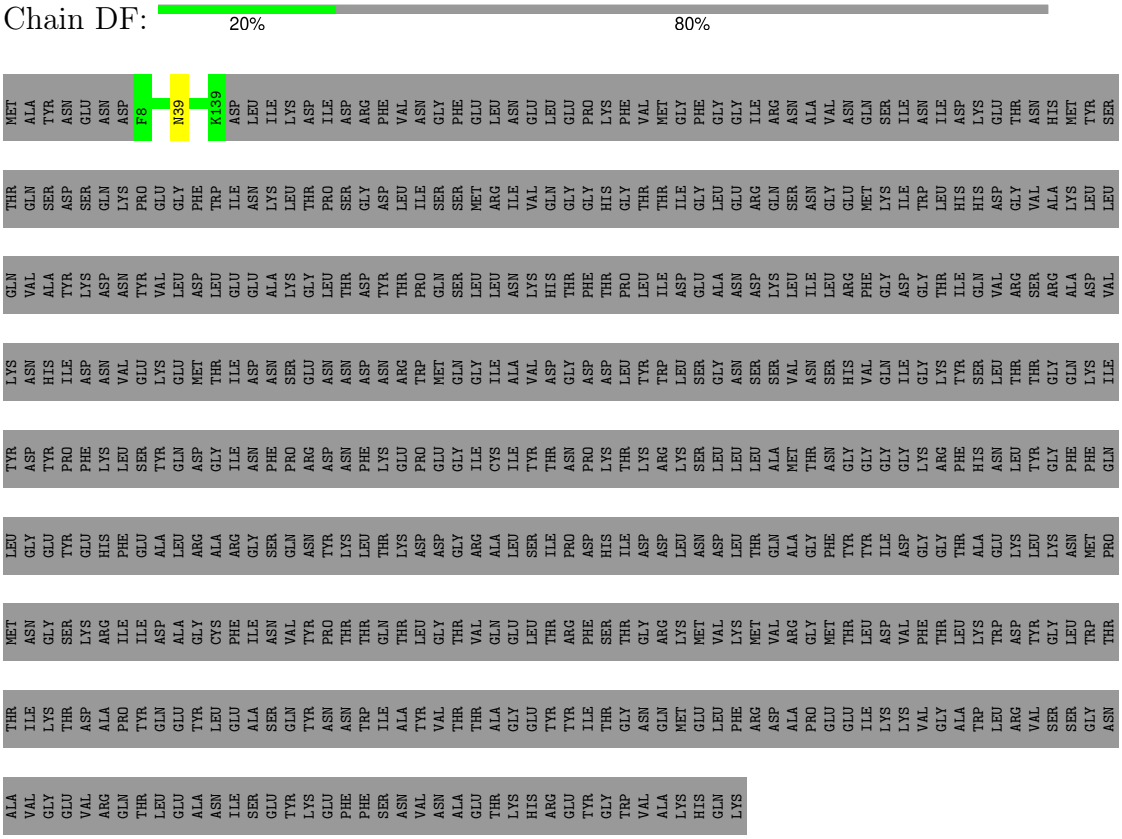
• Molecule 5: Minor structural protein

Chain OC:



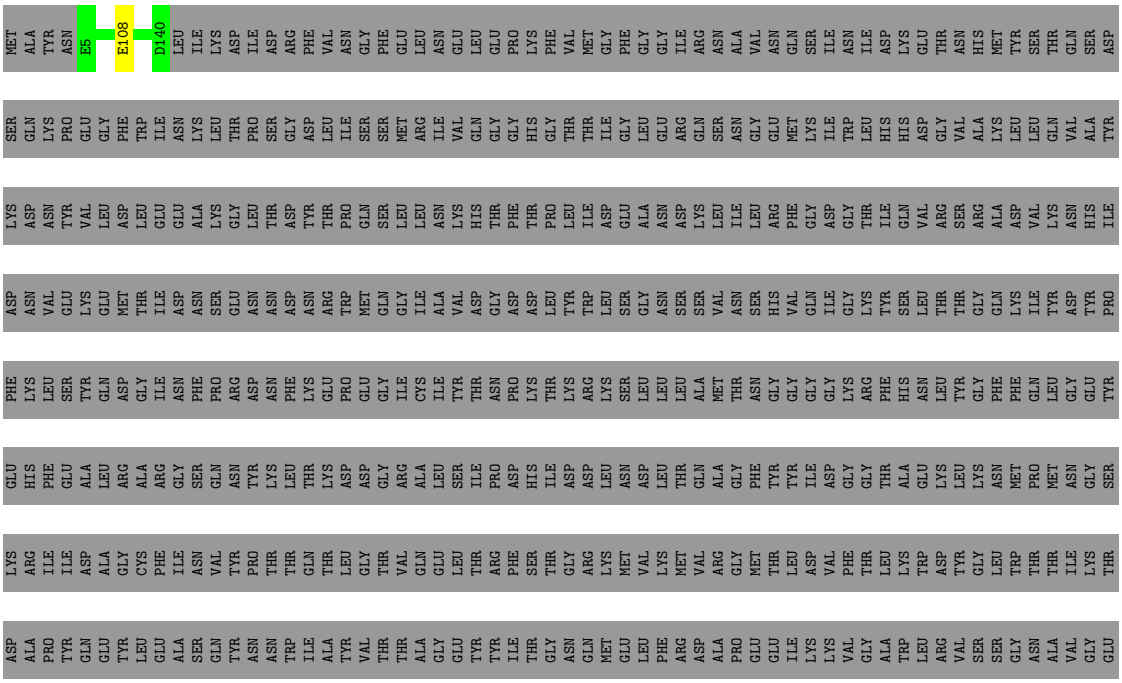
• Molecule 5: Minor structural protein

Chain DF:



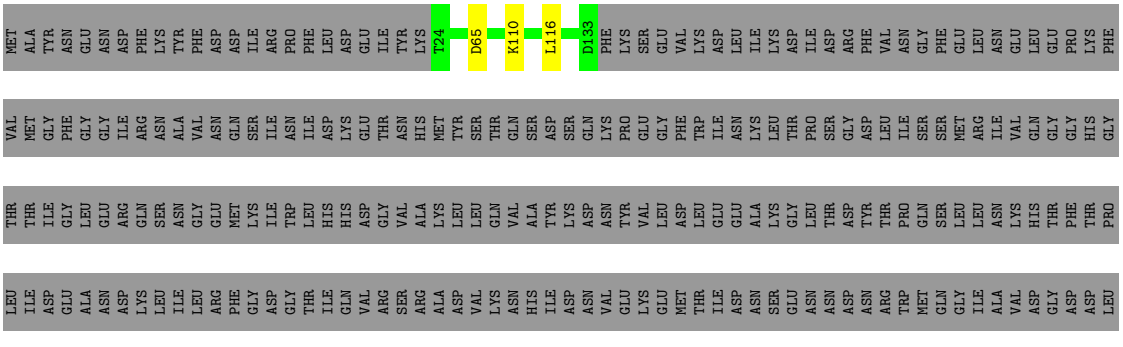
• Molecule 5: Minor structural protein

Chain EF:



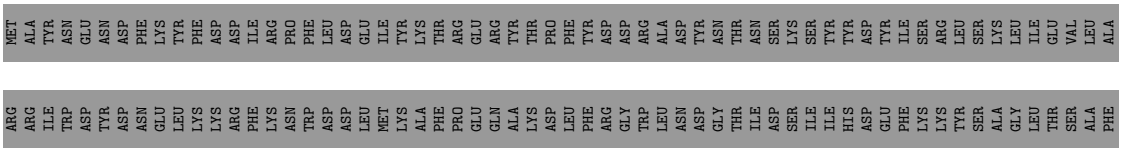
• Molecule 5: Minor structural protein

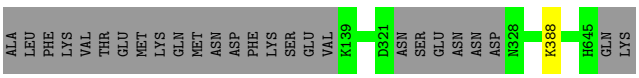
Chain FF:



• Molecule 5: Minor structural protein

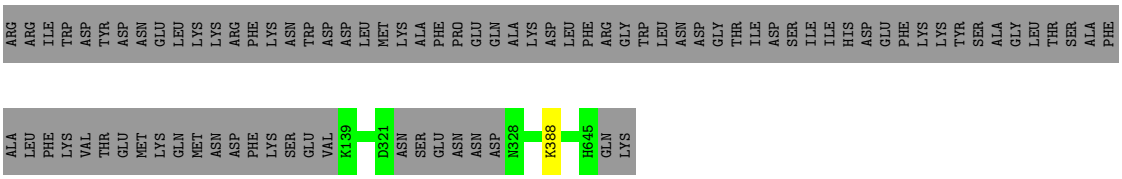
Chain CF:





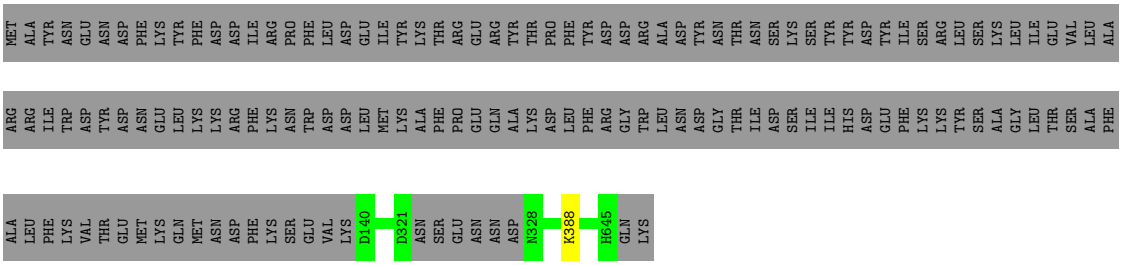
• Molecule 5: Minor structural protein

Chain NF:



• Molecule 5: Minor structural protein

Chain OF:

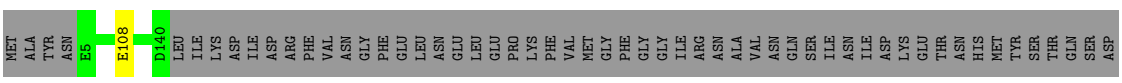


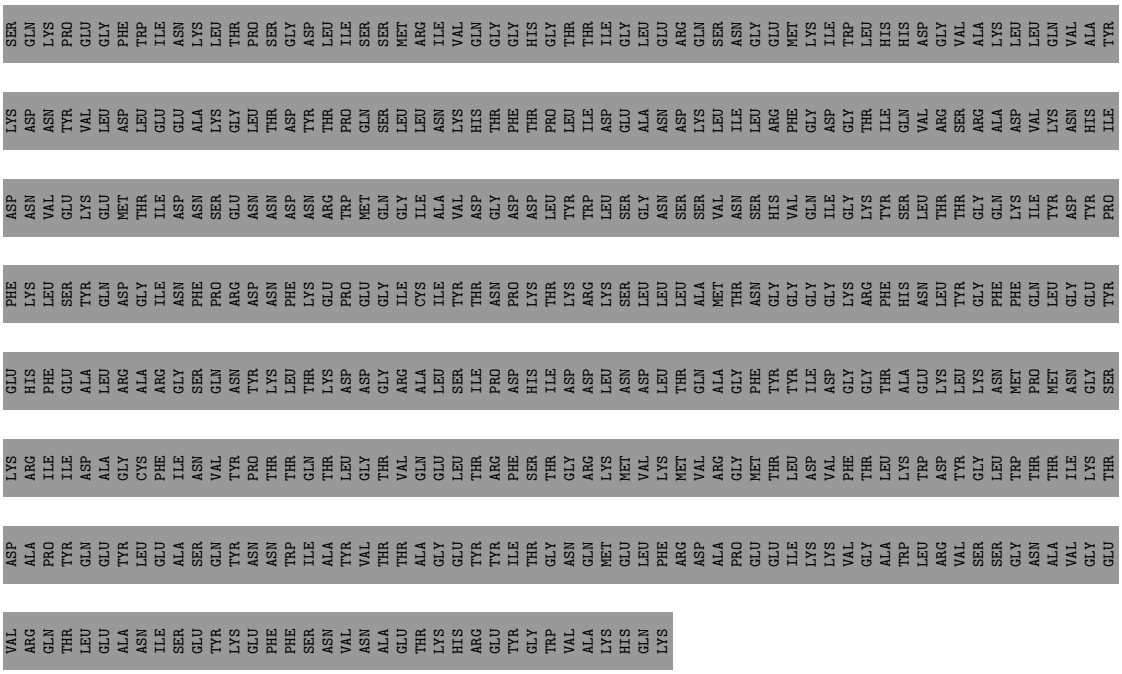
• Molecule 5: Minor structural protein

Chain DH:

• Molecule 5: Minor structural protein

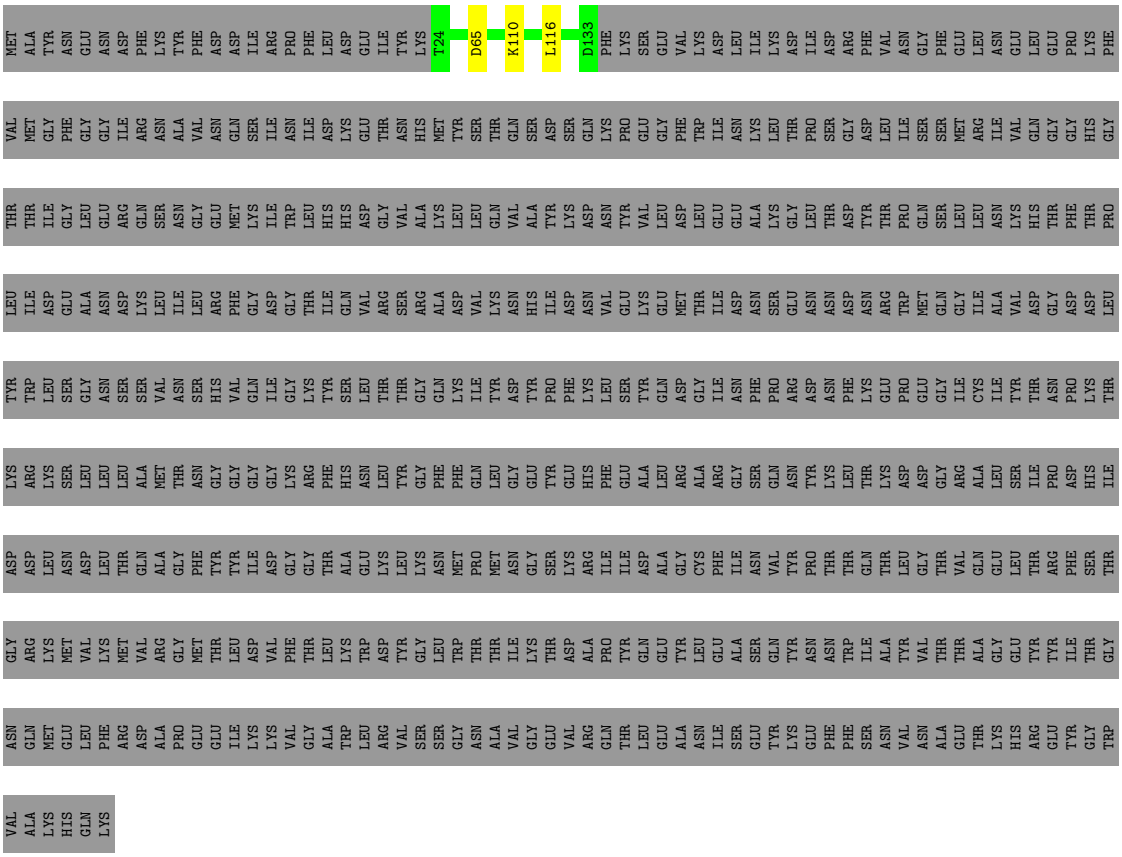
Chain EH:





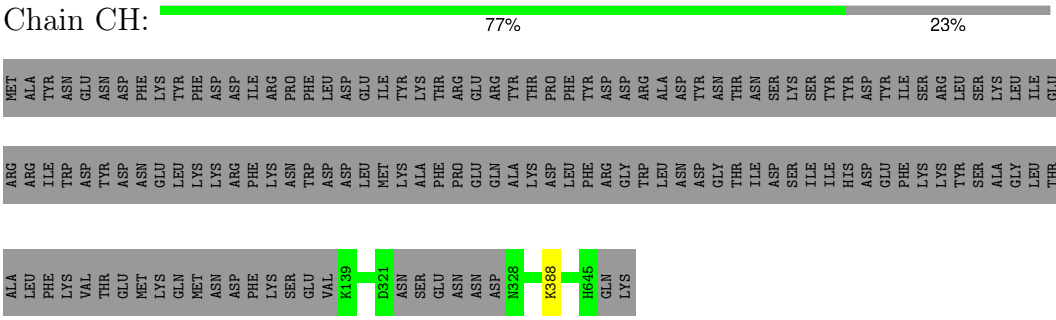
• Molecule 5: Minor structural protein

Chain FH:



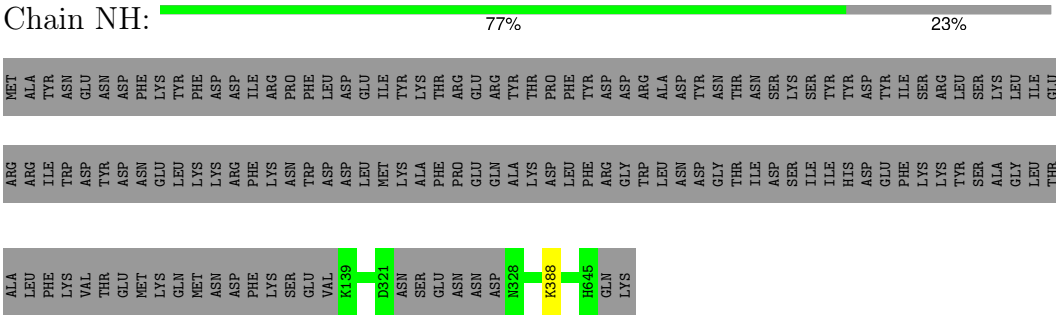
• Molecule 5: Minor structural protein

Chain CH:



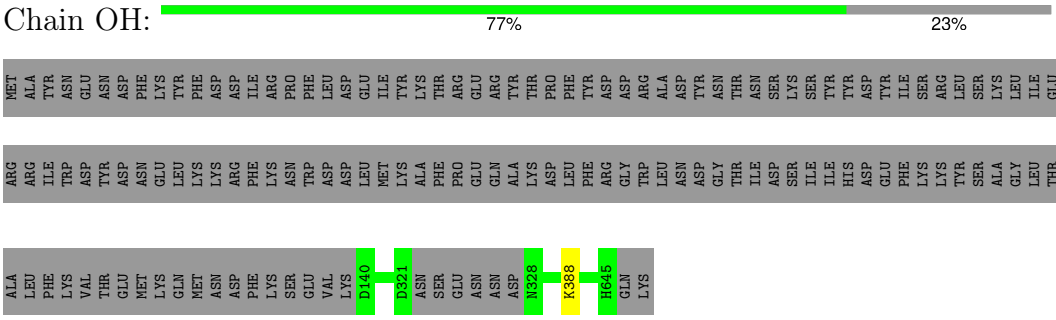
• Molecule 5: Minor structural protein

Chain NH:



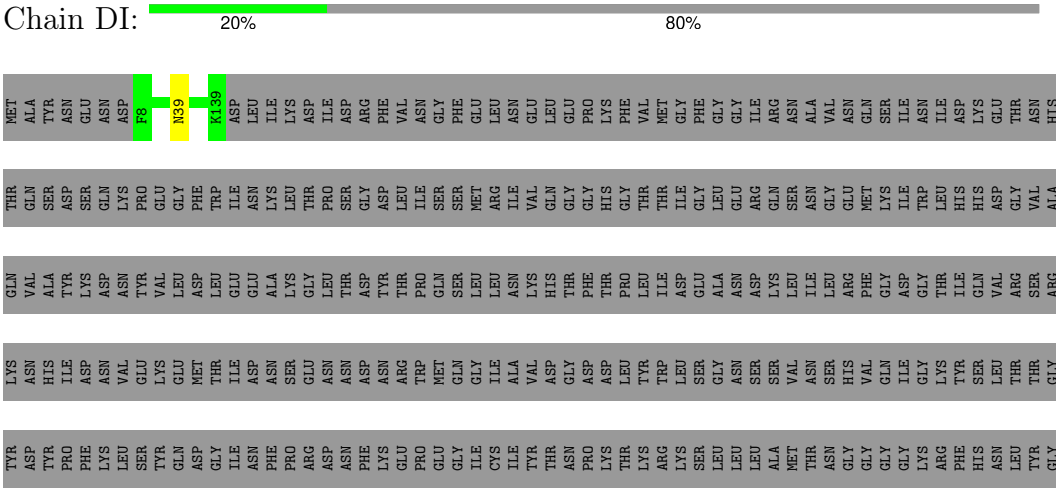
• Molecule 5: Minor structural protein

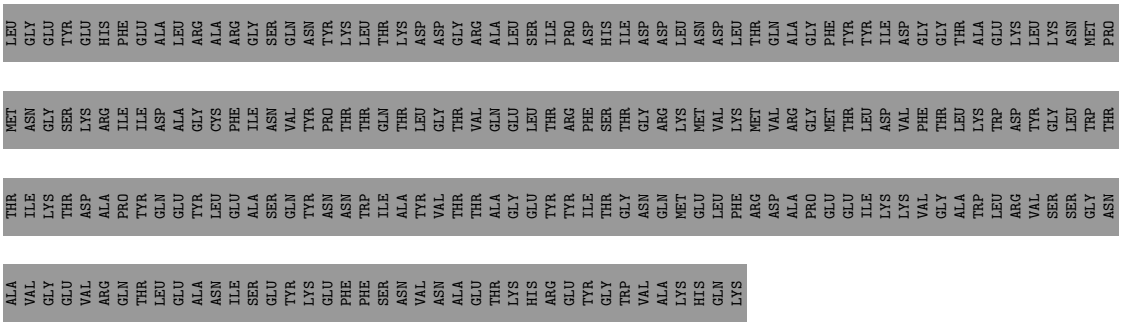
Chain OH:



• Molecule 5: Minor structural protein

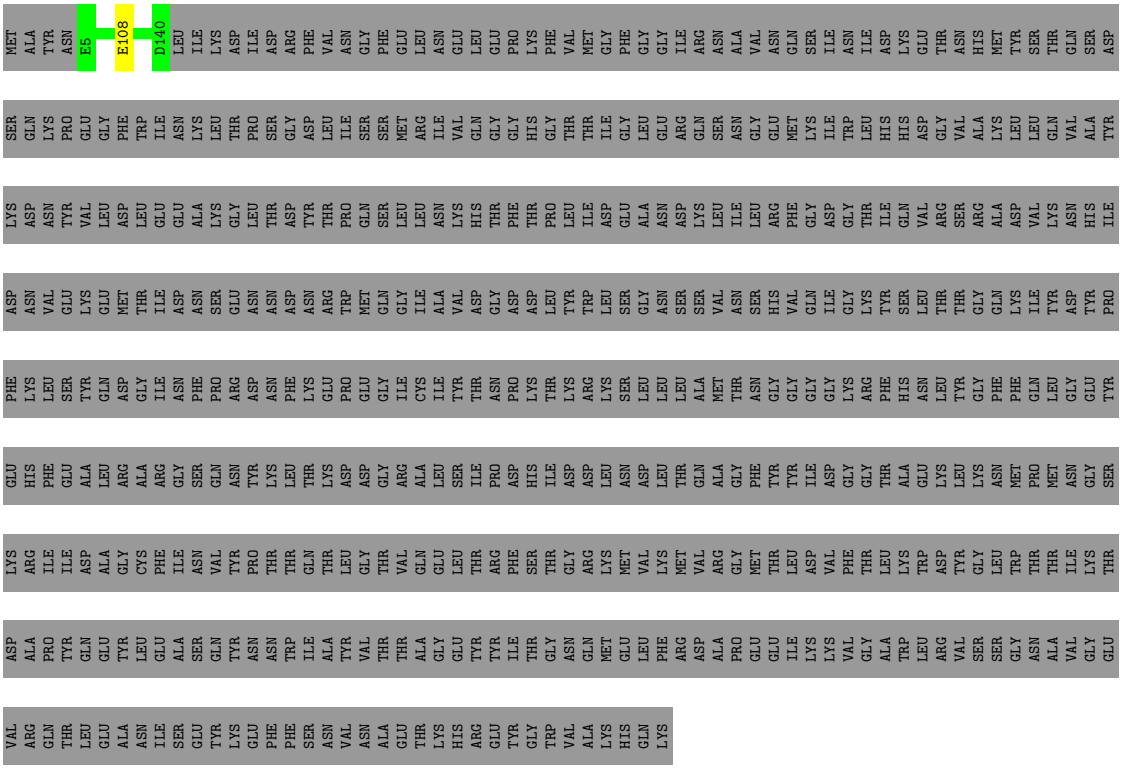
Chain DI:





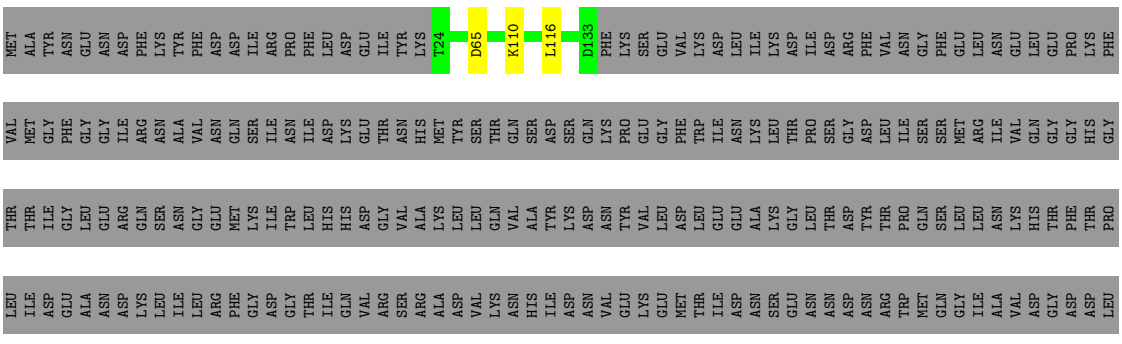
• Molecule 5: Minor structural protein

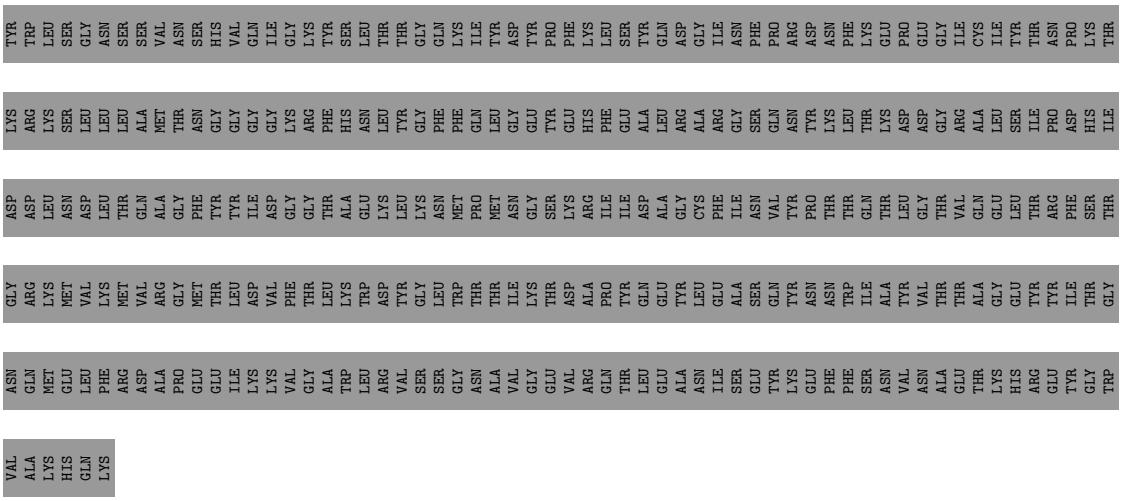
Chain EI:



• Molecule 5: Minor structural protein

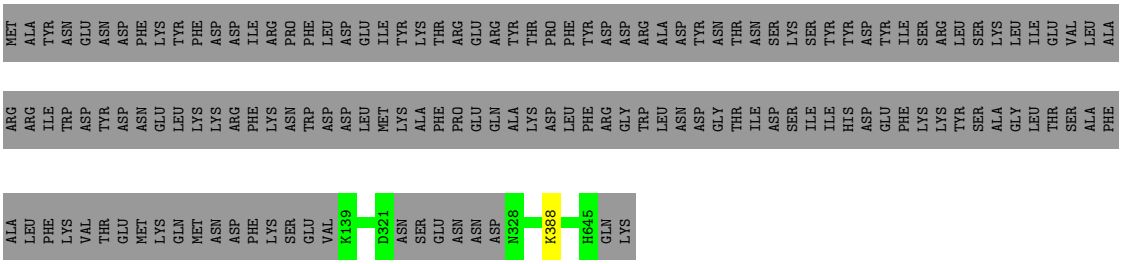
Chain FI:





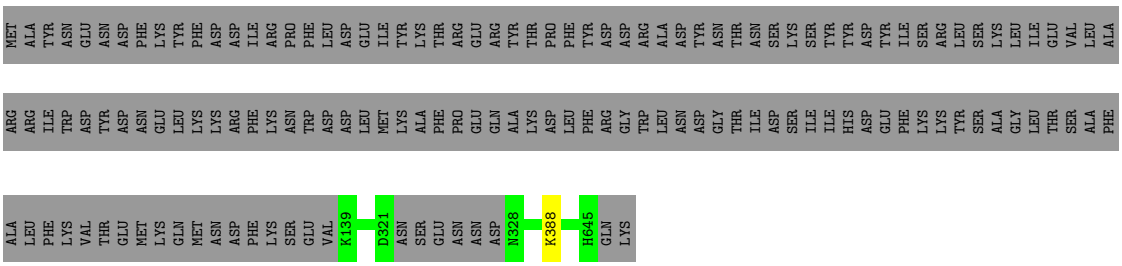
• Molecule 5: Minor structural protein

Chain CI:



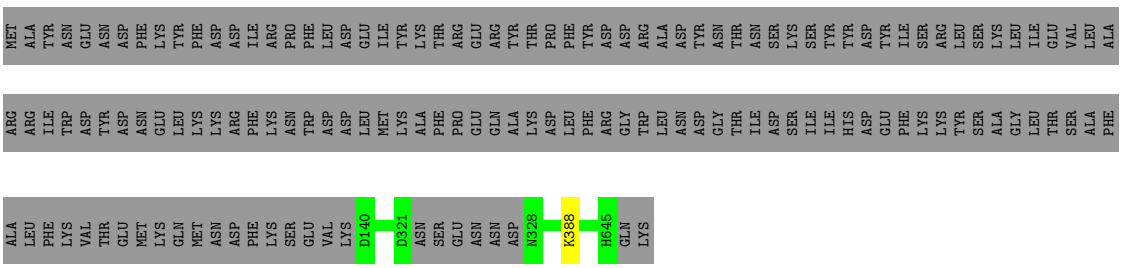
• Molecule 5: Minor structural protein

Chain NI:



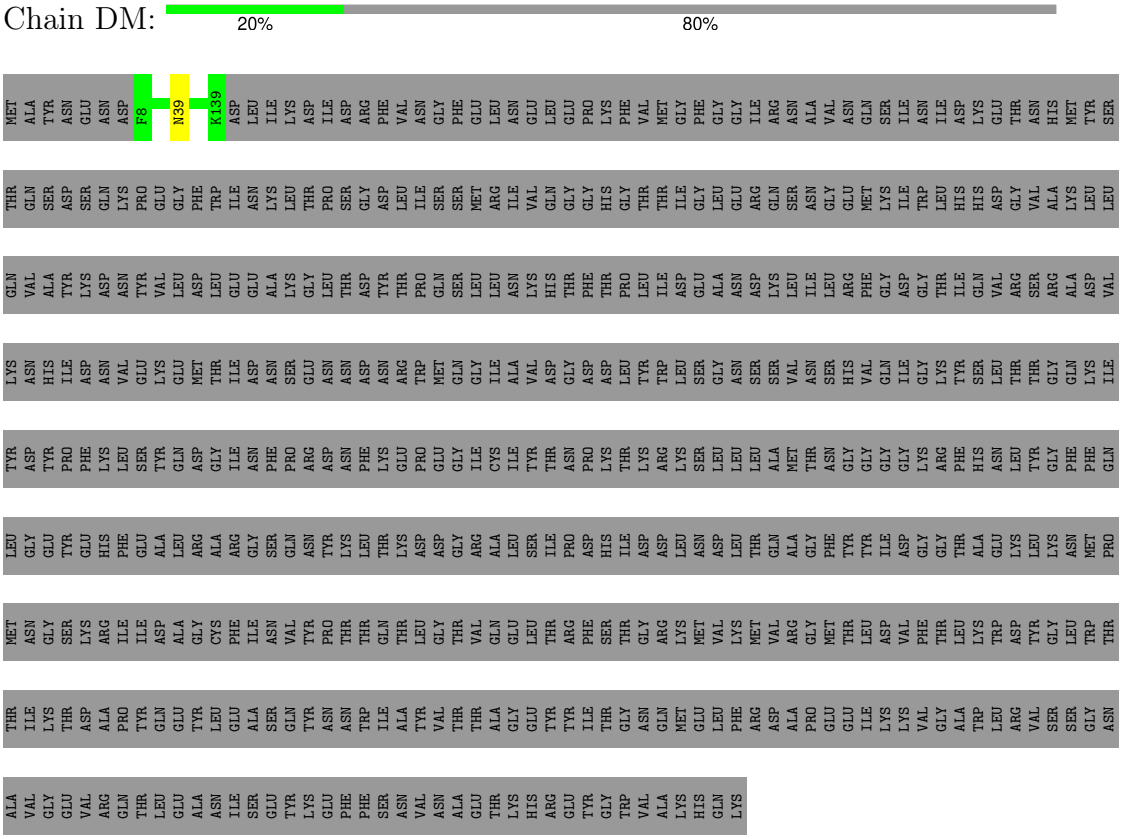
• Molecule 5: Minor structural protein

Chain OI:



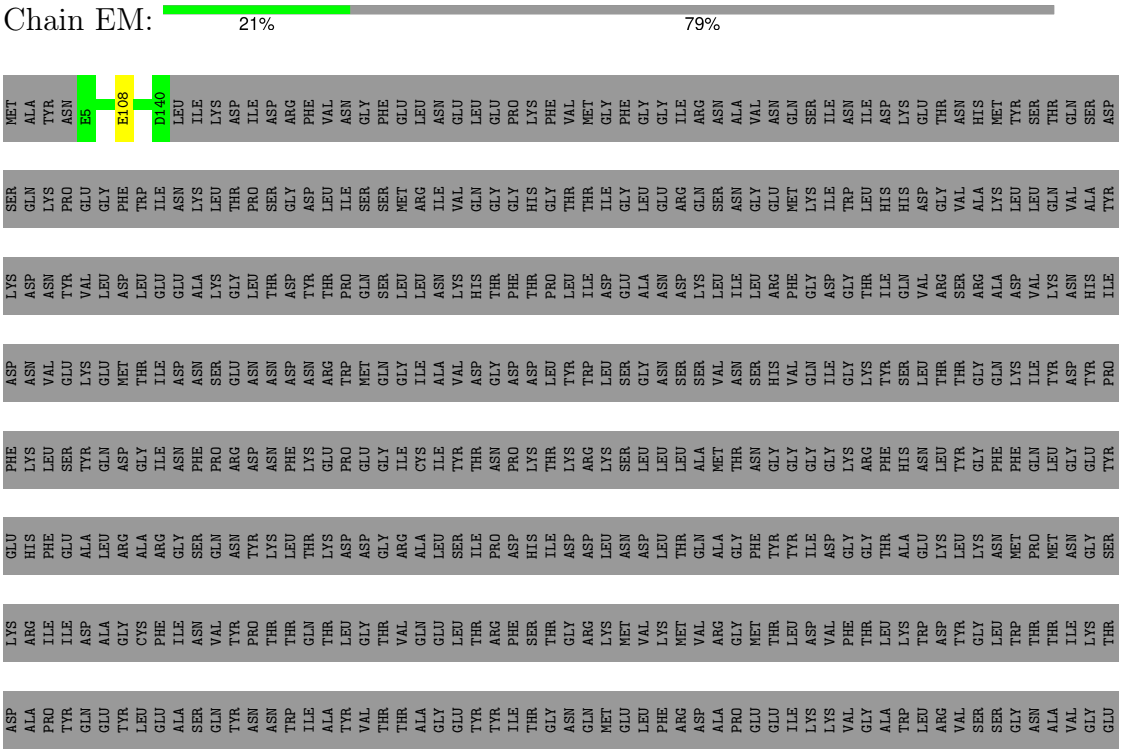
• Molecule 5: Minor structural protein

Chain DM:



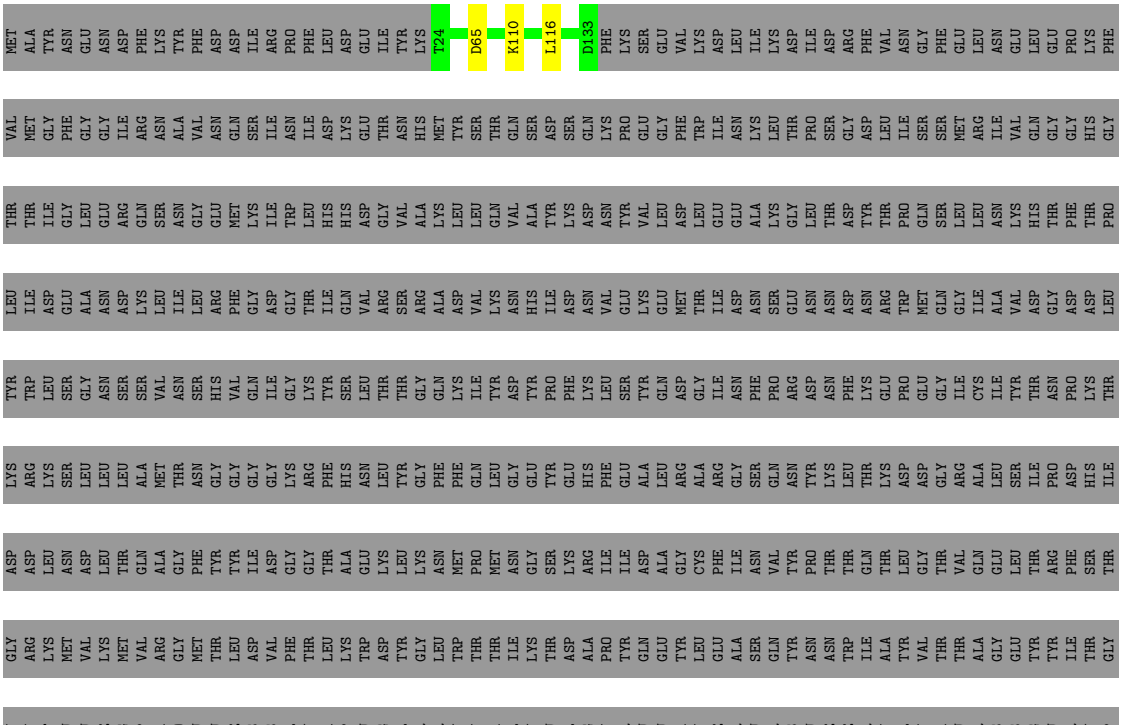
• Molecule 5: Minor structural protein

Chain EM:



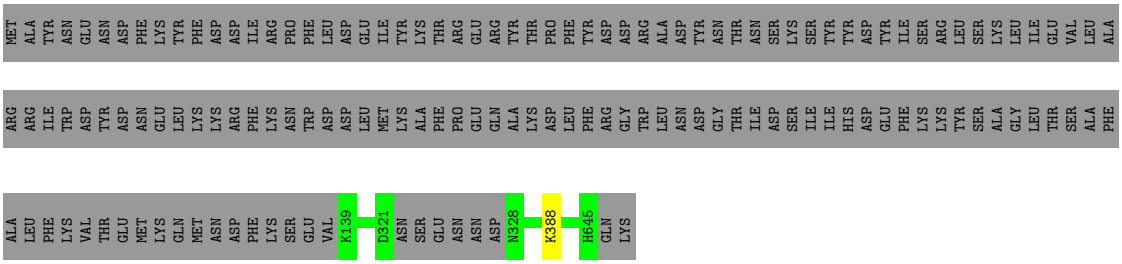
• Molecule 5: Minor structural protein

Chain FM:



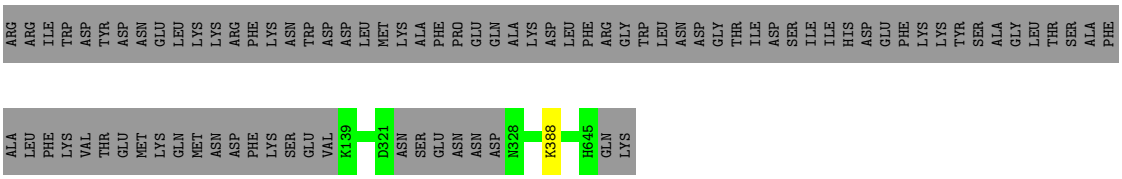
• Molecule 5: Minor structural protein

Chain CM:



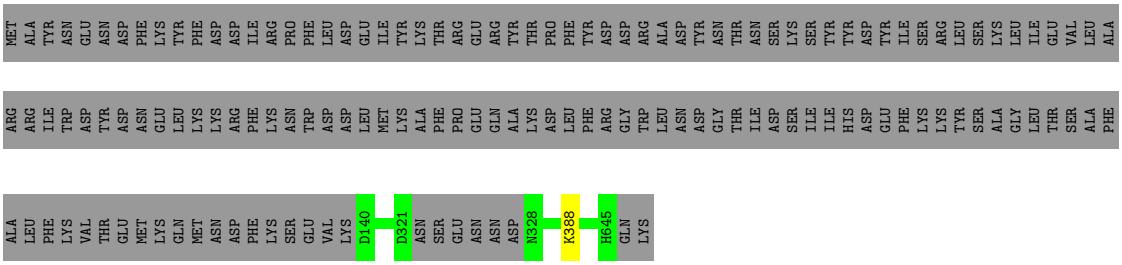
• Molecule 5: Minor structural protein

Chain NM:



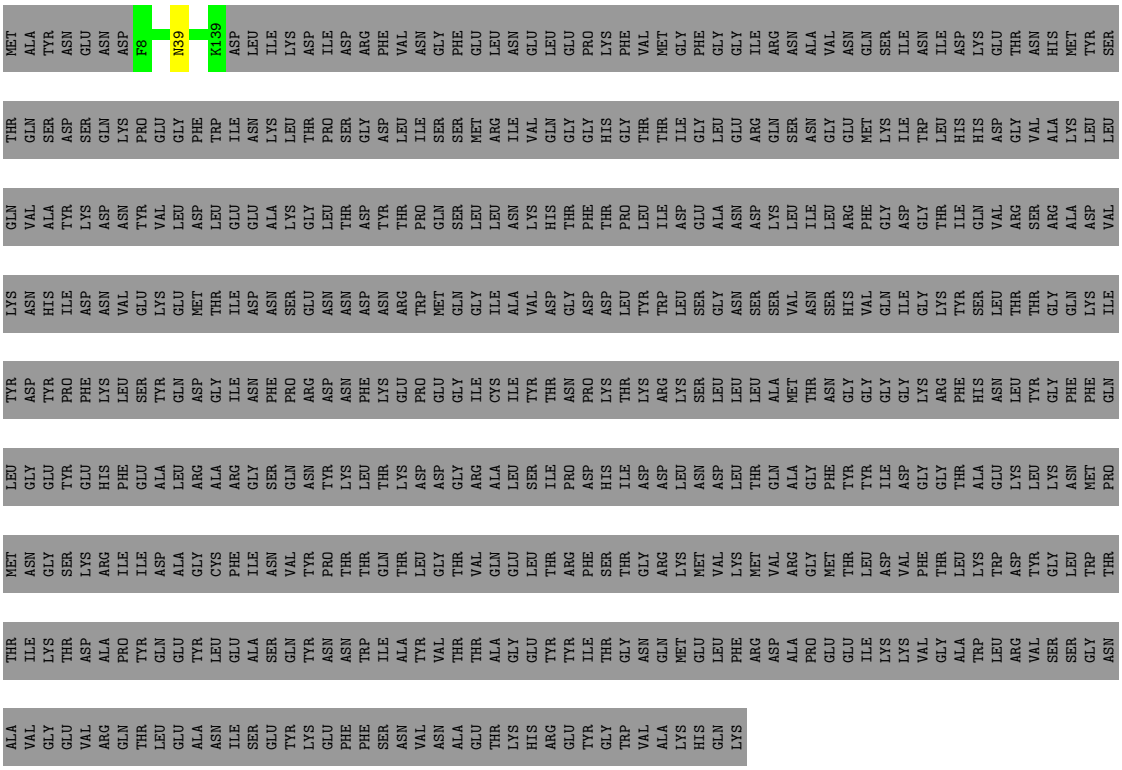
• Molecule 5: Minor structural protein

Chain OM:



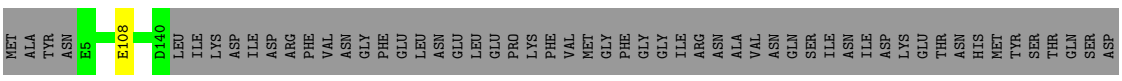
• Molecule 5: Minor structural protein

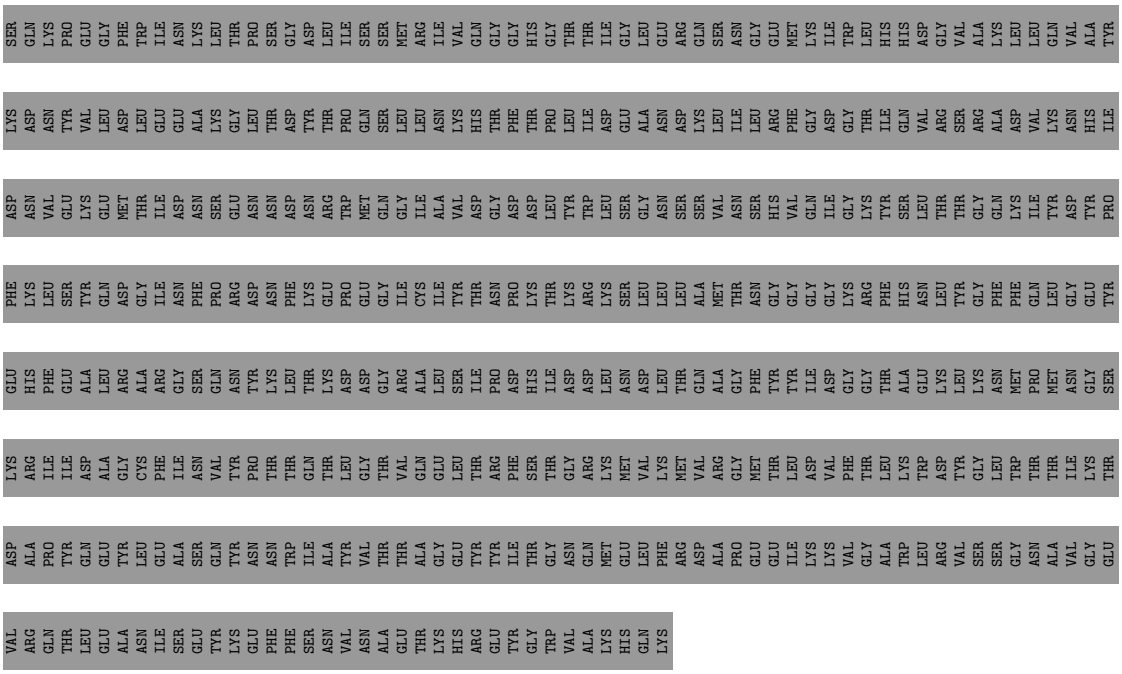
Chain DN:



• Molecule 5: Minor structural protein

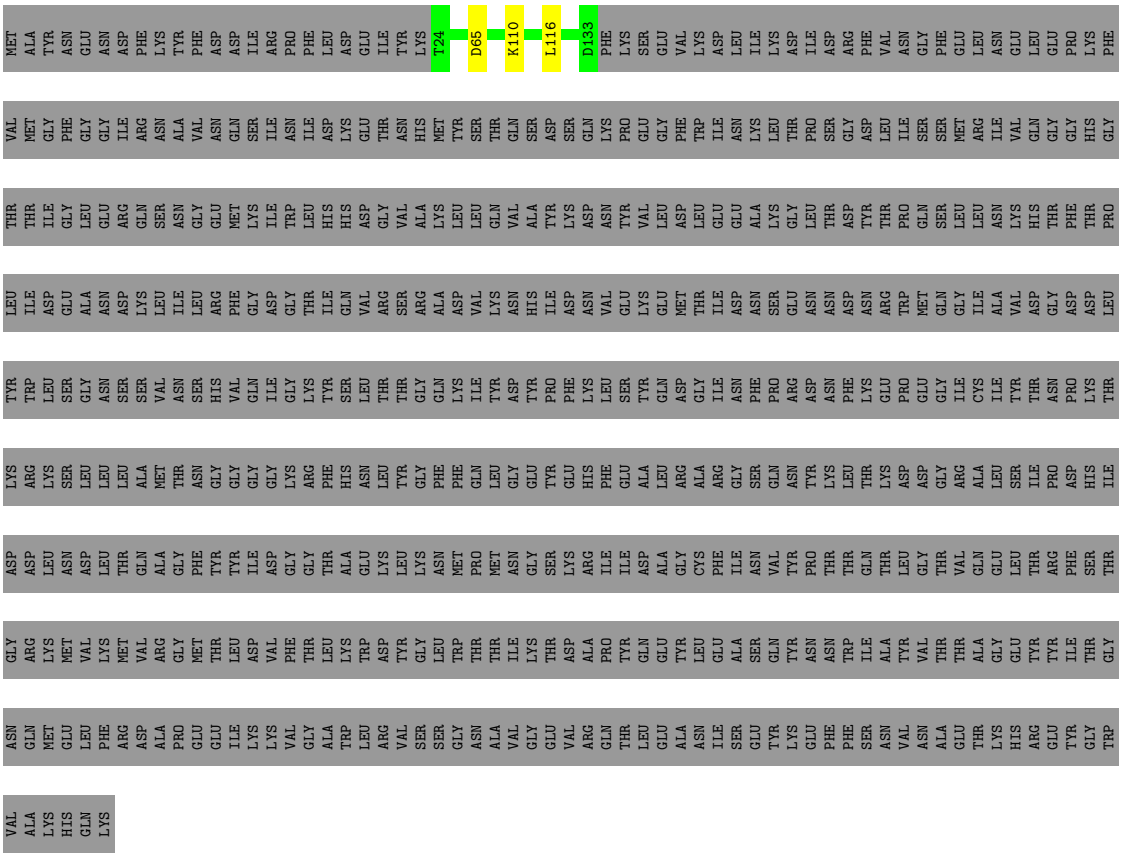
Chain EN:





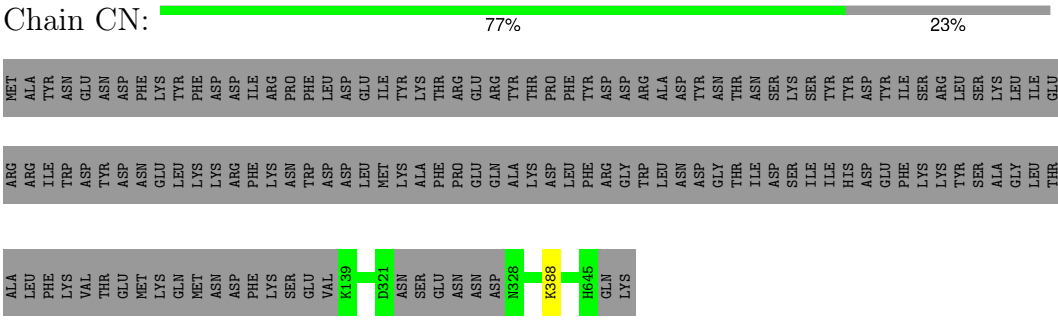
• Molecule 5: Minor structural protein

Chain FN:



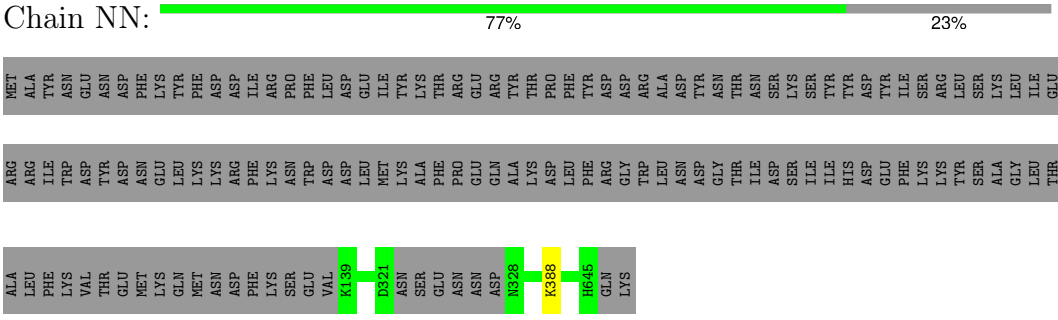
• Molecule 5: Minor structural protein

Chain CN:



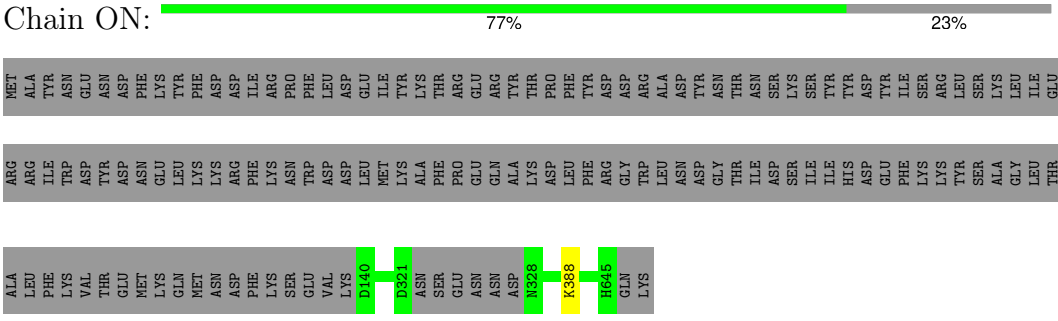
• Molecule 5: Minor structural protein

Chain NN:



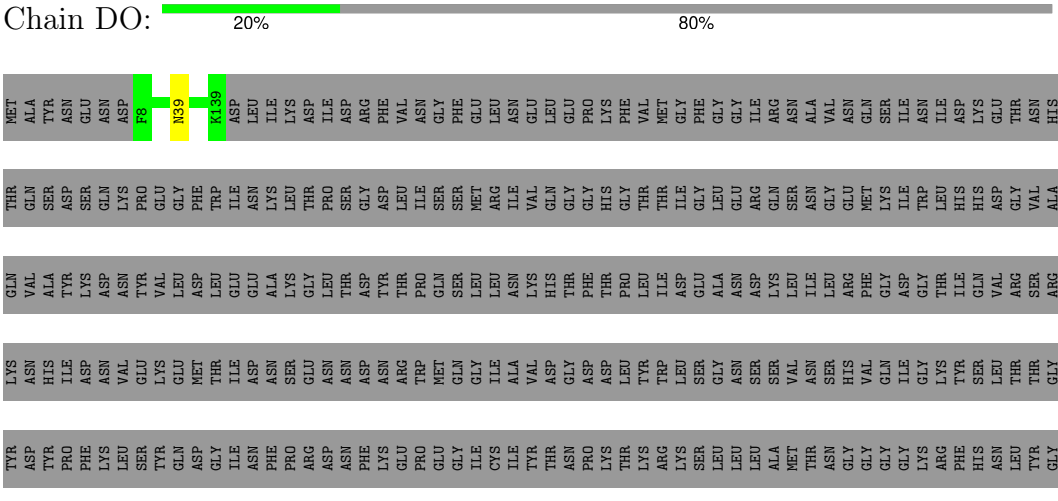
• Molecule 5: Minor structural protein

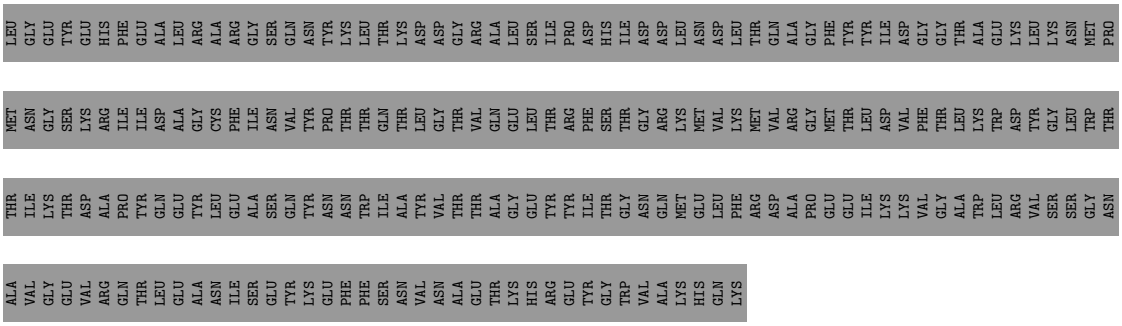
Chain ON:



• Molecule 5: Minor structural protein

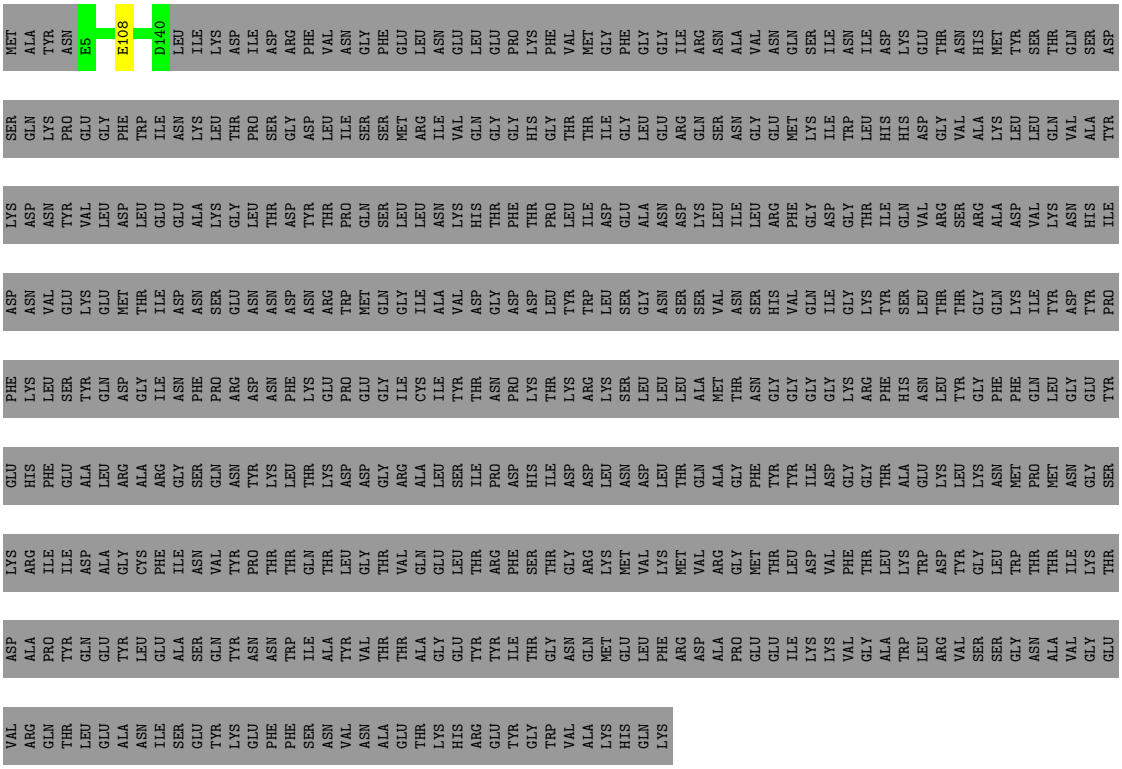
Chain DO:





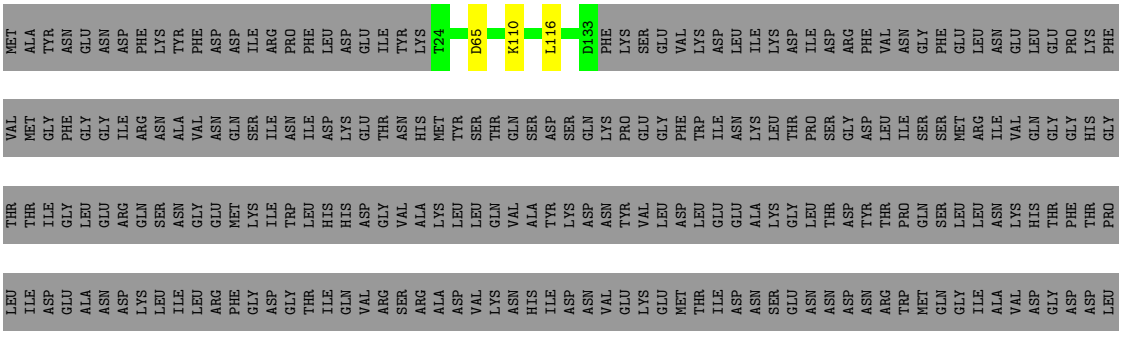
• Molecule 5: Minor structural protein

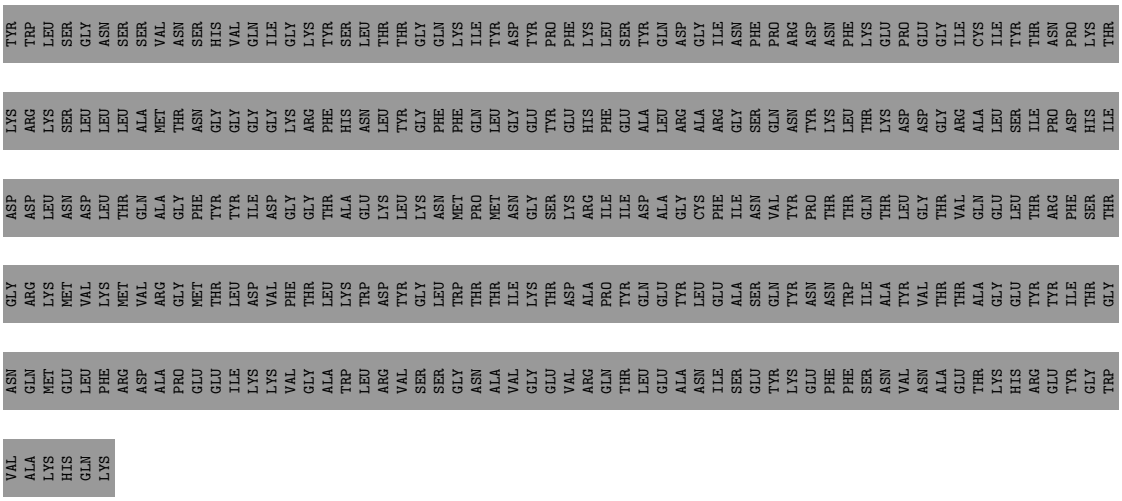
Chain EO:



• Molecule 5: Minor structural protein

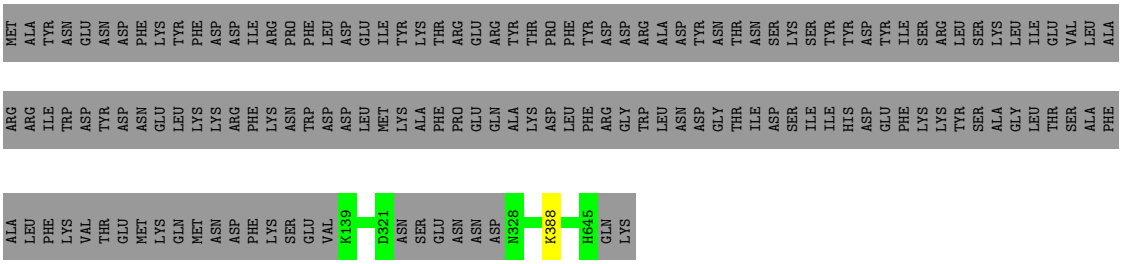
Chain FO:





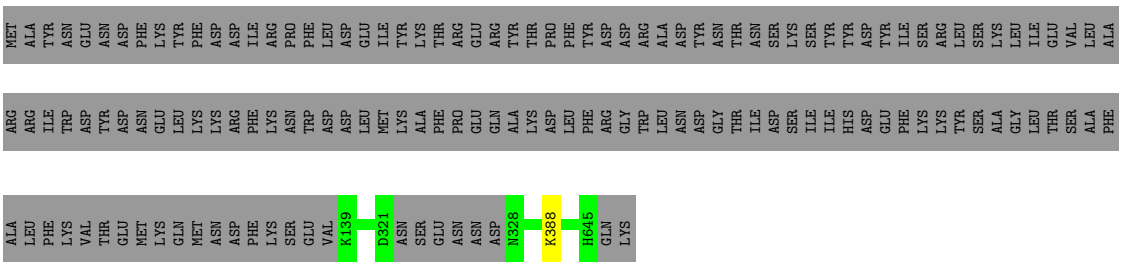
• Molecule 5: Minor structural protein

Chain CO:



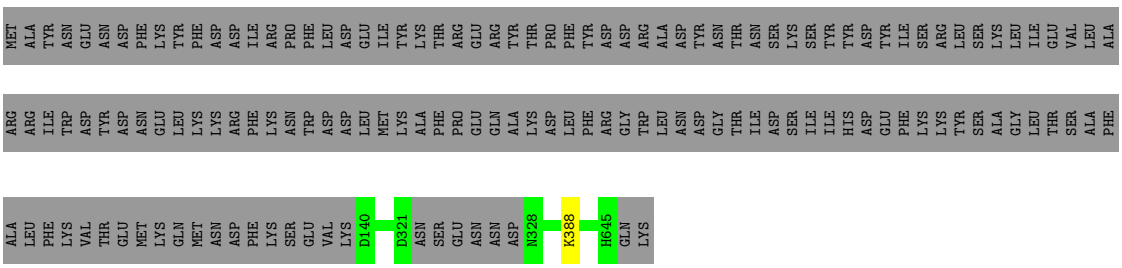
• Molecule 5: Minor structural protein

Chain NO:



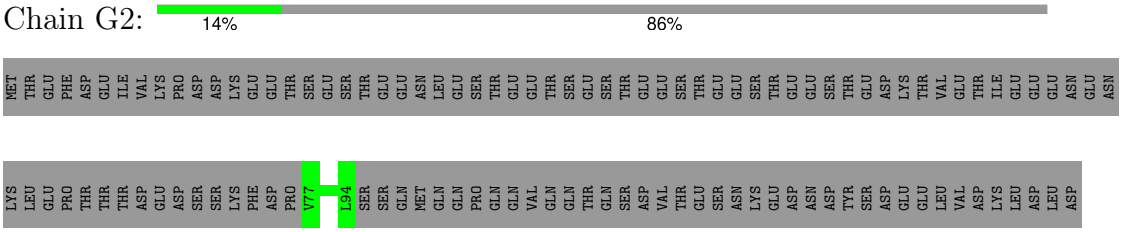
• Molecule 5: Minor structural protein

Chain OO:



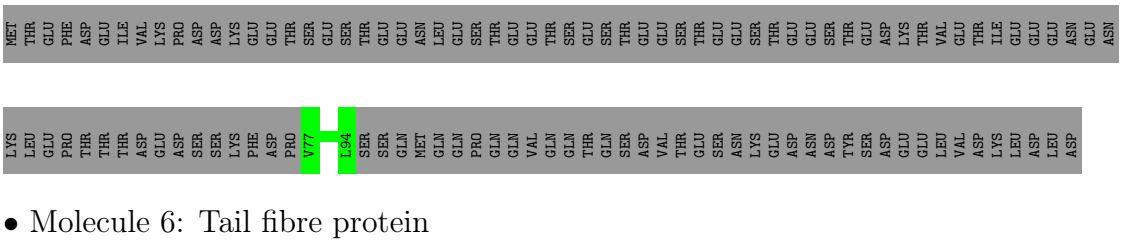
• Molecule 6: Tail fibre protein

Chain G2:



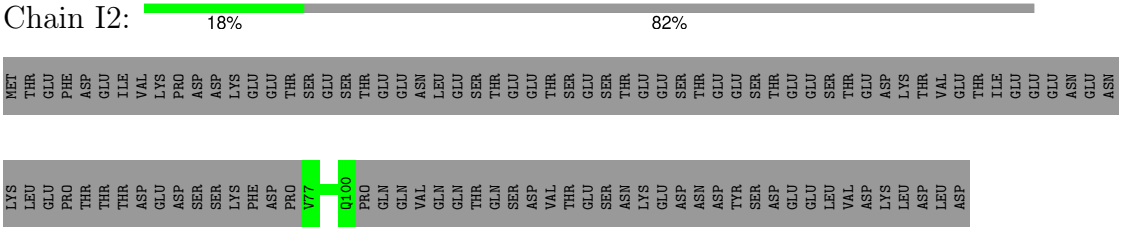
• Molecule 6: Tail fibre protein

Chain H2:



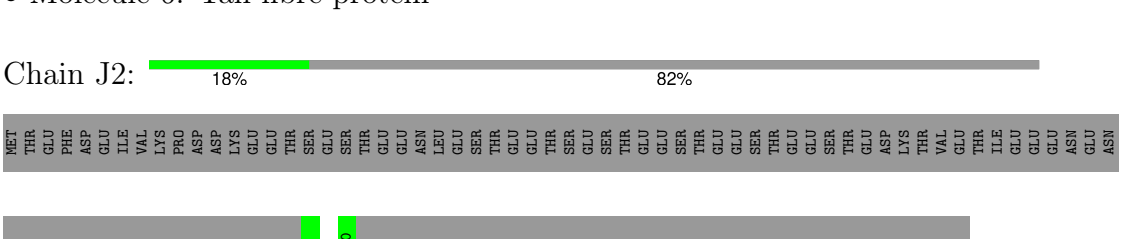
• Molecule 6: Tail fibre protein

Chain I2:



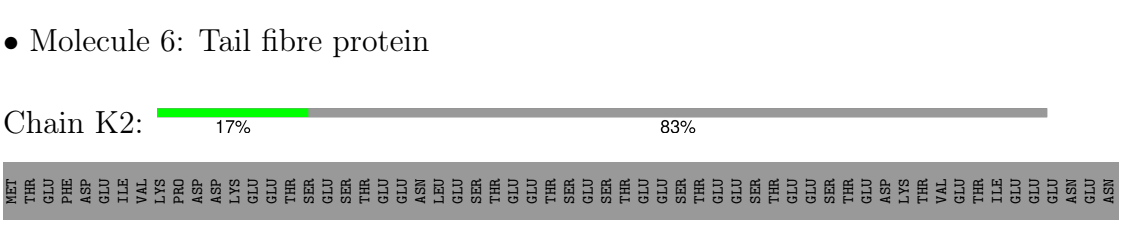
• Molecule 6: Tail fibre protein

Chain J2:



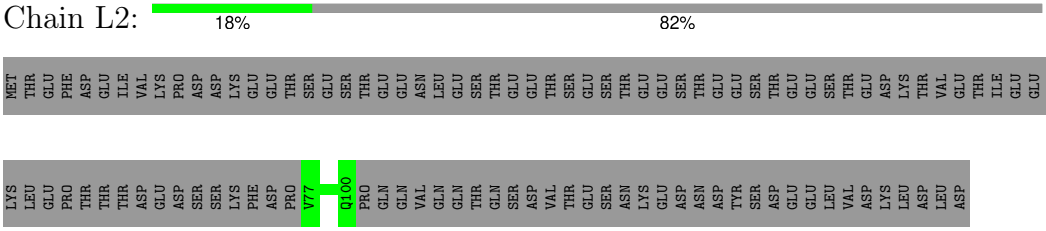
• Molecule 6: Tail fibre protein

Chain K2:



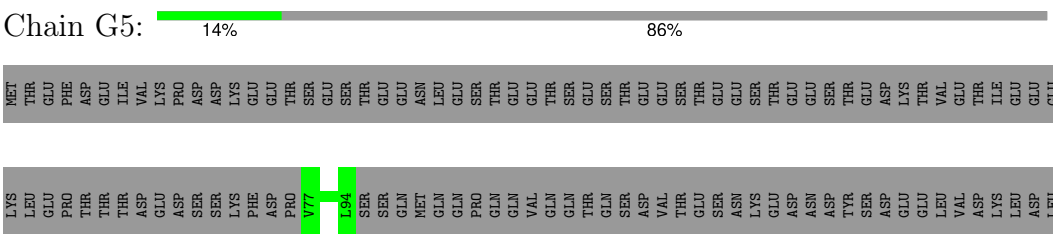
• Molecule 6: Tail fibre protein

Chain L2:



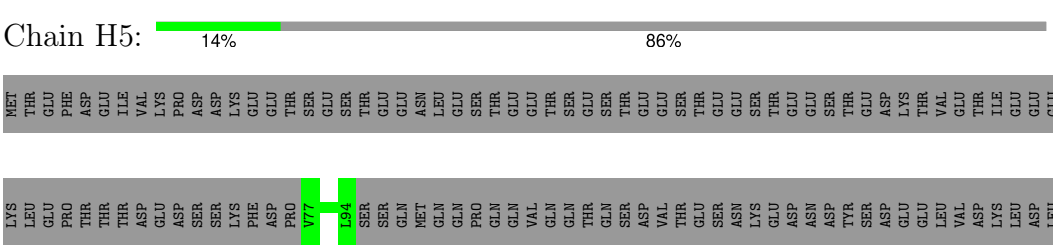
• Molecule 6: Tail fibre protein

Chain G5:



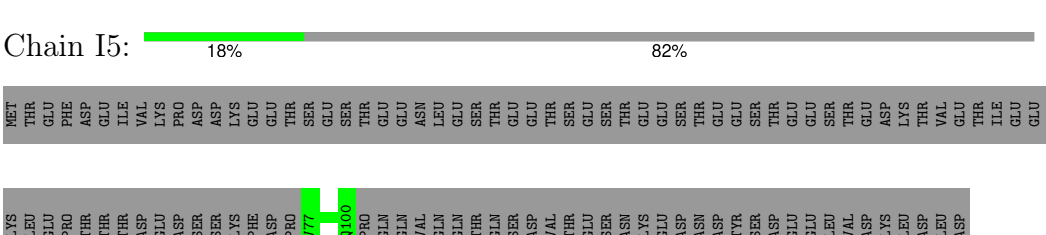
• Molecule 6: Tail fibre protein

Chain H5:



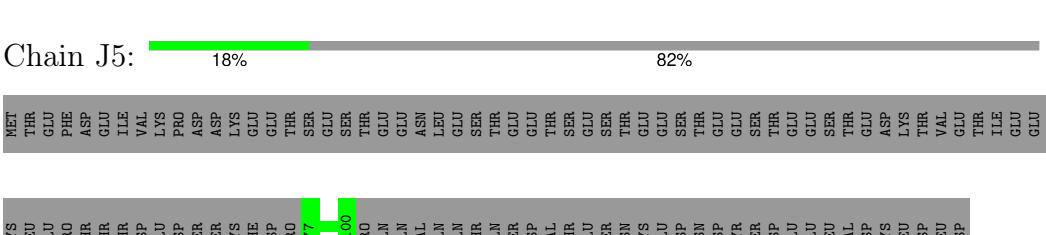
• Molecule 6: Tail fibre protein

Chain I5:



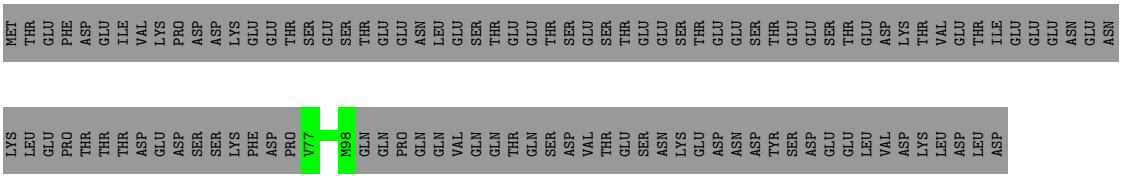
• Molecule 6: Tail fibre protein

Chain J5:



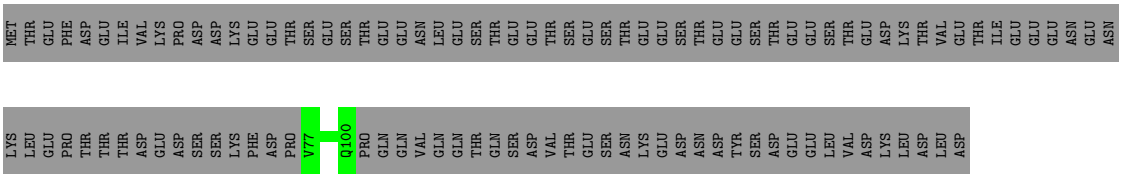
• Molecule 6: Tail fibre protein

Chain K5:



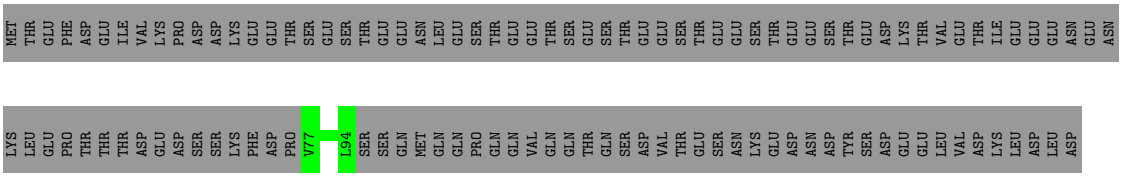
• Molecule 6: Tail fibre protein

Chain L5:



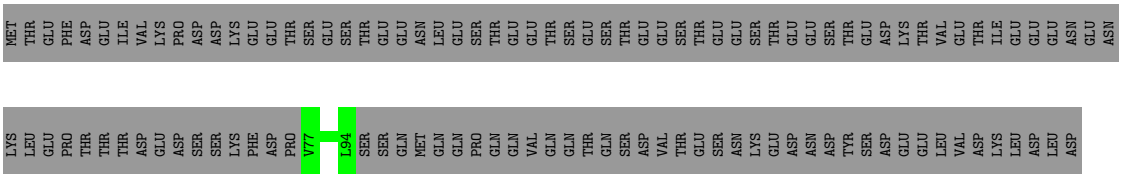
• Molecule 6: Tail fibre protein

Chain G9:



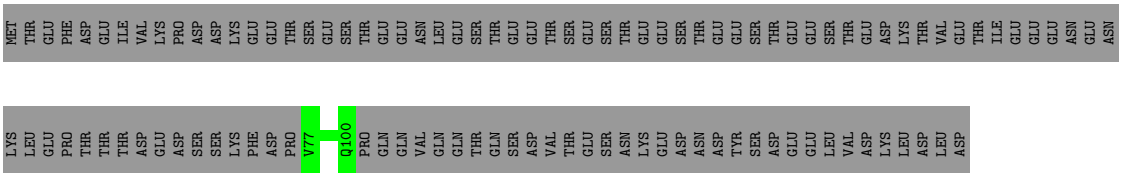
• Molecule 6: Tail fibre protein

Chain H9:



• Molecule 6: Tail fibre protein

Chain I9:



• Molecule 6: Tail fibre protein

Chain J9:

• Molecule 6: Tail fibre protein

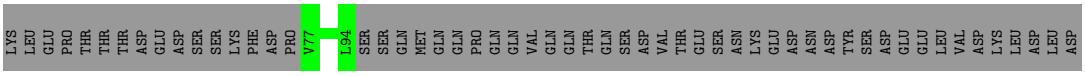
Chain K9:

• Molecule 6: Tail fibre protein

Chain L9:

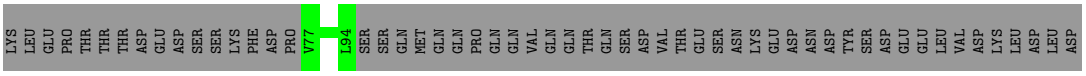
• Molecule 6: Tail fibre protein

Chain GA:



• Molecule 6: Tail fibre protein

Chain HA:

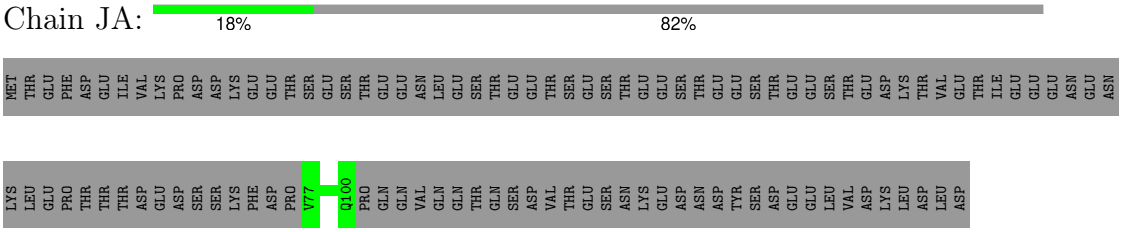


• Molecule 6: Tail fibre protein

Chain IA:

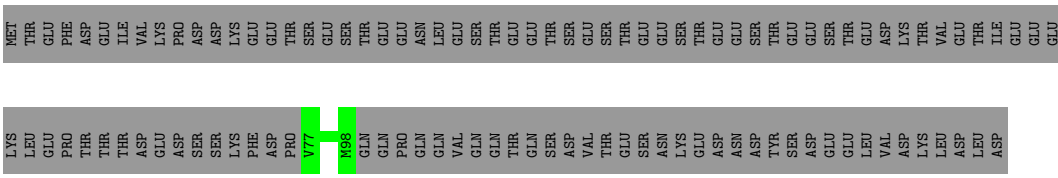
- Molecule 6: Tail fibre protein

Chain JA:



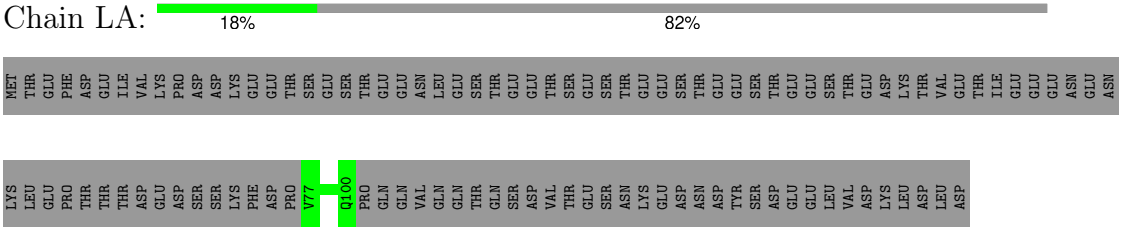
- Molecule 6: Tail fibre protein

Chain KA:



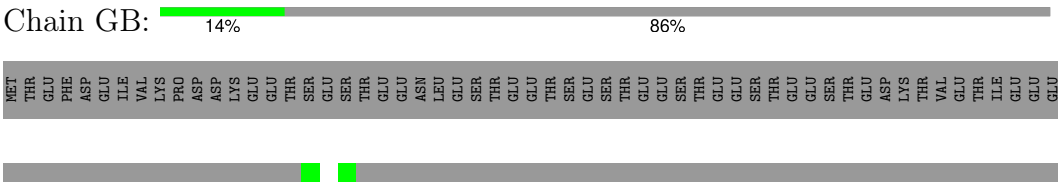
- Molecule 6: Tail fibre protein

Chain LA:



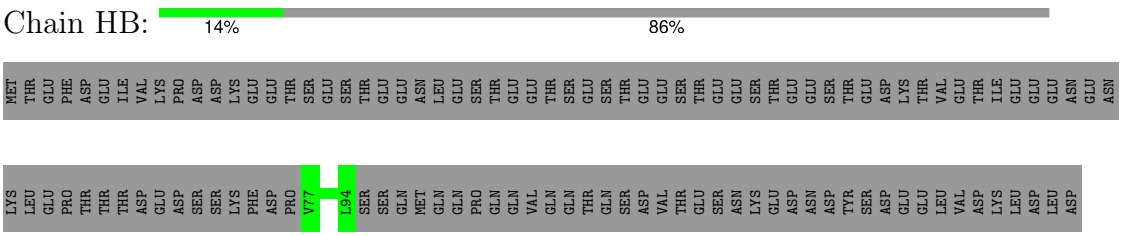
- Molecule 6: Tail fibre protein

Chain GB:



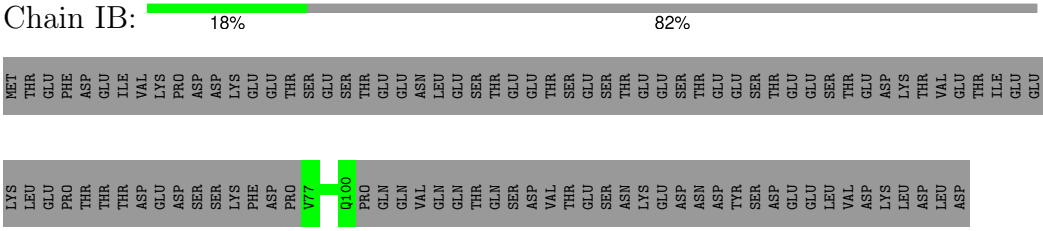
- Molecule 6: Tail fibre protein

Chain HB:



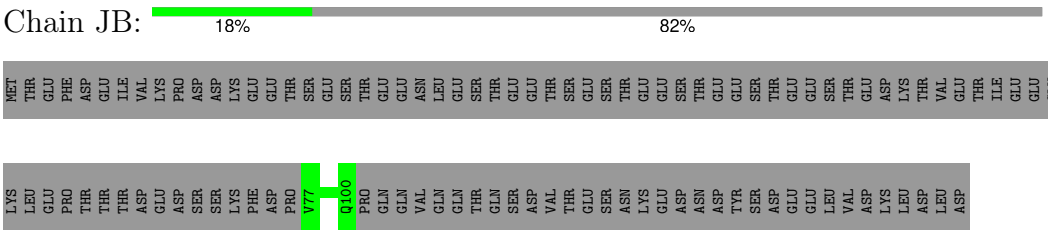
- Molecule 6: Tail fibre protein

Chain IB:



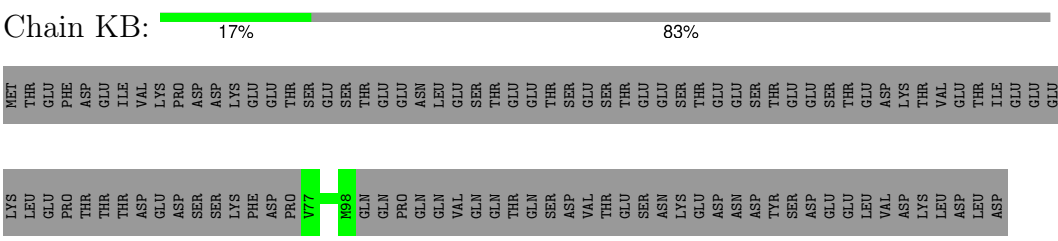
• Molecule 6: Tail fibre protein

Chain JB:



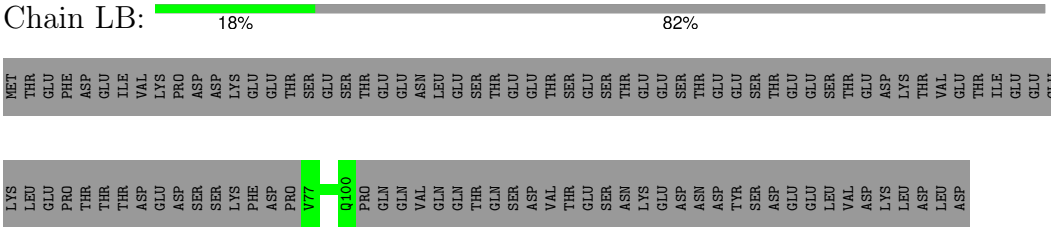
• Molecule 6: Tail fibre protein

Chain KB:



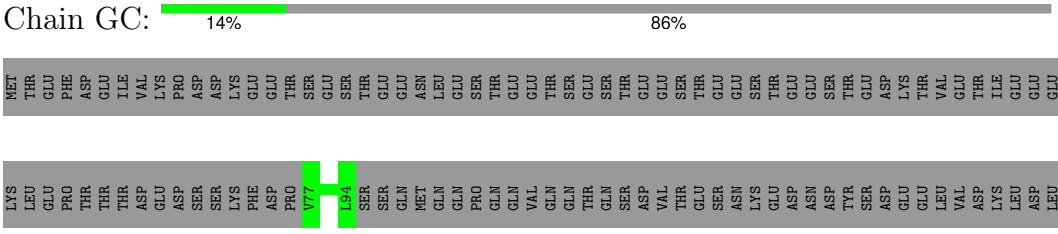
• Molecule 6: Tail fibre protein

Chain LB:



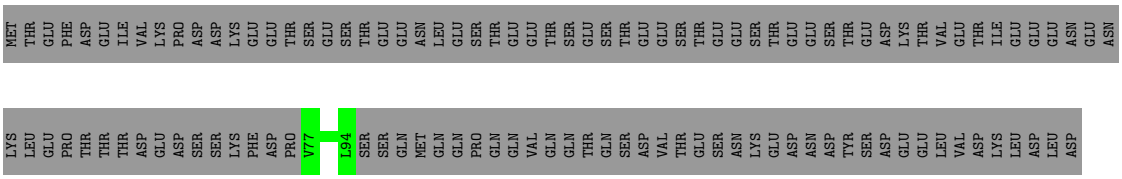
• Molecule 6: Tail fibre protein

Chain GC:



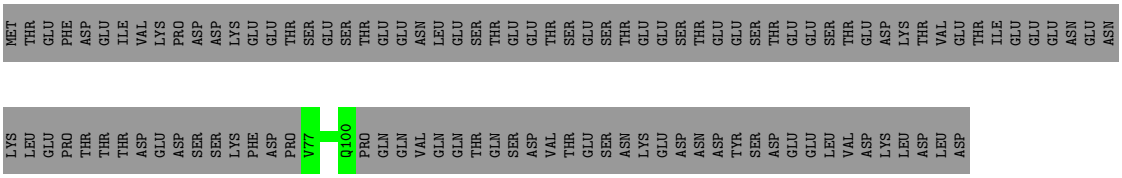
• Molecule 6: Tail fibre protein

Chain HC:



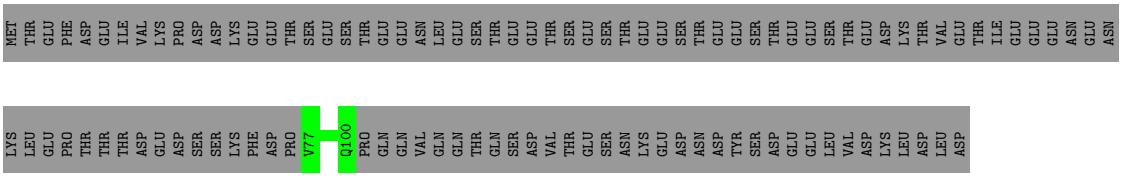
• Molecule 6: Tail fibre protein

Chain IC:



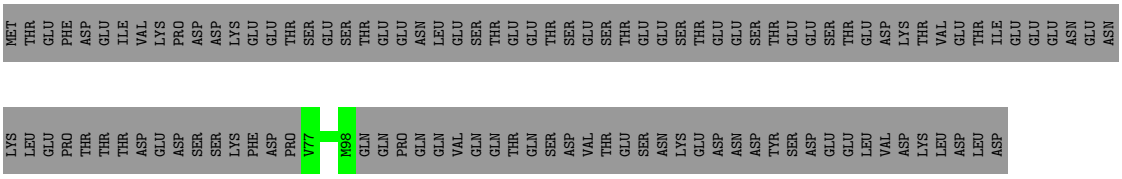
• Molecule 6: Tail fibre protein

Chain JC:



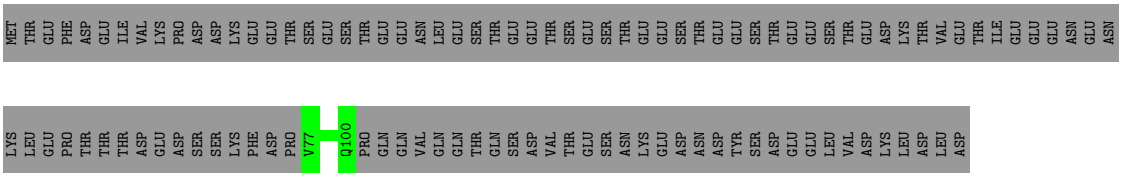
• Molecule 6: Tail fibre protein

Chain KC:



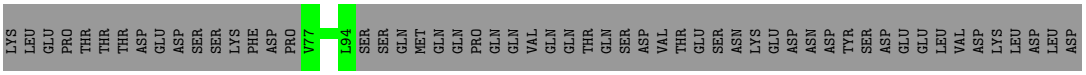
• Molecule 6: Tail fibre protein

Chain LC:



• Molecule 6: Tail fibre protein

Chain GF:



• Molecule 6: Tail fibre protein

Chain HF:

• Molecule 6: Tail fibre protein

Chain IF:

• Molecule 6: Tail fibre protein

Chain JF:

• Molecule 6: Tail fibre protein

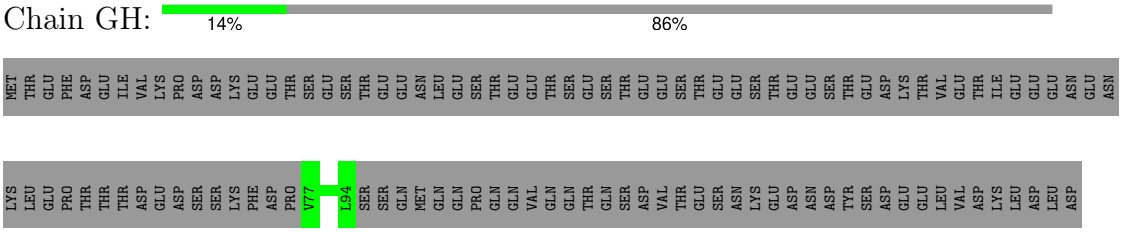
Chain KF:

• Molecule 6: Tail fibre protein

Chain LF:

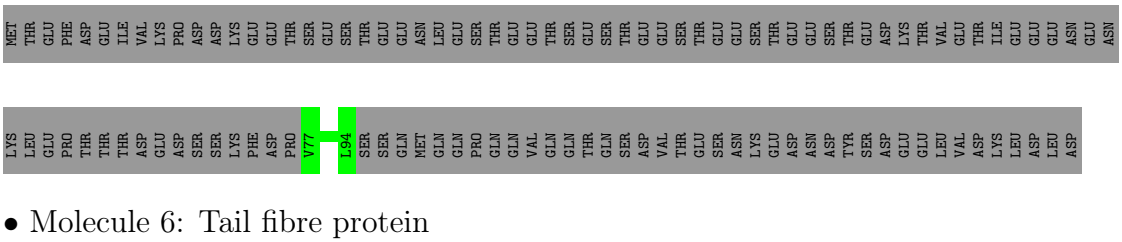
• Molecule 6: Tail fibre protein

Chain GH:



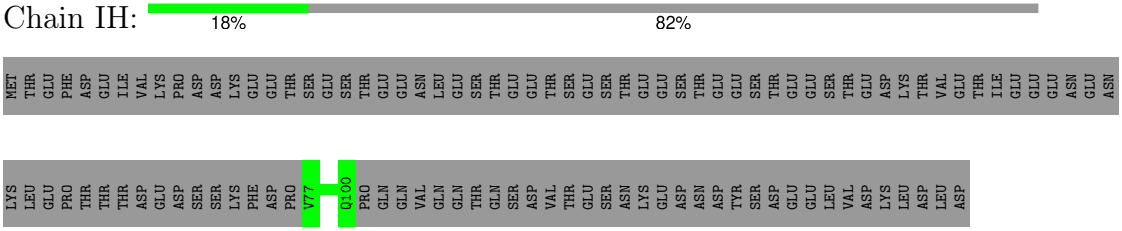
• Molecule 6: Tail fibre protein

Chain HH:



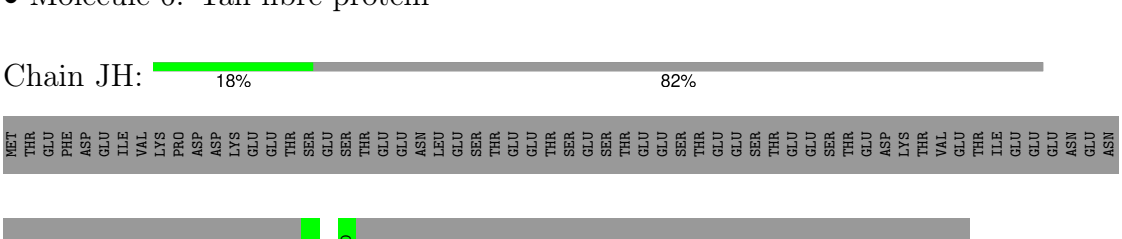
• Molecule 6: Tail fibre protein

Chain IH:



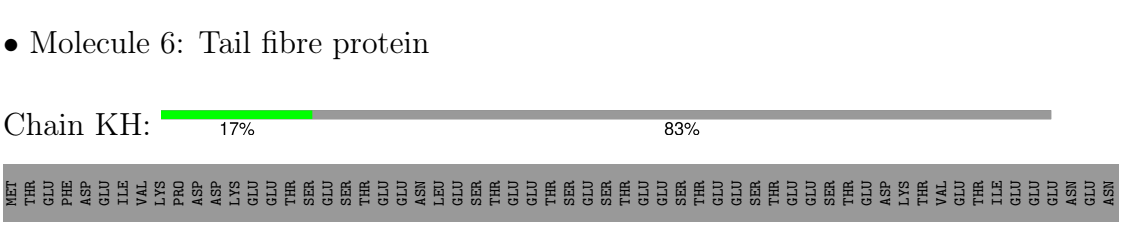
• Molecule 6: Tail fibre protein

Chain JH:



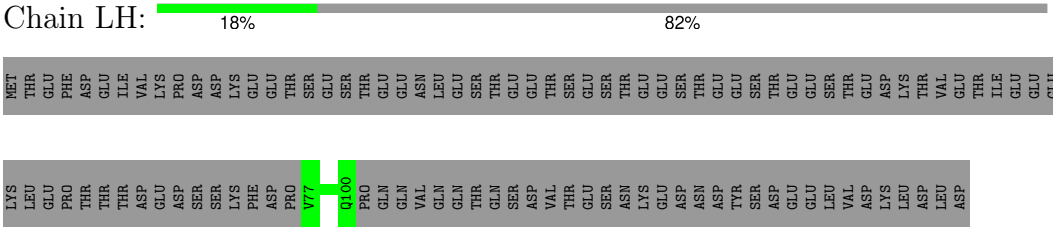
• Molecule 6: Tail fibre protein

Chain KH:



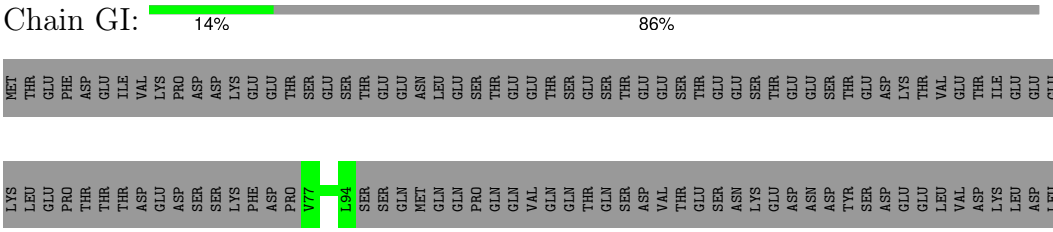
• Molecule 6: Tail fibre protein

Chain LH:



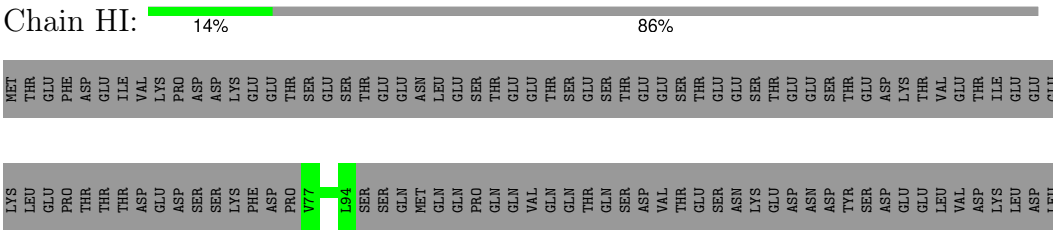
• Molecule 6: Tail fibre protein

Chain GI:



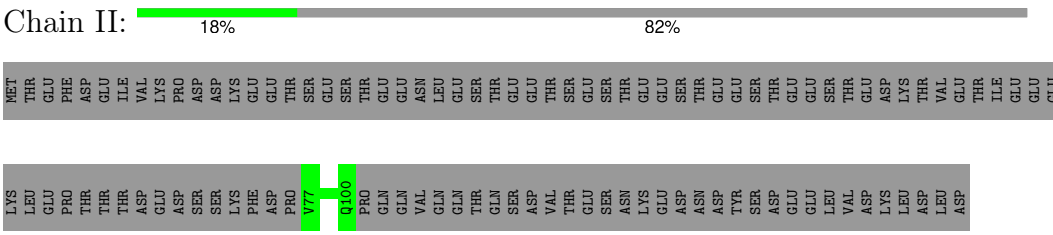
• Molecule 6: Tail fibre protein

Chain HI:



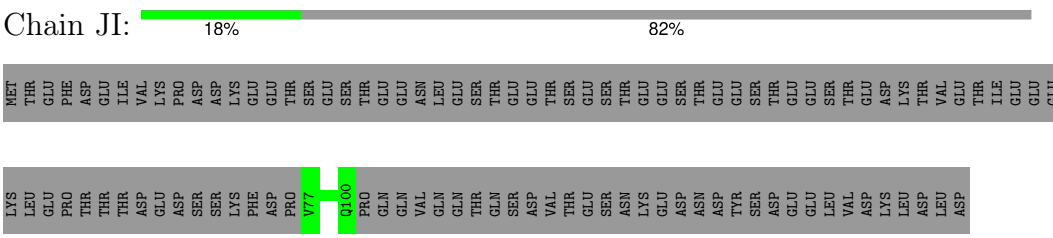
• Molecule 6: Tail fibre protein

Chain II:



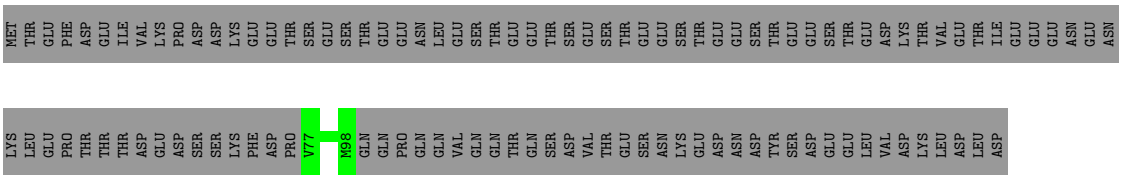
• Molecule 6: Tail fibre protein

Chain JI:



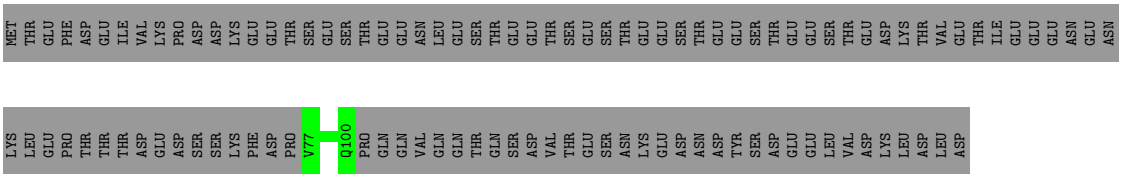
• Molecule 6: Tail fibre protein

Chain KI:



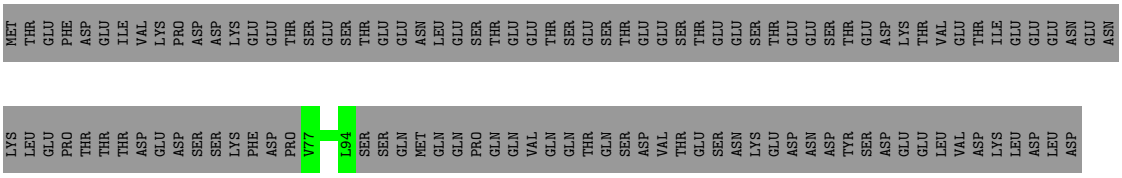
• Molecule 6: Tail fibre protein

Chain LI:



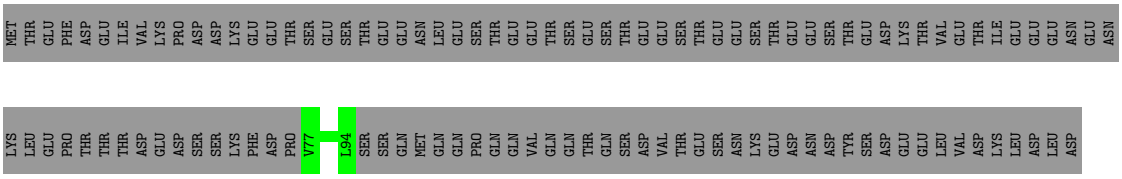
• Molecule 6: Tail fibre protein

Chain GM:



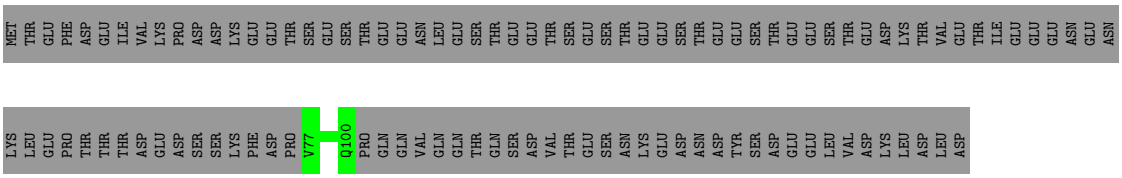
• Molecule 6: Tail fibre protein

Chain HM:



• Molecule 6: Tail fibre protein

Chain IM:



• Molecule 6: Tail fibre protein

Chain JM:

• Molecule 6: Tail fibre protein

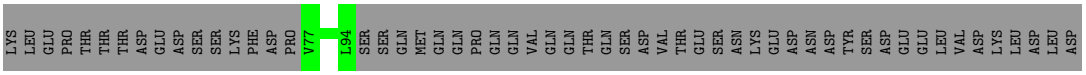
Chain KM:

• Molecule 6: Tail fibre protein

Chain LM:

• Molecule 6: Tail fibre protein

Chain GN:



• Molecule 6: Tail fibre protein

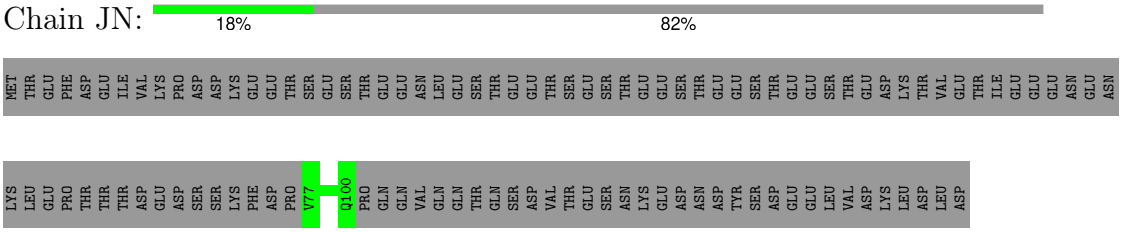
Chain HN:

• Molecule 6: Tail fibre protein

Chain IN:

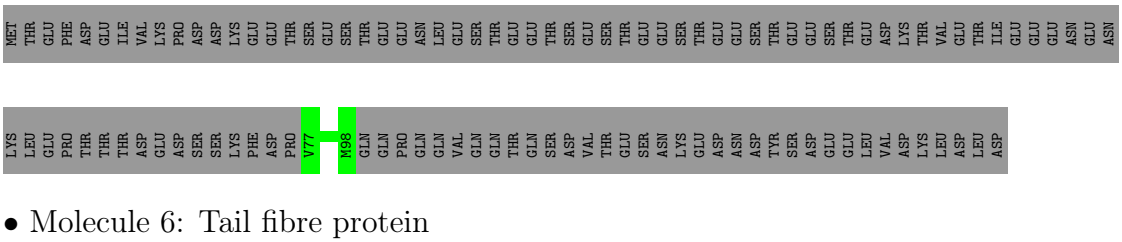
• Molecule 6: Tail fibre protein

Chain JN:



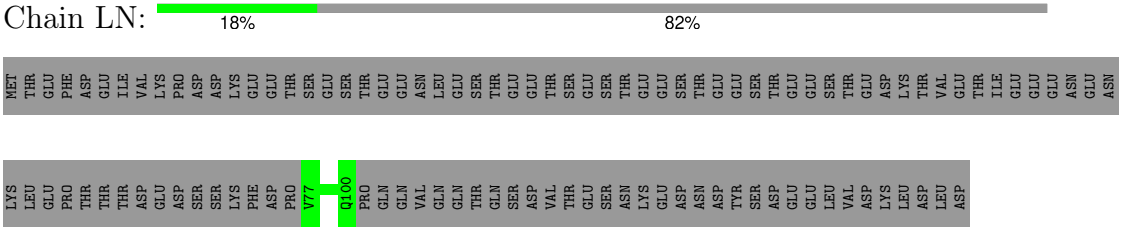
• Molecule 6: Tail fibre protein

Chain KN:



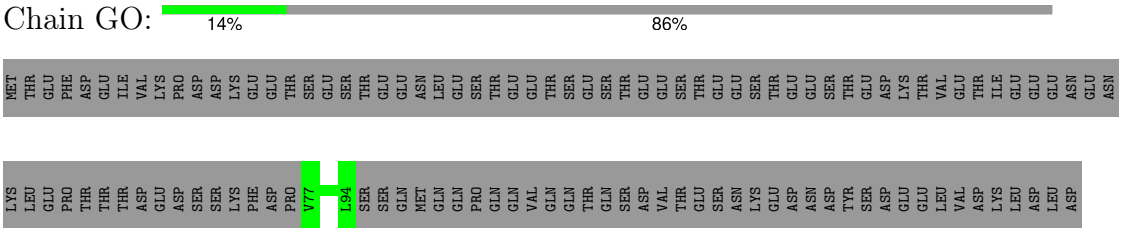
• Molecule 6: Tail fibre protein

Chain LN:



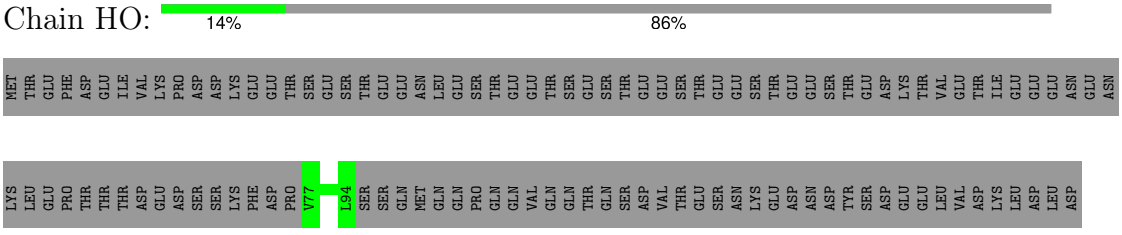
• Molecule 6: Tail fibre protein

Chain GO:



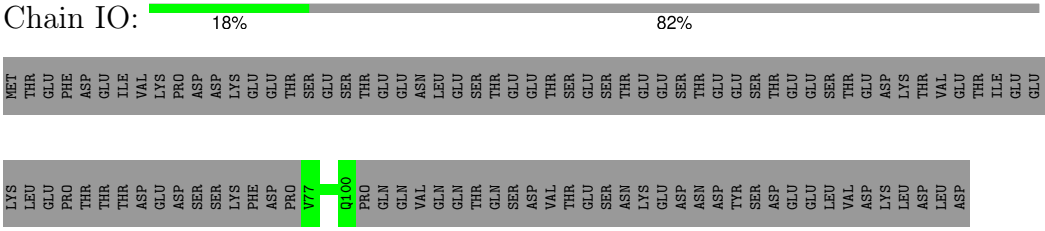
• Molecule 6: Tail fibre protein

Chain HO:



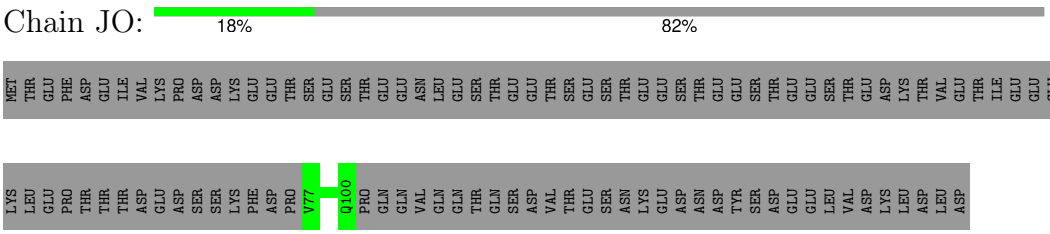
• Molecule 6: Tail fibre protein

Chain IO:



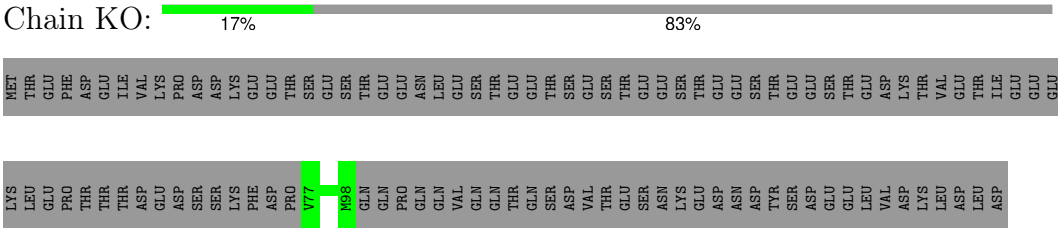
• Molecule 6: Tail fibre protein

Chain JO:



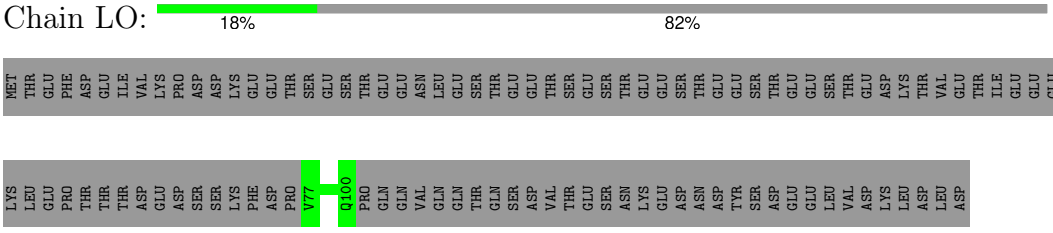
• Molecule 6: Tail fibre protein

Chain KO:



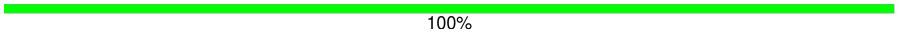
• Molecule 6: Tail fibre protein

Chain LO:



• Molecule 7: Head fiber protein

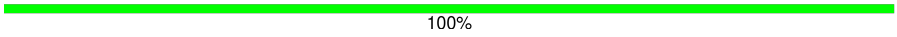
Chain ID:



There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

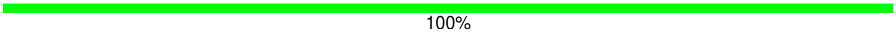
Chain OD:



There are no outlier residues recorded for this chain.

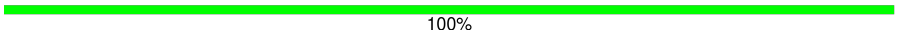
• Molecule 7: Head fiber protein

Chain SD:



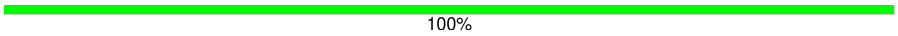
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain IJ: 

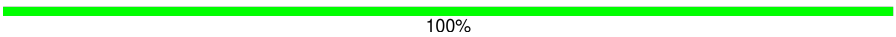
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain OJ: 

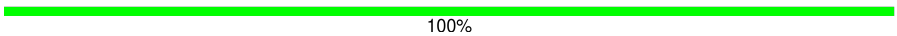
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain SJ: 

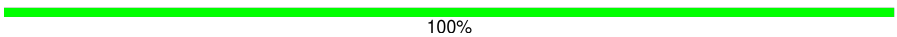
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain IK: 

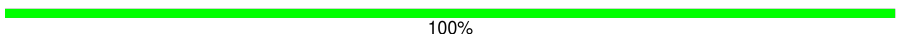
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain OK: 

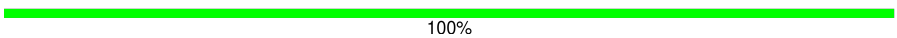
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain SK: 

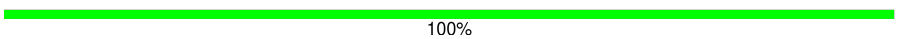
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain IP: 

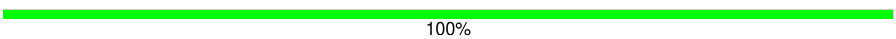
There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain OP: 

There are no outlier residues recorded for this chain.

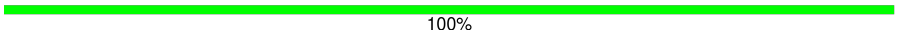
• Molecule 7: Head fiber protein

Chain SP: 

There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

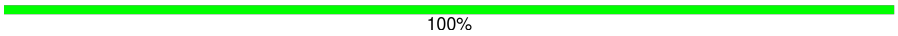
Chain HS:



There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

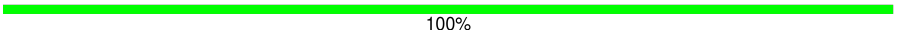
Chain NS:



There are no outlier residues recorded for this chain.

• Molecule 7: Head fiber protein

Chain SS:



There are no outlier residues recorded for this chain.

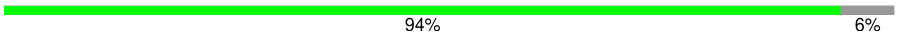
• Molecule 8: Inner core protein

Chain PD:

There are no outlier residues recorded for this chain.

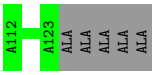
• Molecule 8: Inner core protein

Chain QD:



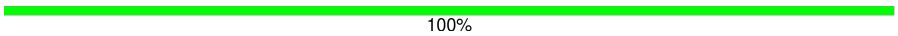
• Molecule 8: Inner core protein

Chain RD:



• Molecule 8: Inner core protein

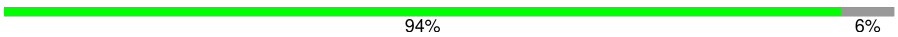
Chain PJ:



There are no outlier residues recorded for this chain.

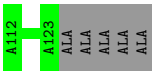
• Molecule 8: Inner core protein

Chain QJ:

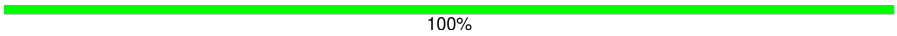


• Molecule 8: Inner core protein

Chain RJ: 

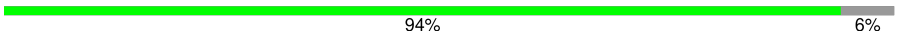


• Molecule 8: Inner core protein

Chain PK: 

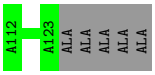
There are no outlier residues recorded for this chain.

• Molecule 8: Inner core protein

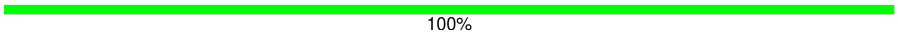
Chain QK: 

• Molecule 8: Inner core protein

Chain RK: 

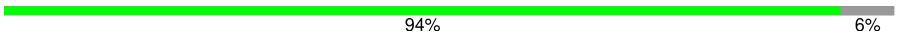


• Molecule 8: Inner core protein

Chain PP: 

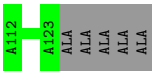
There are no outlier residues recorded for this chain.

• Molecule 8: Inner core protein

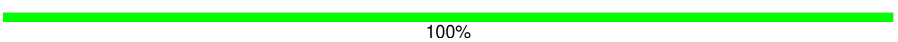
Chain QP: 

• Molecule 8: Inner core protein

Chain RP: 



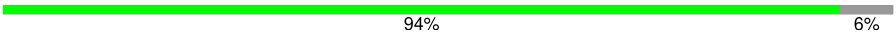
• Molecule 8: Inner core protein

Chain PS: 

There are no outlier residues recorded for this chain.

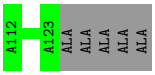
• Molecule 8: Inner core protein

Chain QS:



• Molecule 8: Inner core protein

Chain RS:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33612	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 ($e^-/Å^2$)	21	Depositor
Minimum defocus (nm)	1.0	Depositor
Maximum defocus (nm)	3.0	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A1	0.46	0/3244	0.66	4/4381 (0.1%)
1	A3	0.46	0/3244	0.66	4/4381 (0.1%)
1	A4	0.46	0/3244	0.66	4/4381 (0.1%)
1	A6	0.46	0/3244	0.66	4/4381 (0.1%)
1	A7	0.46	0/3244	0.66	4/4381 (0.1%)
1	A8	0.46	0/3244	0.66	4/4381 (0.1%)
1	AD	0.53	2/2875 (0.1%)	0.80	10/3887 (0.3%)
1	AE	0.47	0/3190	0.66	6/4310 (0.1%)
1	AG	0.46	0/3244	0.66	4/4381 (0.1%)
1	AJ	0.53	2/2875 (0.1%)	0.80	10/3887 (0.3%)
1	AK	0.53	2/2875 (0.1%)	0.80	10/3887 (0.3%)
1	AL	0.46	0/3244	0.66	4/4381 (0.1%)
1	AP	0.53	2/2875 (0.1%)	0.80	10/3887 (0.3%)
1	AQ	0.46	0/3244	0.66	4/4381 (0.1%)
1	AR	0.46	0/3244	0.66	4/4381 (0.1%)
1	AS	0.44	0/3257	0.69	3/4400 (0.1%)
1	B1	0.43	0/3190	0.62	2/4310 (0.0%)
1	B3	0.43	0/3190	0.62	2/4310 (0.0%)
1	B4	0.43	0/3190	0.62	2/4310 (0.0%)
1	B6	0.43	0/3190	0.62	2/4310 (0.0%)
1	B7	0.43	0/3190	0.62	2/4310 (0.0%)
1	B8	0.43	0/3190	0.62	2/4310 (0.0%)
1	BD	0.45	0/3257	0.69	3/4400 (0.1%)
1	BE	0.46	0/3244	0.66	4/4381 (0.1%)
1	BG	0.43	0/3190	0.62	2/4310 (0.0%)
1	BJ	0.45	0/3257	0.69	3/4400 (0.1%)
1	BK	0.45	0/3257	0.69	3/4400 (0.1%)
1	BL	0.43	0/3190	0.62	2/4310 (0.0%)
1	BP	0.45	0/3257	0.69	3/4400 (0.1%)
1	BQ	0.43	0/3190	0.62	2/4310 (0.0%)
1	BR	0.43	0/3190	0.62	2/4310 (0.0%)
1	BS	0.43	0/3202	0.67	4/4326 (0.1%)
1	C1	0.47	0/3190	0.66	6/4310 (0.1%)
1	C3	0.47	0/3190	0.66	6/4310 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	C4	0.47	0/3190	0.66	6/4310 (0.1%)
1	C6	0.47	0/3190	0.66	6/4310 (0.1%)
1	C7	0.47	0/3190	0.66	6/4310 (0.1%)
1	C8	0.47	0/3190	0.66	6/4310 (0.1%)
1	CD	0.43	0/3202	0.67	4/4326 (0.1%)
1	CE	0.43	0/3190	0.62	2/4310 (0.0%)
1	CG	0.47	0/3190	0.66	6/4310 (0.1%)
1	CJ	0.43	0/3202	0.67	4/4326 (0.1%)
1	CK	0.43	0/3202	0.67	4/4326 (0.1%)
1	CL	0.47	0/3190	0.66	6/4310 (0.1%)
1	CP	0.43	0/3202	0.67	4/4326 (0.1%)
1	CQ	0.47	0/3190	0.66	6/4310 (0.1%)
1	CR	0.47	0/3190	0.66	6/4310 (0.1%)
1	CS	0.44	0/3198	0.66	2/4321 (0.0%)
1	D1	0.41	0/3257	0.61	2/4400 (0.0%)
1	D3	0.41	0/3257	0.61	2/4400 (0.0%)
1	D4	0.41	0/3257	0.61	2/4400 (0.0%)
1	D6	0.41	0/3257	0.61	2/4400 (0.0%)
1	D7	0.41	0/3257	0.61	2/4400 (0.0%)
1	D8	0.41	0/3257	0.61	2/4400 (0.0%)
1	DD	0.44	0/3198	0.66	2/4321 (0.0%)
1	DE	0.41	0/3257	0.61	2/4400 (0.0%)
1	DG	0.41	0/3257	0.61	2/4400 (0.0%)
1	DJ	0.44	0/3198	0.66	2/4321 (0.0%)
1	DK	0.44	0/3198	0.66	2/4321 (0.0%)
1	DL	0.41	0/3257	0.61	2/4400 (0.0%)
1	DP	0.44	0/3198	0.66	2/4321 (0.0%)
1	DQ	0.41	0/3257	0.61	2/4400 (0.0%)
1	DR	0.41	0/3257	0.61	2/4400 (0.0%)
1	FE	0.41	0/3257	0.61	2/4400 (0.0%)
1	I1	0.47	0/3190	0.66	6/4310 (0.1%)
1	I3	0.47	0/3190	0.66	6/4310 (0.1%)
1	I4	0.47	0/3190	0.66	6/4310 (0.1%)
1	I6	0.47	0/3190	0.66	6/4310 (0.1%)
1	I7	0.47	0/3190	0.66	6/4310 (0.1%)
1	I8	0.47	0/3190	0.66	6/4310 (0.1%)
1	IG	0.47	0/3190	0.66	6/4310 (0.1%)
1	IL	0.47	0/3190	0.66	6/4310 (0.1%)
1	IQ	0.47	0/3190	0.66	6/4310 (0.1%)
1	IR	0.47	0/3190	0.66	6/4310 (0.1%)
1	IS	0.53	2/2875 (0.1%)	0.80	10/3887 (0.3%)
1	J1	0.46	0/3244	0.66	4/4381 (0.1%)
1	J3	0.46	0/3244	0.66	4/4381 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	J4	0.46	0/3244	0.66	4/4381 (0.1%)
1	J6	0.46	0/3244	0.66	4/4381 (0.1%)
1	J7	0.46	0/3244	0.66	4/4381 (0.1%)
1	J8	0.46	0/3244	0.66	4/4381 (0.1%)
1	JG	0.46	0/3244	0.66	4/4381 (0.1%)
1	JL	0.46	0/3244	0.66	4/4381 (0.1%)
1	JQ	0.46	0/3244	0.66	4/4381 (0.1%)
1	JR	0.46	0/3244	0.66	4/4381 (0.1%)
1	JS	0.42	0/3168	0.70	4/4279 (0.1%)
1	K1	0.43	0/3190	0.62	2/4310 (0.0%)
1	K3	0.43	0/3190	0.62	2/4310 (0.0%)
1	K4	0.43	0/3190	0.62	2/4310 (0.0%)
1	K6	0.43	0/3190	0.62	2/4310 (0.0%)
1	K7	0.43	0/3190	0.62	2/4310 (0.0%)
1	K8	0.43	0/3190	0.62	2/4310 (0.0%)
1	KD	0.42	0/3168	0.70	4/4279 (0.1%)
1	KE	0.47	0/3190	0.66	6/4310 (0.1%)
1	KG	0.43	0/3190	0.62	2/4310 (0.0%)
1	KJ	0.42	0/3168	0.70	4/4279 (0.1%)
1	KK	0.42	0/3168	0.70	4/4279 (0.1%)
1	KL	0.43	0/3190	0.62	2/4310 (0.0%)
1	KP	0.42	0/3168	0.70	4/4279 (0.1%)
1	KQ	0.43	0/3190	0.62	2/4310 (0.0%)
1	KR	0.43	0/3190	0.62	2/4310 (0.0%)
1	KS	0.43	0/3202	0.67	4/4326 (0.1%)
1	L1	0.41	0/3257	0.61	2/4400 (0.0%)
1	L3	0.41	0/3257	0.61	2/4400 (0.0%)
1	L4	0.41	0/3257	0.61	2/4400 (0.0%)
1	L6	0.41	0/3257	0.61	2/4400 (0.0%)
1	L7	0.41	0/3257	0.61	2/4400 (0.0%)
1	L8	0.41	0/3257	0.61	2/4400 (0.0%)
1	LD	0.44	0/3202	0.67	4/4326 (0.1%)
1	LE	0.46	0/3244	0.66	4/4381 (0.1%)
1	LG	0.41	0/3257	0.61	2/4400 (0.0%)
1	LJ	0.43	0/3202	0.67	4/4326 (0.1%)
1	LK	0.44	0/3202	0.67	4/4326 (0.1%)
1	LL	0.41	0/3257	0.61	2/4400 (0.0%)
1	LP	0.44	0/3202	0.67	4/4326 (0.1%)
1	LQ	0.41	0/3257	0.61	2/4400 (0.0%)
1	LR	0.41	0/3257	0.61	2/4400 (0.0%)
1	ME	0.43	0/3190	0.62	2/4310 (0.0%)
1	NE	0.41	0/3257	0.61	2/4400 (0.0%)
1	Q1	0.47	0/3190	0.66	6/4310 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Q3	0.47	0/3190	0.66	6/4310 (0.1%)
1	Q4	0.47	0/3190	0.66	6/4310 (0.1%)
1	Q6	0.47	0/3190	0.66	6/4310 (0.1%)
1	Q7	0.47	0/3190	0.66	6/4310 (0.1%)
1	Q8	0.47	0/3190	0.66	6/4310 (0.1%)
1	QG	0.47	0/3190	0.66	6/4310 (0.1%)
1	QL	0.47	0/3190	0.66	6/4310 (0.1%)
1	QQ	0.47	0/3190	0.66	6/4310 (0.1%)
1	QR	0.47	0/3190	0.66	6/4310 (0.1%)
1	R1	0.46	0/3244	0.66	4/4381 (0.1%)
1	R3	0.46	0/3244	0.66	4/4381 (0.1%)
1	R4	0.46	0/3244	0.66	4/4381 (0.1%)
1	R6	0.46	0/3244	0.66	4/4381 (0.1%)
1	R7	0.46	0/3244	0.66	4/4381 (0.1%)
1	R8	0.46	0/3244	0.66	4/4381 (0.1%)
1	RG	0.46	0/3244	0.66	4/4381 (0.1%)
1	RL	0.46	0/3244	0.66	4/4381 (0.1%)
1	RQ	0.46	0/3244	0.66	4/4381 (0.1%)
1	RR	0.46	0/3244	0.66	4/4381 (0.1%)
1	S1	0.43	0/3190	0.62	2/4310 (0.0%)
1	S3	0.43	0/3190	0.62	2/4310 (0.0%)
1	S4	0.43	0/3190	0.62	2/4310 (0.0%)
1	S6	0.43	0/3190	0.62	2/4310 (0.0%)
1	S7	0.43	0/3190	0.62	2/4310 (0.0%)
1	S8	0.43	0/3190	0.62	2/4310 (0.0%)
1	SE	0.47	0/3190	0.66	6/4310 (0.1%)
1	SG	0.43	0/3190	0.62	2/4310 (0.0%)
1	SL	0.43	0/3190	0.62	2/4310 (0.0%)
1	SQ	0.43	0/3190	0.62	2/4310 (0.0%)
1	SR	0.43	0/3190	0.62	2/4310 (0.0%)
1	T1	0.41	0/3257	0.61	2/4400 (0.0%)
1	T3	0.41	0/3257	0.61	2/4400 (0.0%)
1	T4	0.41	0/3257	0.61	2/4400 (0.0%)
1	T6	0.41	0/3257	0.61	2/4400 (0.0%)
1	T7	0.41	0/3257	0.61	2/4400 (0.0%)
1	T8	0.41	0/3257	0.61	2/4400 (0.0%)
1	TE	0.46	0/3244	0.66	4/4381 (0.1%)
1	TG	0.41	0/3257	0.61	2/4400 (0.0%)
1	TL	0.41	0/3257	0.61	2/4400 (0.0%)
1	TQ	0.41	0/3257	0.61	2/4400 (0.0%)
1	TR	0.41	0/3257	0.61	2/4400 (0.0%)
1	UE	0.43	0/3190	0.62	2/4310 (0.0%)
1	VE	0.41	0/3257	0.61	2/4400 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	X1	0.47	0/3190	0.66	6/4310 (0.1%)
1	X4	0.47	0/3190	0.66	6/4310 (0.1%)
1	Y1	0.46	0/3244	0.66	4/4381 (0.1%)
1	Y3	0.41	0/3257	0.61	2/4400 (0.0%)
1	Y4	0.46	0/3244	0.66	4/4381 (0.1%)
1	Y6	0.47	0/3190	0.66	6/4310 (0.1%)
1	Y7	0.47	0/3190	0.66	6/4310 (0.1%)
1	Y8	0.47	0/3190	0.66	6/4310 (0.1%)
1	YG	0.47	0/3190	0.66	6/4310 (0.1%)
1	YL	0.47	0/3190	0.66	6/4310 (0.1%)
1	YQ	0.41	0/3257	0.61	2/4400 (0.0%)
1	YR	0.47	0/3190	0.66	6/4310 (0.1%)
1	Z1	0.43	0/3190	0.62	2/4310 (0.0%)
1	Z4	0.43	0/3190	0.62	2/4310 (0.0%)
1	Z6	0.46	0/3244	0.66	4/4381 (0.1%)
1	Z7	0.46	0/3244	0.66	4/4381 (0.1%)
1	Z8	0.46	0/3244	0.66	4/4381 (0.1%)
1	ZG	0.46	0/3244	0.66	4/4381 (0.1%)
1	ZL	0.46	0/3244	0.66	4/4381 (0.1%)
1	ZR	0.46	0/3244	0.66	4/4381 (0.1%)
1	a1	0.41	0/3257	0.61	2/4400 (0.0%)
1	a4	0.41	0/3257	0.61	2/4400 (0.0%)
1	a6	0.43	0/3190	0.62	2/4310 (0.0%)
1	a7	0.43	0/3190	0.62	2/4310 (0.0%)
1	a8	0.43	0/3190	0.62	2/4310 (0.0%)
1	aE	0.47	0/3190	0.66	6/4310 (0.1%)
1	aG	0.43	0/3190	0.62	2/4310 (0.0%)
1	aL	0.43	0/3190	0.62	2/4310 (0.0%)
1	aR	0.43	0/3190	0.62	2/4310 (0.0%)
1	b3	0.41	0/3257	0.61	2/4400 (0.0%)
1	b6	0.41	0/3257	0.61	2/4400 (0.0%)
1	b7	0.41	0/3257	0.61	2/4400 (0.0%)
1	b8	0.41	0/3257	0.61	2/4400 (0.0%)
1	bE	0.46	0/3244	0.66	4/4381 (0.1%)
1	bG	0.41	0/3257	0.61	2/4400 (0.0%)
1	bL	0.41	0/3257	0.61	2/4400 (0.0%)
1	bQ	0.47	0/3190	0.66	6/4310 (0.1%)
1	bR	0.41	0/3257	0.61	2/4400 (0.0%)
1	cE	0.43	0/3190	0.62	2/4310 (0.0%)
1	cQ	0.46	0/3244	0.66	4/4381 (0.1%)
1	dE	0.41	0/3257	0.61	2/4400 (0.0%)
1	dQ	0.43	0/3190	0.62	2/4310 (0.0%)
1	eQ	0.41	0/3257	0.61	2/4400 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	f1	0.47	0/3190	0.66	6/4310 (0.1%)
1	f4	0.47	0/3190	0.66	6/4310 (0.1%)
1	g1	0.46	0/3244	0.66	4/4381 (0.1%)
1	g4	0.46	0/3244	0.66	4/4381 (0.1%)
1	g6	0.47	0/3190	0.66	6/4310 (0.1%)
1	g7	0.47	0/3190	0.66	6/4310 (0.1%)
1	g8	0.47	0/3190	0.66	6/4310 (0.1%)
1	gG	0.47	0/3190	0.66	6/4310 (0.1%)
1	gL	0.41	0/3257	0.61	2/4400 (0.0%)
1	gR	0.47	0/3190	0.66	6/4310 (0.1%)
1	h1	0.43	0/3190	0.62	2/4310 (0.0%)
1	h4	0.43	0/3190	0.62	2/4310 (0.0%)
1	h6	0.46	0/3244	0.66	4/4381 (0.1%)
1	h7	0.46	0/3244	0.66	4/4381 (0.1%)
1	h8	0.46	0/3244	0.66	4/4381 (0.1%)
1	hG	0.46	0/3244	0.66	4/4381 (0.1%)
1	hR	0.46	0/3244	0.66	4/4381 (0.1%)
1	i1	0.41	0/3257	0.61	2/4400 (0.0%)
1	i4	0.41	0/3257	0.61	2/4400 (0.0%)
1	i6	0.43	0/3190	0.62	2/4310 (0.0%)
1	i7	0.43	0/3190	0.62	2/4310 (0.0%)
1	i8	0.43	0/3190	0.62	2/4310 (0.0%)
1	iG	0.43	0/3190	0.62	2/4310 (0.0%)
1	iR	0.43	0/3190	0.62	2/4310 (0.0%)
1	j6	0.41	0/3257	0.61	2/4400 (0.0%)
1	j7	0.41	0/3257	0.61	2/4400 (0.0%)
1	j8	0.41	0/3257	0.61	2/4400 (0.0%)
1	jG	0.41	0/3257	0.61	2/4400 (0.0%)
1	jR	0.41	0/3257	0.61	2/4400 (0.0%)
2	DS	0.37	0/441	0.72	0/587
2	E1	0.56	0/436	1.03	3/581 (0.5%)
2	E3	0.56	0/436	1.03	3/581 (0.5%)
2	E4	0.56	0/436	1.03	3/581 (0.5%)
2	E6	0.56	0/436	1.03	3/581 (0.5%)
2	E7	0.56	0/436	1.03	3/581 (0.5%)
2	E8	0.56	0/436	1.03	3/581 (0.5%)
2	ED	0.37	0/441	0.71	0/587
2	EE	0.56	0/436	1.03	3/581 (0.5%)
2	EG	0.56	0/436	1.03	3/581 (0.5%)
2	EJ	0.37	0/441	0.71	0/587
2	EK	0.37	0/441	0.72	0/587
2	EL	0.56	0/436	1.03	3/581 (0.5%)
2	EP	0.37	0/441	0.72	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	EQ	0.56	0/436	1.03	3/581 (0.5%)
2	ER	0.56	0/436	1.03	3/581 (0.5%)
2	ES	0.36	0/441	0.93	1/587 (0.2%)
2	F1	0.39	0/440	0.79	1/586 (0.2%)
2	F3	0.39	0/440	0.79	1/586 (0.2%)
2	F4	0.39	0/440	0.79	1/586 (0.2%)
2	F6	0.39	0/440	0.79	1/586 (0.2%)
2	F7	0.39	0/440	0.79	1/586 (0.2%)
2	F8	0.39	0/440	0.79	1/586 (0.2%)
2	FD	0.36	0/441	0.93	1/587 (0.2%)
2	FG	0.39	0/440	0.79	1/586 (0.2%)
2	FJ	0.36	0/441	0.93	1/587 (0.2%)
2	FK	0.36	0/441	0.93	1/587 (0.2%)
2	FL	0.39	0/440	0.79	1/586 (0.2%)
2	FP	0.36	0/441	0.93	1/587 (0.2%)
2	FQ	0.39	0/440	0.79	1/586 (0.2%)
2	FR	0.39	0/440	0.79	1/586 (0.2%)
2	FS	0.40	0/239	0.78	0/320
2	G1	0.33	0/222	0.69	0/293
2	G3	0.33	0/222	0.68	0/293
2	G4	0.33	0/222	0.69	0/293
2	G6	0.33	0/222	0.69	0/293
2	G7	0.33	0/222	0.69	0/293
2	G8	0.33	0/222	0.68	0/293
2	GD	0.40	0/239	0.78	0/320
2	GE	0.33	0/222	0.69	0/293
2	GG	0.33	0/222	0.69	0/293
2	GJ	0.40	0/239	0.78	0/320
2	GK	0.40	0/239	0.78	0/320
2	GL	0.33	0/222	0.69	0/293
2	GP	0.40	0/239	0.78	0/320
2	GQ	0.33	0/222	0.69	0/293
2	GR	0.33	0/222	0.68	0/293
2	GS	0.35	0/437	0.82	0/582
2	H1	0.41	0/439	0.76	0/585
2	H3	0.41	0/439	0.76	0/585
2	H4	0.41	0/439	0.76	0/585
2	H6	0.41	0/439	0.76	0/585
2	H7	0.41	0/439	0.76	0/585
2	H8	0.41	0/439	0.76	0/585
2	HD	0.36	0/437	0.82	0/582
2	HE	0.39	0/440	0.79	1/586 (0.2%)
2	HG	0.41	0/439	0.76	0/585

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	HJ	0.36	0/437	0.82	0/582
2	HK	0.36	0/437	0.82	0/582
2	HL	0.41	0/439	0.76	0/585
2	HP	0.36	0/437	0.82	0/582
2	HQ	0.41	0/439	0.76	0/585
2	HR	0.41	0/439	0.76	0/585
2	IE	0.33	0/222	0.68	0/293
2	JE	0.41	0/439	0.76	0/585
2	LS	0.37	0/441	0.79	0/587
2	M1	0.56	0/436	1.03	3/581 (0.5%)
2	M3	0.56	0/436	1.03	3/581 (0.5%)
2	M4	0.56	0/436	1.03	3/581 (0.5%)
2	M6	0.56	0/436	1.03	3/581 (0.5%)
2	M7	0.56	0/436	1.03	3/581 (0.5%)
2	M8	0.56	0/436	1.03	3/581 (0.5%)
2	MD	0.37	0/441	0.79	0/587
2	MG	0.56	0/436	1.03	3/581 (0.5%)
2	MJ	0.37	0/441	0.79	0/587
2	MK	0.37	0/441	0.79	0/587
2	ML	0.56	0/436	1.03	3/581 (0.5%)
2	MP	0.37	0/441	0.79	0/587
2	MQ	0.56	0/436	1.03	3/581 (0.5%)
2	MR	0.56	0/436	1.03	3/581 (0.5%)
2	MS	0.40	0/441	0.88	1/587 (0.2%)
2	N1	0.39	0/440	0.79	1/586 (0.2%)
2	N3	0.39	0/440	0.79	1/586 (0.2%)
2	N4	0.39	0/440	0.79	1/586 (0.2%)
2	N6	0.39	0/440	0.79	1/586 (0.2%)
2	N7	0.39	0/440	0.79	1/586 (0.2%)
2	N8	0.39	0/440	0.79	1/586 (0.2%)
2	ND	0.40	0/441	0.88	1/587 (0.2%)
2	NG	0.39	0/440	0.79	1/586 (0.2%)
2	NJ	0.40	0/441	0.88	1/587 (0.2%)
2	NK	0.40	0/441	0.88	1/587 (0.2%)
2	NL	0.39	0/440	0.79	1/586 (0.2%)
2	NP	0.40	0/441	0.88	1/587 (0.2%)
2	NQ	0.39	0/440	0.79	1/586 (0.2%)
2	NR	0.39	0/440	0.79	1/586 (0.2%)
2	O1	0.33	0/222	0.68	0/293
2	O3	0.33	0/222	0.69	0/293
2	O4	0.33	0/222	0.68	0/293
2	O6	0.33	0/222	0.69	0/293
2	O7	0.33	0/222	0.69	0/293

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	O8	0.33	0/222	0.68	0/293
2	OE	0.56	0/436	1.03	3/581 (0.5%)
2	OG	0.33	0/222	0.68	0/293
2	OL	0.33	0/222	0.69	0/293
2	OQ	0.33	0/222	0.68	0/293
2	OR	0.33	0/222	0.69	0/293
2	P1	0.41	0/439	0.76	0/585
2	P3	0.41	0/439	0.76	0/585
2	P4	0.41	0/439	0.76	0/585
2	P6	0.41	0/439	0.76	0/585
2	P7	0.41	0/439	0.76	0/585
2	P8	0.41	0/439	0.76	0/585
2	PE	0.39	0/440	0.79	1/586 (0.2%)
2	PG	0.41	0/439	0.76	0/585
2	PL	0.41	0/439	0.76	0/585
2	PQ	0.41	0/439	0.76	0/585
2	PR	0.41	0/439	0.76	0/585
2	QE	0.33	0/222	0.68	0/293
2	RE	0.41	0/439	0.76	0/585
2	U1	0.39	0/440	0.79	1/586 (0.2%)
2	U3	0.56	0/436	1.03	3/581 (0.5%)
2	U4	0.39	0/440	0.79	1/586 (0.2%)
2	U6	0.56	0/436	1.03	3/581 (0.5%)
2	U7	0.56	0/436	1.03	3/581 (0.5%)
2	U8	0.56	0/436	1.03	3/581 (0.5%)
2	UG	0.56	0/436	1.03	3/581 (0.5%)
2	UL	0.56	0/436	1.03	3/581 (0.5%)
2	UQ	0.56	0/436	1.03	3/581 (0.5%)
2	UR	0.56	0/436	1.03	3/581 (0.5%)
2	V1	0.33	0/222	0.69	0/293
2	V3	0.39	0/440	0.79	1/586 (0.2%)
2	V4	0.33	0/222	0.69	0/293
2	V6	0.39	0/440	0.79	1/586 (0.2%)
2	V7	0.39	0/440	0.79	1/586 (0.2%)
2	V8	0.39	0/440	0.79	1/586 (0.2%)
2	VG	0.39	0/440	0.79	1/586 (0.2%)
2	VL	0.39	0/440	0.79	1/586 (0.2%)
2	VQ	0.39	0/440	0.79	1/586 (0.2%)
2	VR	0.39	0/440	0.79	1/586 (0.2%)
2	W1	0.41	0/439	0.76	0/585
2	W3	0.33	0/222	0.68	0/293
2	W4	0.41	0/439	0.76	0/585
2	W6	0.33	0/222	0.69	0/293

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	W7	0.33	0/222	0.69	0/293
2	W8	0.33	0/222	0.69	0/293
2	WE	0.56	0/436	1.03	3/581 (0.5%)
2	WG	0.33	0/222	0.69	0/293
2	WL	0.33	0/222	0.69	0/293
2	WQ	0.33	0/222	0.69	0/293
2	WR	0.33	0/222	0.69	0/293
2	X3	0.41	0/439	0.76	0/585
2	X6	0.41	0/439	0.76	0/585
2	X7	0.41	0/439	0.76	0/585
2	X8	0.41	0/439	0.76	0/585
2	XE	0.39	0/440	0.79	1/586 (0.2%)
2	XG	0.41	0/439	0.76	0/585
2	XL	0.41	0/439	0.76	0/585
2	XQ	0.41	0/439	0.76	0/585
2	XR	0.41	0/439	0.76	0/585
2	YE	0.33	0/222	0.68	0/293
2	Z3	0.56	0/436	1.03	3/581 (0.5%)
2	ZE	0.41	0/439	0.76	0/585
2	ZQ	0.56	0/436	1.03	3/581 (0.5%)
2	a3	0.33	0/222	0.68	0/293
2	aQ	0.33	0/222	0.69	0/293
2	b1	0.56	0/436	1.03	3/581 (0.5%)
2	b4	0.56	0/436	1.03	3/581 (0.5%)
2	c1	0.39	0/440	0.79	1/586 (0.2%)
2	c3	0.56	0/436	1.03	3/581 (0.5%)
2	c4	0.39	0/440	0.79	1/586 (0.2%)
2	c6	0.56	0/436	1.03	3/581 (0.5%)
2	c7	0.56	0/436	1.03	3/581 (0.5%)
2	c8	0.56	0/436	1.03	3/581 (0.5%)
2	cG	0.56	0/436	1.03	3/581 (0.5%)
2	cL	0.56	0/436	1.03	3/581 (0.5%)
2	cR	0.56	0/436	1.03	3/581 (0.5%)
2	d1	0.33	0/222	0.69	0/293
2	d3	0.33	0/222	0.68	0/293
2	d4	0.33	0/222	0.68	0/293
2	d6	0.39	0/440	0.79	1/586 (0.2%)
2	d7	0.39	0/440	0.79	1/586 (0.2%)
2	d8	0.39	0/440	0.79	1/586 (0.2%)
2	dG	0.39	0/440	0.79	1/586 (0.2%)
2	dL	0.39	0/440	0.79	1/586 (0.2%)
2	dR	0.39	0/440	0.79	1/586 (0.2%)
2	e1	0.41	0/439	0.76	0/585

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	e4	0.41	0/439	0.76	0/585
2	e6	0.33	0/222	0.68	0/293
2	e7	0.33	0/222	0.69	0/293
2	e8	0.33	0/222	0.68	0/293
2	eE	0.56	0/436	1.03	3/581 (0.5%)
2	eG	0.33	0/222	0.68	0/293
2	eL	0.33	0/222	0.69	0/293
2	eR	0.33	0/222	0.69	0/293
2	f6	0.41	0/439	0.76	0/585
2	f7	0.41	0/439	0.76	0/585
2	f8	0.41	0/439	0.76	0/585
2	fE	0.39	0/440	0.79	1/586 (0.2%)
2	fG	0.41	0/439	0.76	0/585
2	fL	0.41	0/439	0.76	0/585
2	fQ	0.56	0/436	1.03	3/581 (0.5%)
2	fR	0.41	0/439	0.76	0/585
2	gE	0.33	0/222	0.68	0/293
2	gQ	0.39	0/440	0.79	1/586 (0.2%)
2	hE	0.41	0/439	0.76	0/585
2	hL	0.56	0/436	1.03	3/581 (0.5%)
2	hQ	0.33	0/222	0.69	0/293
2	iL	0.33	0/222	0.69	0/293
2	iQ	0.41	0/439	0.76	0/585
2	j1	0.56	0/436	1.03	3/581 (0.5%)
2	j4	0.39	0/440	0.79	1/586 (0.2%)
2	k1	0.39	0/440	0.79	1/586 (0.2%)
2	k4	0.33	0/222	0.68	0/293
2	k6	0.56	0/436	1.03	3/581 (0.5%)
2	k7	0.56	0/436	1.03	3/581 (0.5%)
2	k8	0.56	0/436	1.03	3/581 (0.5%)
2	kG	0.56	0/436	1.03	3/581 (0.5%)
2	kR	0.39	0/440	0.79	1/586 (0.2%)
2	l1	0.33	0/222	0.69	0/293
2	l4	0.41	0/439	0.76	0/585
2	l6	0.39	0/440	0.79	1/586 (0.2%)
2	l7	0.39	0/440	0.79	1/586 (0.2%)
2	l8	0.39	0/440	0.79	1/586 (0.2%)
2	lG	0.39	0/440	0.79	1/586 (0.2%)
2	lR	0.33	0/222	0.69	0/293
2	m1	0.41	0/439	0.76	0/585
2	m6	0.33	0/222	0.68	0/293
2	m7	0.33	0/222	0.68	0/293
2	m8	0.33	0/222	0.69	0/293

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	mG	0.33	0/222	0.69	0/293
2	mR	0.41	0/439	0.76	0/585
2	n6	0.41	0/439	0.76	0/585
2	n7	0.41	0/439	0.76	0/585
2	n8	0.41	0/439	0.76	0/585
2	nG	0.41	0/439	0.76	0/585
3	A2	0.55	0/2386	0.81	8/3223 (0.2%)
3	A5	0.55	0/2386	0.81	8/3223 (0.2%)
3	A9	0.55	0/2386	0.81	8/3223 (0.2%)
3	AA	0.55	0/2386	0.81	8/3223 (0.2%)
3	AB	0.55	0/2386	0.81	8/3223 (0.2%)
3	AC	0.55	0/2386	0.81	7/3223 (0.2%)
3	AF	0.55	0/2386	0.81	8/3223 (0.2%)
3	AH	0.55	0/2386	0.81	7/3223 (0.2%)
3	AI	0.55	0/2386	0.81	7/3223 (0.2%)
3	AM	0.55	0/2386	0.81	7/3223 (0.2%)
3	AN	0.55	0/2386	0.81	7/3223 (0.2%)
3	AO	0.55	0/2386	0.81	8/3223 (0.2%)
4	B2	0.48	0/1791	0.70	1/2411 (0.0%)
4	B5	0.48	0/1791	0.70	1/2411 (0.0%)
4	B9	0.48	0/1791	0.70	1/2411 (0.0%)
4	BA	0.48	0/1791	0.70	1/2411 (0.0%)
4	BB	0.48	0/1791	0.69	1/2411 (0.0%)
4	BC	0.48	0/1791	0.70	1/2411 (0.0%)
4	BF	0.48	0/1791	0.70	1/2411 (0.0%)
4	BH	0.48	0/1791	0.70	1/2411 (0.0%)
4	BI	0.48	0/1791	0.70	1/2411 (0.0%)
4	BM	0.48	0/1791	0.70	1/2411 (0.0%)
4	BN	0.48	0/1791	0.70	1/2411 (0.0%)
4	BO	0.48	0/1791	0.70	1/2411 (0.0%)
5	C2	0.26	0/4109	0.48	0/5550
5	C5	0.26	0/4109	0.48	0/5550
5	C9	0.26	0/4109	0.48	0/5550
5	CA	0.26	0/4109	0.48	0/5550
5	CB	0.26	0/4109	0.48	0/5550
5	CC	0.26	0/4109	0.48	0/5550
5	CF	0.26	0/4109	0.48	0/5550
5	CH	0.26	0/4109	0.48	0/5550
5	CI	0.26	0/4109	0.48	0/5550
5	CM	0.26	0/4109	0.48	0/5550
5	CN	0.26	0/4109	0.48	0/5550
5	CO	0.26	0/4109	0.48	0/5550
5	D2	0.48	0/1135	0.65	0/1529

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	D5	0.48	0/1135	0.65	0/1529
5	D9	0.47	0/1135	0.65	0/1529
5	DA	0.47	0/1135	0.65	0/1529
5	DB	0.47	0/1135	0.65	0/1529
5	DC	0.48	0/1135	0.65	0/1529
5	DF	0.47	0/1135	0.65	0/1529
5	DH	0.48	0/1135	0.65	0/1529
5	DI	0.48	0/1135	0.65	0/1529
5	DM	0.48	0/1135	0.65	0/1529
5	DN	0.48	0/1135	0.65	0/1529
5	DO	0.47	0/1135	0.65	0/1529
5	E2	0.49	0/1203	0.68	0/1617
5	E5	0.48	0/1203	0.68	0/1617
5	E9	0.48	0/1203	0.68	0/1617
5	EA	0.48	0/1203	0.68	0/1617
5	EB	0.49	0/1203	0.68	0/1617
5	EC	0.49	0/1203	0.68	0/1617
5	EF	0.48	0/1203	0.68	0/1617
5	EH	0.49	0/1203	0.68	0/1617
5	EI	0.48	0/1203	0.68	0/1617
5	EM	0.48	0/1203	0.68	0/1617
5	EN	0.49	0/1203	0.68	0/1617
5	EO	0.49	0/1203	0.68	0/1617
5	F2	0.55	0/950	0.73	2/1279 (0.2%)
5	F5	0.55	0/950	0.73	2/1279 (0.2%)
5	F9	0.55	0/950	0.73	2/1279 (0.2%)
5	FA	0.55	0/950	0.73	2/1279 (0.2%)
5	FB	0.55	0/950	0.73	2/1279 (0.2%)
5	FC	0.55	0/950	0.73	2/1279 (0.2%)
5	FF	0.55	0/950	0.73	2/1279 (0.2%)
5	FH	0.55	0/950	0.73	2/1279 (0.2%)
5	FI	0.55	0/950	0.73	2/1279 (0.2%)
5	FM	0.55	0/950	0.73	2/1279 (0.2%)
5	FN	0.55	0/950	0.73	2/1279 (0.2%)
5	FO	0.55	0/950	0.73	2/1279 (0.2%)
5	N2	0.26	0/4109	0.48	0/5550
5	N5	0.26	0/4109	0.48	0/5550
5	N9	0.26	0/4109	0.48	0/5550
5	NA	0.26	0/4109	0.48	0/5550
5	NB	0.26	0/4109	0.48	0/5550
5	NC	0.26	0/4109	0.48	0/5550
5	NF	0.26	0/4109	0.48	0/5550
5	NH	0.26	0/4109	0.48	0/5550

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	NI	0.26	0/4109	0.48	0/5550
5	NM	0.26	0/4109	0.48	0/5550
5	NN	0.26	0/4109	0.48	0/5550
5	NO	0.26	0/4109	0.48	0/5550
5	O2	0.26	0/4100	0.48	0/5539
5	O5	0.26	0/4100	0.48	0/5539
5	O9	0.26	0/4100	0.48	0/5539
5	OA	0.26	0/4100	0.48	0/5539
5	OB	0.26	0/4100	0.48	0/5539
5	OC	0.26	0/4100	0.48	0/5539
5	OF	0.26	0/4100	0.48	0/5539
5	OH	0.26	0/4100	0.48	0/5539
5	OI	0.26	0/4100	0.48	0/5539
5	OM	0.26	0/4100	0.48	0/5539
5	ON	0.26	0/4100	0.48	0/5539
5	OO	0.26	0/4100	0.48	0/5539
6	G2	0.24	0/89	0.38	0/123
6	G5	0.24	0/89	0.38	0/123
6	G9	0.24	0/89	0.38	0/123
6	GA	0.24	0/89	0.38	0/123
6	GB	0.24	0/89	0.38	0/123
6	GC	0.24	0/89	0.38	0/123
6	GF	0.24	0/89	0.38	0/123
6	GH	0.24	0/89	0.38	0/123
6	GI	0.24	0/89	0.38	0/123
6	GM	0.24	0/89	0.38	0/123
6	GN	0.24	0/89	0.38	0/123
6	GO	0.23	0/89	0.38	0/123
6	H2	0.24	0/89	0.38	0/123
6	H5	0.25	0/89	0.38	0/123
6	H9	0.24	0/89	0.38	0/123
6	HA	0.25	0/89	0.38	0/123
6	HB	0.24	0/89	0.38	0/123
6	HC	0.24	0/89	0.38	0/123
6	HF	0.25	0/89	0.38	0/123
6	HH	0.24	0/89	0.38	0/123
6	HI	0.24	0/89	0.38	0/123
6	HM	0.24	0/89	0.38	0/123
6	HN	0.25	0/89	0.38	0/123
6	HO	0.24	0/89	0.38	0/123
6	I2	0.24	0/119	0.42	0/165
6	I5	0.24	0/119	0.42	0/165
6	I9	0.24	0/119	0.42	0/165

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	IA	0.24	0/119	0.42	0/165
6	IB	0.24	0/119	0.42	0/165
6	IC	0.24	0/119	0.42	0/165
6	IF	0.24	0/119	0.42	0/165
6	IH	0.24	0/119	0.42	0/165
6	II	0.24	0/119	0.42	0/165
6	IM	0.24	0/119	0.42	0/165
6	IN	0.24	0/119	0.42	0/165
6	IO	0.24	0/119	0.42	0/165
6	J2	0.26	0/119	0.41	0/165
6	J5	0.26	0/119	0.41	0/165
6	J9	0.26	0/119	0.41	0/165
6	JA	0.26	0/119	0.41	0/165
6	JB	0.25	0/119	0.41	0/165
6	JC	0.26	0/119	0.41	0/165
6	JF	0.26	0/119	0.41	0/165
6	JH	0.26	0/119	0.41	0/165
6	JI	0.26	0/119	0.41	0/165
6	JM	0.26	0/119	0.41	0/165
6	JN	0.26	0/119	0.41	0/165
6	JO	0.25	0/119	0.41	0/165
6	K2	0.21	0/111	0.44	0/154
6	K5	0.21	0/111	0.45	0/154
6	K9	0.21	0/111	0.45	0/154
6	KA	0.21	0/111	0.45	0/154
6	KB	0.21	0/111	0.45	0/154
6	KC	0.21	0/111	0.45	0/154
6	KF	0.21	0/111	0.45	0/154
6	KH	0.21	0/111	0.45	0/154
6	KI	0.21	0/111	0.45	0/154
6	KM	0.21	0/111	0.45	0/154
6	KN	0.21	0/111	0.45	0/154
6	KO	0.21	0/111	0.45	0/154
6	L2	0.25	0/119	0.40	0/165
6	L5	0.25	0/119	0.40	0/165
6	L9	0.25	0/119	0.40	0/165
6	LA	0.25	0/119	0.40	0/165
6	LB	0.25	0/119	0.40	0/165
6	LC	0.25	0/119	0.40	0/165
6	LF	0.25	0/119	0.40	0/165
6	LH	0.25	0/119	0.40	0/165
6	LI	0.25	0/119	0.40	0/165
6	LM	0.25	0/119	0.40	0/165

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	LN	0.25	0/119	0.40	0/165
6	LO	0.25	0/119	0.40	0/165
7	HS	0.31	0/274	0.58	0/382
7	ID	0.31	0/274	0.58	0/382
7	IJ	0.31	0/274	0.58	0/382
7	IK	0.31	0/274	0.58	0/382
7	IP	0.31	0/274	0.58	0/382
7	NS	0.31	0/274	0.58	0/382
7	OD	0.30	0/274	0.58	0/382
7	OJ	0.31	0/274	0.58	0/382
7	OK	0.31	0/274	0.58	0/382
7	OP	0.31	0/274	0.58	0/382
7	SD	0.31	0/274	0.58	0/382
7	SJ	0.31	0/274	0.58	0/382
7	SK	0.31	0/274	0.58	0/382
7	SP	0.31	0/274	0.58	0/382
7	SS	0.31	0/274	0.58	0/382
8	PD	0.27	0/84	0.47	0/116
8	PJ	0.27	0/84	0.47	0/116
8	PK	0.27	0/84	0.47	0/116
8	PP	0.27	0/84	0.47	0/116
8	PS	0.27	0/84	0.47	0/116
8	QD	0.26	0/78	0.49	0/107
8	QJ	0.26	0/78	0.49	0/107
8	QK	0.26	0/78	0.49	0/107
8	QP	0.25	0/78	0.49	0/107
8	QS	0.25	0/78	0.49	0/107
8	RD	0.27	0/53	0.57	0/69
8	RJ	0.27	0/53	0.57	0/69
8	RK	0.27	0/53	0.57	0/69
8	RP	0.27	0/53	0.57	0/69
8	RS	0.27	0/53	0.57	0/69
All	All	0.43	10/1095338 (0.0%)	0.65	1182/1478016 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	2
1	A3	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A4	0	2
1	A6	0	2
1	A7	0	2
1	A8	0	2
1	AD	0	1
1	AE	0	1
1	AG	0	2
1	AJ	0	1
1	AK	0	1
1	AL	0	2
1	AP	0	1
1	AQ	0	2
1	AR	0	2
1	AS	0	2
1	B1	0	1
1	B3	0	1
1	B4	0	1
1	B6	0	1
1	B7	0	1
1	B8	0	1
1	BD	0	2
1	BE	0	2
1	BG	0	1
1	BJ	0	2
1	BK	0	2
1	BL	0	1
1	BP	0	2
1	BQ	0	1
1	BR	0	1
1	C1	0	1
1	C3	0	1
1	C4	0	1
1	C6	0	1
1	C7	0	1
1	C8	0	1
1	CE	0	1
1	CG	0	1
1	CL	0	1
1	CQ	0	1
1	CR	0	1
1	CS	0	2
1	DD	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DJ	0	2
1	DK	0	2
1	DP	0	2
1	I1	0	1
1	I3	0	1
1	I4	0	1
1	I6	0	1
1	I7	0	1
1	I8	0	1
1	IG	0	1
1	IL	0	1
1	IQ	0	1
1	IR	0	1
1	IS	0	1
1	J1	0	2
1	J3	0	2
1	J4	0	2
1	J6	0	2
1	J7	0	2
1	J8	0	2
1	JG	0	2
1	JL	0	2
1	JQ	0	2
1	JR	0	2
1	JS	0	1
1	K1	0	1
1	K3	0	1
1	K4	0	1
1	K6	0	1
1	K7	0	1
1	K8	0	1
1	KD	0	1
1	KE	0	1
1	KG	0	1
1	KJ	0	2
1	KK	0	1
1	KL	0	1
1	KP	0	1
1	KQ	0	1
1	KR	0	1
1	KS	0	1
1	LD	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	LE	0	2
1	LJ	0	1
1	LK	0	1
1	LP	0	1
1	ME	0	1
1	Q1	0	1
1	Q3	0	1
1	Q4	0	1
1	Q6	0	1
1	Q7	0	1
1	Q8	0	1
1	QG	0	1
1	QL	0	1
1	QQ	0	1
1	QR	0	1
1	R1	0	2
1	R3	0	2
1	R4	0	2
1	R6	0	2
1	R7	0	2
1	R8	0	2
1	RG	0	2
1	RL	0	2
1	RQ	0	2
1	RR	0	2
1	S1	0	1
1	S3	0	1
1	S4	0	1
1	S6	0	1
1	S7	0	1
1	S8	0	1
1	SE	0	1
1	SG	0	1
1	SL	0	1
1	SQ	0	1
1	SR	0	1
1	TE	0	2
1	UE	0	1
1	X1	0	1
1	X4	0	1
1	Y1	0	2
1	Y4	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y6	0	1
1	Y7	0	1
1	Y8	0	1
1	YG	0	1
1	YL	0	1
1	YR	0	1
1	Z1	0	1
1	Z4	0	1
1	Z6	0	2
1	Z7	0	2
1	Z8	0	2
1	ZG	0	2
1	ZL	0	2
1	ZR	0	2
1	a6	0	1
1	a7	0	1
1	a8	0	1
1	aE	0	1
1	aG	0	1
1	aL	0	1
1	aR	0	1
1	bE	0	2
1	bQ	0	1
1	cE	0	1
1	cQ	0	2
1	dQ	0	1
1	f1	0	1
1	f4	0	1
1	g1	0	2
1	g4	0	2
1	g6	0	1
1	g7	0	1
1	g8	0	1
1	gG	0	1
1	gR	0	1
1	h1	0	1
1	h4	0	1
1	h6	0	2
1	h7	0	2
1	h8	0	2
1	hG	0	2
1	hR	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	i6	0	1
1	i7	0	1
1	i8	0	1
1	iG	0	1
1	iR	0	1
2	DS	0	3
2	E1	0	1
2	E3	0	1
2	E4	0	1
2	E6	0	1
2	E7	0	1
2	E8	0	1
2	ED	0	3
2	EE	0	1
2	EG	0	1
2	EJ	0	3
2	EK	0	3
2	EL	0	1
2	EP	0	3
2	EQ	0	1
2	ER	0	1
2	ES	0	2
2	F1	0	2
2	F3	0	2
2	F4	0	2
2	F6	0	2
2	F7	0	2
2	F8	0	2
2	FD	0	2
2	FG	0	2
2	FJ	0	2
2	FK	0	2
2	FL	0	2
2	FP	0	2
2	FQ	0	2
2	FR	0	2
2	G1	0	3
2	G3	0	3
2	G4	0	3
2	G6	0	3
2	G7	0	3
2	G8	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	GE	0	3
2	GG	0	3
2	GL	0	3
2	GQ	0	3
2	GR	0	3
2	H1	0	1
2	H3	0	1
2	H4	0	1
2	H6	0	1
2	H7	0	1
2	H8	0	1
2	HE	0	2
2	HG	0	1
2	HL	0	1
2	HQ	0	1
2	HR	0	1
2	IE	0	3
2	JE	0	1
2	LS	0	1
2	M1	0	1
2	M3	0	1
2	M4	0	1
2	M6	0	1
2	M7	0	1
2	M8	0	1
2	MD	0	1
2	MG	0	1
2	MJ	0	1
2	MK	0	1
2	ML	0	1
2	MP	0	1
2	MQ	0	1
2	MR	0	1
2	MS	0	1
2	N1	0	2
2	N3	0	2
2	N4	0	2
2	N6	0	2
2	N7	0	2
2	N8	0	2
2	ND	0	1
2	NG	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	NJ	0	1
2	NK	0	1
2	NL	0	2
2	NP	0	1
2	NQ	0	2
2	NR	0	2
2	O1	0	3
2	O3	0	3
2	O4	0	3
2	O6	0	3
2	O7	0	3
2	O8	0	3
2	OE	0	1
2	OG	0	3
2	OL	0	3
2	OQ	0	3
2	OR	0	3
2	P1	0	1
2	P3	0	1
2	P4	0	1
2	P6	0	1
2	P7	0	1
2	P8	0	1
2	PE	0	2
2	PG	0	1
2	PL	0	1
2	PQ	0	1
2	PR	0	1
2	QE	0	3
2	RE	0	1
2	U1	0	2
2	U3	0	1
2	U4	0	2
2	U6	0	1
2	U7	0	1
2	U8	0	1
2	UG	0	1
2	UL	0	1
2	UQ	0	1
2	UR	0	1
2	V1	0	3
2	V3	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V4	0	3
2	V6	0	2
2	V7	0	2
2	V8	0	2
2	VG	0	2
2	VL	0	2
2	VQ	0	2
2	VR	0	2
2	W1	0	1
2	W3	0	3
2	W4	0	1
2	W6	0	3
2	W7	0	3
2	W8	0	3
2	WE	0	1
2	WG	0	3
2	WL	0	3
2	WQ	0	3
2	WR	0	3
2	X3	0	1
2	X6	0	1
2	X7	0	1
2	X8	0	1
2	XE	0	2
2	XG	0	1
2	XL	0	1
2	XQ	0	1
2	XR	0	1
2	YE	0	3
2	Z3	0	1
2	ZE	0	1
2	ZQ	0	1
2	a3	0	3
2	aQ	0	3
2	b1	0	1
2	b4	0	1
2	c1	0	2
2	c3	0	1
2	c4	0	2
2	c6	0	1
2	c7	0	1
2	c8	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	cG	0	1
2	cL	0	1
2	cR	0	1
2	d1	0	3
2	d3	0	3
2	d4	0	3
2	d6	0	2
2	d7	0	2
2	d8	0	2
2	dG	0	2
2	dL	0	2
2	dR	0	2
2	e1	0	1
2	e4	0	1
2	e6	0	3
2	e7	0	3
2	e8	0	3
2	eE	0	1
2	eG	0	3
2	eL	0	3
2	eR	0	3
2	f6	0	1
2	f7	0	1
2	f8	0	1
2	fE	0	2
2	fG	0	1
2	fL	0	1
2	fQ	0	1
2	fR	0	1
2	gE	0	3
2	gQ	0	2
2	hE	0	1
2	hL	0	1
2	hQ	0	3
2	iL	0	3
2	iQ	0	1
2	j1	0	1
2	j4	0	2
2	k1	0	2
2	k4	0	3
2	k6	0	1
2	k7	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	k8	0	1
2	kG	0	1
2	kR	0	2
2	l1	0	3
2	l4	0	1
2	l6	0	2
2	l7	0	2
2	l8	0	2
2	lG	0	2
2	lR	0	3
2	m1	0	1
2	m6	0	3
2	m7	0	3
2	m8	0	3
2	mG	0	3
2	mR	0	1
2	n6	0	1
2	n7	0	1
2	n8	0	1
2	nG	0	1
3	A2	0	5
3	A5	0	5
3	A9	0	5
3	AA	0	5
3	AB	0	5
3	AC	0	5
3	AF	0	5
3	AH	0	5
3	AI	0	5
3	AM	0	5
3	AN	0	5
3	AO	0	5
4	B2	0	2
4	B5	0	2
4	B9	0	2
4	BA	0	2
4	BB	0	2
4	BC	0	2
4	BF	0	2
4	BH	0	2
4	BI	0	2
4	BM	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	BN	0	2
4	BO	0	2
5	F2	0	1
5	F5	0	1
5	F9	0	1
5	FA	0	1
5	FB	0	1
5	FC	0	1
5	FF	0	1
5	FH	0	1
5	FI	0	1
5	FM	0	1
5	FN	0	1
5	FO	0	1
All	All	0	732

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AD	49	PHE	CA-C	-7.83	1.32	1.52
1	AJ	49	PHE	CA-C	-7.82	1.32	1.52
1	IS	49	PHE	CA-C	-7.81	1.32	1.52
1	AP	49	PHE	CA-C	-7.81	1.32	1.52
1	AK	49	PHE	CA-C	-7.79	1.32	1.52

The worst 5 of 1182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	62	LEU	N-CA-C	9.00	135.31	111.00
1	J3	62	LEU	N-CA-C	9.00	135.31	111.00
1	A4	62	LEU	N-CA-C	9.00	135.31	111.00
1	R4	62	LEU	N-CA-C	9.00	135.31	111.00
1	A6	62	LEU	N-CA-C	9.00	135.31	111.00

There are no chirality outliers.

5 of 732 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	204	ALA	Peptide
1	A1	61	THR	Mainchain
1	B1	61	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C1	347	ILE	Peptide
2	E1	9	SER	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	A3	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	A4	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	A6	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	A7	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	A8	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	AD	352/408 (86%)	310 (88%)	40 (11%)	2 (1%)	25	62
1	AE	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	AG	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	AJ	352/408 (86%)	309 (88%)	41 (12%)	2 (1%)	25	62
1	AK	352/408 (86%)	310 (88%)	40 (11%)	2 (1%)	25	62
1	AL	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	AP	352/408 (86%)	310 (88%)	40 (11%)	2 (1%)	25	62
1	AQ	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	AR	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	AS	391/408 (96%)	352 (90%)	39 (10%)	0	100	100
1	B1	383/408 (94%)	350 (91%)	33 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B3	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	B4	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	B6	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	B7	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	B8	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	BD	391/408 (96%)	352 (90%)	39 (10%)	0	100	100
1	BE	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	BG	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	BJ	391/408 (96%)	352 (90%)	39 (10%)	0	100	100
1	BK	391/408 (96%)	352 (90%)	39 (10%)	0	100	100
1	BL	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	BP	391/408 (96%)	352 (90%)	39 (10%)	0	100	100
1	BQ	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	BR	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	BS	384/408 (94%)	345 (90%)	39 (10%)	0	100	100
1	C1	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	C3	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	C4	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	C6	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	C7	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	C8	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	CD	384/408 (94%)	345 (90%)	39 (10%)	0	100	100
1	CE	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	CG	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	CJ	384/408 (94%)	344 (90%)	40 (10%)	0	100	100
1	CK	384/408 (94%)	345 (90%)	39 (10%)	0	100	100
1	CL	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	CP	384/408 (94%)	344 (90%)	40 (10%)	0	100	100
1	CQ	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	CR	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	CS	384/408 (94%)	344 (90%)	39 (10%)	1 (0%)	41	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D1	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	D3	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	D4	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	D6	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	D7	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	D8	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	DD	384/408 (94%)	345 (90%)	38 (10%)	1 (0%)	41	74
1	DE	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	DG	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	DJ	384/408 (94%)	344 (90%)	39 (10%)	1 (0%)	41	74
1	DK	384/408 (94%)	344 (90%)	39 (10%)	1 (0%)	41	74
1	DL	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	DP	384/408 (94%)	344 (90%)	39 (10%)	1 (0%)	41	74
1	DQ	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	DR	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	FE	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	I1	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	I3	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	I4	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	I6	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	I7	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	I8	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	IG	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	IL	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	IQ	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	IR	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	IS	352/408 (86%)	309 (88%)	41 (12%)	2 (1%)	25	62
1	J1	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	J3	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	J4	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	J6	388/408 (95%)	360 (93%)	28 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J7	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	J8	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	JG	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	JL	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	JQ	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	JR	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	JS	378/408 (93%)	338 (89%)	40 (11%)	0	100	100
1	K1	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	K3	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	K4	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	K6	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	K7	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	K8	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	KD	378/408 (93%)	337 (89%)	41 (11%)	0	100	100
1	KE	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	KG	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	KJ	378/408 (93%)	337 (89%)	41 (11%)	0	100	100
1	KK	378/408 (93%)	337 (89%)	41 (11%)	0	100	100
1	KL	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	KP	378/408 (93%)	337 (89%)	41 (11%)	0	100	100
1	KQ	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	KR	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	KS	384/408 (94%)	347 (90%)	36 (9%)	1 (0%)	41	74
1	L1	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	L3	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	L4	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	L6	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	L7	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	L8	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	LD	384/408 (94%)	347 (90%)	36 (9%)	1 (0%)	41	74
1	LE	388/408 (95%)	360 (93%)	28 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LG	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	LJ	384/408 (94%)	347 (90%)	36 (9%)	1 (0%)	41	74
1	LK	384/408 (94%)	348 (91%)	35 (9%)	1 (0%)	41	74
1	LL	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	LP	384/408 (94%)	348 (91%)	35 (9%)	1 (0%)	41	74
1	LQ	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	LR	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	ME	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	NE	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	Q1	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Q3	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Q4	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Q6	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Q7	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Q8	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	QG	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	QL	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	QQ	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	QR	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	R1	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	R3	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	R4	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	R6	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	R7	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	R8	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	RG	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	RL	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	RQ	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	RR	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	S1	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	S3	383/408 (94%)	350 (91%)	33 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S4	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	S6	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	S7	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	S8	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	SE	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	SG	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	SL	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	SQ	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	SR	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	T1	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	T3	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	T4	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	T6	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	T7	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	T8	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	TE	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	TG	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	TL	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	TQ	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	TR	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	UE	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	VE	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	X1	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	X4	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Y1	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	Y3	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	Y4	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	Y6	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Y7	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Y8	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	YG	383/408 (94%)	357 (93%)	26 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	YL	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	YQ	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	YR	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	Z1	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	Z4	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	Z6	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	Z7	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	Z8	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	ZG	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	ZL	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	ZR	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	a1	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	a4	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	a6	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	a7	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	a8	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	aE	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	aG	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	aL	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	aR	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	b3	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	b6	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	b7	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	b8	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	bE	388/408 (95%)	360 (93%)	28 (7%)	0	100	100
1	bG	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	bL	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	bQ	383/408 (94%)	357 (93%)	26 (7%)	0	100	100
1	bR	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41	74
1	cE	383/408 (94%)	350 (91%)	33 (9%)	0	100	100
1	cQ	388/408 (95%)	360 (93%)	28 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	dE	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	dQ	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	eQ	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	f1	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	f4	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	g1	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	g4	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	g6	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	g7	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	g8	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	gG	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	gL	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	gR	383/408 (94%)	357 (93%)	26 (7%)	0	100 100
1	h1	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	h4	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	h6	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	h7	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	h8	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	hG	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	hR	388/408 (95%)	360 (93%)	28 (7%)	0	100 100
1	i1	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	i4	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	i6	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	i7	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	i8	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	iG	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	iR	383/408 (94%)	350 (91%)	33 (9%)	0	100 100
1	j6	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	j7	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	j8	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
1	jG	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	jR	391/408 (96%)	368 (94%)	22 (6%)	1 (0%)	41 74
2	DS	53/60 (88%)	42 (79%)	11 (21%)	0	100 100
2	E1	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	E3	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	E4	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	E6	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	E7	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	E8	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	ED	53/60 (88%)	42 (79%)	11 (21%)	0	100 100
2	EE	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	EG	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	EJ	53/60 (88%)	42 (79%)	11 (21%)	0	100 100
2	EK	53/60 (88%)	42 (79%)	11 (21%)	0	100 100
2	EL	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	EP	53/60 (88%)	42 (79%)	11 (21%)	0	100 100
2	EQ	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	ER	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	ES	53/60 (88%)	40 (76%)	12 (23%)	1 (2%)	8 42
2	F1	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	F3	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	F4	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	F6	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	F7	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	F8	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	FD	53/60 (88%)	40 (76%)	12 (23%)	1 (2%)	8 42
2	FG	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	FJ	53/60 (88%)	39 (74%)	13 (24%)	1 (2%)	8 42
2	FK	53/60 (88%)	40 (76%)	12 (23%)	1 (2%)	8 42
2	FL	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	FP	53/60 (88%)	40 (76%)	12 (23%)	1 (2%)	8 42
2	FQ	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	FR	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	FS	28/60 (47%)	18 (64%)	10 (36%)	0	100 100
2	G1	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	G3	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	G4	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	G6	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	G7	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	G8	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GD	28/60 (47%)	18 (64%)	10 (36%)	0	100 100
2	GE	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GG	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GJ	28/60 (47%)	18 (64%)	10 (36%)	0	100 100
2	GK	28/60 (47%)	18 (64%)	10 (36%)	0	100 100
2	GL	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GP	28/60 (47%)	18 (64%)	10 (36%)	0	100 100
2	GQ	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GR	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	GS	52/60 (87%)	38 (73%)	14 (27%)	0	100 100
2	H1	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	H3	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	H4	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	H6	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	H7	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	H8	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	HD	52/60 (87%)	38 (73%)	14 (27%)	0	100 100
2	HE	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	HG	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	HJ	52/60 (87%)	38 (73%)	14 (27%)	0	100 100
2	HK	52/60 (87%)	38 (73%)	14 (27%)	0	100 100
2	HL	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	HP	52/60 (87%)	38 (73%)	14 (27%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	HQ	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	HR	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	IE	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	JE	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	LS	53/60 (88%)	40 (76%)	13 (24%)	0	100 100
2	M1	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	M3	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	M4	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	M6	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	M7	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	M8	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	MD	53/60 (88%)	40 (76%)	13 (24%)	0	100 100
2	MG	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	MJ	53/60 (88%)	40 (76%)	13 (24%)	0	100 100
2	MK	53/60 (88%)	40 (76%)	13 (24%)	0	100 100
2	ML	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	MP	53/60 (88%)	40 (76%)	13 (24%)	0	100 100
2	MQ	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	MR	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	MS	53/60 (88%)	41 (77%)	10 (19%)	2 (4%)	3 29
2	N1	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	N3	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	N4	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	N6	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	N7	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	N8	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	ND	53/60 (88%)	40 (76%)	11 (21%)	2 (4%)	3 29
2	NG	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	NJ	53/60 (88%)	41 (77%)	10 (19%)	2 (4%)	3 29
2	NK	53/60 (88%)	41 (77%)	10 (19%)	2 (4%)	3 29
2	NL	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	NP	53/60 (88%)	41 (77%)	10 (19%)	2 (4%)	3 29
2	NQ	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	NR	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	O1	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	O3	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	O4	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	O6	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	O7	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	O8	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	OE	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	OG	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	OL	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	OQ	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	OR	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	P1	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	P3	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	P4	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	P6	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	P7	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	P8	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	PE	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	PG	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	PL	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	PQ	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	PR	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	QE	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	RE	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	U1	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	U3	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	U4	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	U6	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	U7	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	U8	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	UG	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	UL	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	UQ	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	UR	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	V1	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	V3	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	V4	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	V6	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	V7	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	V8	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	VG	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	VL	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	VQ	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	VR	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	W1	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	W3	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	W4	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	W6	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	W7	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	W8	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	WE	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	WG	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	WL	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	WQ	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	WR	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	X3	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	X6	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	X7	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	X8	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	XE	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	XG	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	XL	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	XQ	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	XR	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	YE	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	Z3	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	ZE	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	ZQ	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	a3	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	aQ	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	b1	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	b4	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	c1	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	c3	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	c4	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	c6	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	c7	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	c8	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	cG	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	cL	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	cR	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	d1	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	d3	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	d4	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	d6	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	d7	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	d8	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	dG	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	dL	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	dR	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	e1	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	e4	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	e6	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	e7	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	e8	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	eE	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	eG	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	eL	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	eR	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	f6	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	f7	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	f8	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	fE	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	fG	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	fL	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	fQ	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	fR	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	gE	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	gQ	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	hE	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	hL	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	hQ	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	iL	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	iQ	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	j1	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	j4	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	k1	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	k4	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	k6	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	k7	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	k8	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	kG	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	8 42
2	kR	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	l1	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	l4	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	l6	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	l7	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	l8	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	lG	53/60 (88%)	35 (66%)	15 (28%)	3 (6%)	1 21
2	lR	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	m1	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	m6	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	m7	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	m8	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	mG	25/60 (42%)	20 (80%)	5 (20%)	0	100 100
2	mR	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	n6	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	n7	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	n8	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
2	nG	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	8 42
3	A2	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	A5	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	A9	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	AA	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	AB	295/327 (90%)	245 (83%)	50 (17%)	0	100 100
3	AC	295/327 (90%)	245 (83%)	49 (17%)	1 (0%)	41 74
3	AF	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	AH	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	AI	295/327 (90%)	245 (83%)	50 (17%)	0	100 100
3	AM	295/327 (90%)	245 (83%)	49 (17%)	1 (0%)	41 74
3	AN	295/327 (90%)	244 (83%)	51 (17%)	0	100 100
3	AO	295/327 (90%)	244 (83%)	51 (17%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B2	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	B5	216/251 (86%)	179 (83%)	37 (17%)	0	100	100
4	B9	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BA	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BB	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BC	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BF	216/251 (86%)	179 (83%)	37 (17%)	0	100	100
4	BH	216/251 (86%)	179 (83%)	37 (17%)	0	100	100
4	BI	216/251 (86%)	179 (83%)	37 (17%)	0	100	100
4	BM	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BN	216/251 (86%)	180 (83%)	36 (17%)	0	100	100
4	BO	216/251 (86%)	179 (83%)	37 (17%)	0	100	100
5	C2	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	C5	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	C9	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CA	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CB	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CC	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CF	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CH	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CI	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CM	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CN	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	CO	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	D2	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	D5	130/647 (20%)	119 (92%)	10 (8%)	1 (1%)	19	57
5	D9	130/647 (20%)	119 (92%)	10 (8%)	1 (1%)	19	57
5	DA	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DB	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DC	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DF	130/647 (20%)	119 (92%)	10 (8%)	1 (1%)	19	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	DH	130/647 (20%)	119 (92%)	10 (8%)	1 (1%)	19	57
5	DI	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DM	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DN	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	DO	130/647 (20%)	120 (92%)	9 (7%)	1 (1%)	19	57
5	E2	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	E5	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	E9	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	EA	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	EB	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	EC	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	EF	134/647 (21%)	121 (90%)	12 (9%)	1 (1%)	22	60
5	EH	134/647 (21%)	120 (90%)	13 (10%)	1 (1%)	22	60
5	EI	134/647 (21%)	120 (90%)	13 (10%)	1 (1%)	22	60
5	EM	134/647 (21%)	120 (90%)	13 (10%)	1 (1%)	22	60
5	EN	134/647 (21%)	120 (90%)	13 (10%)	1 (1%)	22	60
5	EO	134/647 (21%)	120 (90%)	13 (10%)	1 (1%)	22	60
5	F2	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	F5	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	F9	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FA	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FB	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FC	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FF	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FH	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FI	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FM	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FN	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	FO	108/647 (17%)	98 (91%)	10 (9%)	0	100	100
5	N2	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	N5	497/647 (77%)	483 (97%)	14 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N9	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NA	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NB	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NC	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NF	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NH	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NI	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NM	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NN	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	NO	497/647 (77%)	483 (97%)	14 (3%)	0	100	100
5	O2	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	O5	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	O9	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OA	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OB	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OC	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OF	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OH	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OI	496/647 (77%)	481 (97%)	15 (3%)	0	100	100
5	OM	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	ON	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
5	OO	496/647 (77%)	482 (97%)	14 (3%)	0	100	100
6	G2	16/133 (12%)	16 (100%)	0	0	100	100
6	G5	16/133 (12%)	16 (100%)	0	0	100	100
6	G9	16/133 (12%)	16 (100%)	0	0	100	100
6	GA	16/133 (12%)	16 (100%)	0	0	100	100
6	GB	16/133 (12%)	16 (100%)	0	0	100	100
6	GC	16/133 (12%)	16 (100%)	0	0	100	100
6	GF	16/133 (12%)	16 (100%)	0	0	100	100
6	GH	16/133 (12%)	16 (100%)	0	0	100	100
6	GI	16/133 (12%)	16 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	GM	16/133 (12%)	16 (100%)	0	0	100	100
6	GN	16/133 (12%)	16 (100%)	0	0	100	100
6	GO	16/133 (12%)	16 (100%)	0	0	100	100
6	H2	16/133 (12%)	16 (100%)	0	0	100	100
6	H5	16/133 (12%)	16 (100%)	0	0	100	100
6	H9	16/133 (12%)	16 (100%)	0	0	100	100
6	HA	16/133 (12%)	16 (100%)	0	0	100	100
6	HB	16/133 (12%)	16 (100%)	0	0	100	100
6	HC	16/133 (12%)	16 (100%)	0	0	100	100
6	HF	16/133 (12%)	16 (100%)	0	0	100	100
6	HH	16/133 (12%)	16 (100%)	0	0	100	100
6	HI	16/133 (12%)	16 (100%)	0	0	100	100
6	HM	16/133 (12%)	16 (100%)	0	0	100	100
6	HN	16/133 (12%)	16 (100%)	0	0	100	100
6	HO	16/133 (12%)	16 (100%)	0	0	100	100
6	I2	22/133 (16%)	22 (100%)	0	0	100	100
6	I5	22/133 (16%)	22 (100%)	0	0	100	100
6	I9	22/133 (16%)	22 (100%)	0	0	100	100
6	IA	22/133 (16%)	22 (100%)	0	0	100	100
6	IB	22/133 (16%)	22 (100%)	0	0	100	100
6	IC	22/133 (16%)	22 (100%)	0	0	100	100
6	IF	22/133 (16%)	22 (100%)	0	0	100	100
6	IH	22/133 (16%)	22 (100%)	0	0	100	100
6	II	22/133 (16%)	22 (100%)	0	0	100	100
6	IM	22/133 (16%)	22 (100%)	0	0	100	100
6	IN	22/133 (16%)	22 (100%)	0	0	100	100
6	IO	22/133 (16%)	22 (100%)	0	0	100	100
6	J2	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	J5	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	J9	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JA	22/133 (16%)	21 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	JB	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JC	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JF	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JH	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JI	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JM	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JN	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	JO	22/133 (16%)	21 (96%)	1 (4%)	0	100	100
6	K2	20/133 (15%)	20 (100%)	0	0	100	100
6	K5	20/133 (15%)	20 (100%)	0	0	100	100
6	K9	20/133 (15%)	20 (100%)	0	0	100	100
6	KA	20/133 (15%)	20 (100%)	0	0	100	100
6	KB	20/133 (15%)	20 (100%)	0	0	100	100
6	KC	20/133 (15%)	20 (100%)	0	0	100	100
6	KF	20/133 (15%)	20 (100%)	0	0	100	100
6	KH	20/133 (15%)	20 (100%)	0	0	100	100
6	KI	20/133 (15%)	20 (100%)	0	0	100	100
6	KM	20/133 (15%)	20 (100%)	0	0	100	100
6	KN	20/133 (15%)	20 (100%)	0	0	100	100
6	KO	20/133 (15%)	20 (100%)	0	0	100	100
6	L2	22/133 (16%)	22 (100%)	0	0	100	100
6	L5	22/133 (16%)	22 (100%)	0	0	100	100
6	L9	22/133 (16%)	22 (100%)	0	0	100	100
6	LA	22/133 (16%)	22 (100%)	0	0	100	100
6	LB	22/133 (16%)	22 (100%)	0	0	100	100
6	LC	22/133 (16%)	22 (100%)	0	0	100	100
6	LF	22/133 (16%)	22 (100%)	0	0	100	100
6	LH	22/133 (16%)	22 (100%)	0	0	100	100
6	LI	22/133 (16%)	22 (100%)	0	0	100	100
6	LM	22/133 (16%)	22 (100%)	0	0	100	100
6	LN	22/133 (16%)	22 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LO	22/133 (16%)	22 (100%)	0	0	100	100
7	HS	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	ID	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	IJ	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	IK	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	IP	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	NS	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	OD	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	OJ	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	OK	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	OP	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	SD	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	SJ	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	SK	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	SP	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
7	SS	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
8	PD	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
8	PJ	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
8	PK	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
8	PP	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
8	PS	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
8	QD	14/17 (82%)	14 (100%)	0	0	100	100
8	QJ	14/17 (82%)	14 (100%)	0	0	100	100
8	QK	14/17 (82%)	14 (100%)	0	0	100	100
8	QP	14/17 (82%)	14 (100%)	0	0	100	100
8	QS	14/17 (82%)	14 (100%)	0	0	100	100
8	RD	10/17 (59%)	9 (90%)	1 (10%)	0	100	100
8	RJ	10/17 (59%)	9 (90%)	1 (10%)	0	100	100
8	RK	10/17 (59%)	9 (90%)	1 (10%)	0	100	100
8	RP	10/17 (59%)	9 (90%)	1 (10%)	0	100	100
8	RS	10/17 (59%)	9 (90%)	1 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	132187/174156 (76%)	120358 (91%)	11463 (9%)	366 (0%)	44 74

5 of 366 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F1	44	GLN
2	N1	44	GLN
2	U1	44	GLN
2	c1	44	GLN
2	k1	44	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A1	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	A3	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	A4	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	A6	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	A7	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	A8	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	AD	304/367 (83%)	294 (97%)	10 (3%)	38 65
1	AE	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	AG	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	AJ	304/367 (83%)	294 (97%)	10 (3%)	38 65
1	AK	304/367 (83%)	294 (97%)	10 (3%)	38 65
1	AL	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	AP	304/367 (83%)	294 (97%)	10 (3%)	38 65
1	AQ	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	AR	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	AS	353/367 (96%)	344 (98%)	9 (2%)	47 70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	B3	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	B4	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	B6	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	B7	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	B8	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	BD	353/367 (96%)	344 (98%)	9 (2%)	47	70
1	BE	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	BG	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	BJ	353/367 (96%)	344 (98%)	9 (2%)	47	70
1	BK	353/367 (96%)	344 (98%)	9 (2%)	47	70
1	BL	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	BP	353/367 (96%)	344 (98%)	9 (2%)	47	70
1	BQ	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	BR	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	BS	346/367 (94%)	339 (98%)	7 (2%)	55	75
1	C1	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	C3	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	C4	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	C6	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	C7	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	C8	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	CD	346/367 (94%)	339 (98%)	7 (2%)	55	75
1	CE	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	CG	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	CJ	346/367 (94%)	339 (98%)	7 (2%)	55	75
1	CK	346/367 (94%)	339 (98%)	7 (2%)	55	75
1	CL	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	CP	346/367 (94%)	339 (98%)	7 (2%)	55	75
1	CQ	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	CR	344/367 (94%)	340 (99%)	4 (1%)	71	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CS	345/367 (94%)	336 (97%)	9 (3%)	46	69
1	D1	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	D3	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	D4	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	D6	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	D7	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	D8	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	DD	345/367 (94%)	336 (97%)	9 (3%)	46	69
1	DE	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	DG	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	DJ	345/367 (94%)	336 (97%)	9 (3%)	46	69
1	DK	345/367 (94%)	336 (97%)	9 (3%)	46	69
1	DL	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	DP	345/367 (94%)	336 (97%)	9 (3%)	46	69
1	DQ	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	DR	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	FE	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	I1	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	I3	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	I4	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	I6	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	I7	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	I8	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	IG	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	IL	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	IQ	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	IR	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	IS	304/367 (83%)	294 (97%)	10 (3%)	38	65
1	J1	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	J3	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	J4	351/367 (96%)	344 (98%)	7 (2%)	55	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J6	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	J7	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	J8	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	JG	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	JL	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	JQ	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	JR	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	JS	343/367 (94%)	336 (98%)	7 (2%)	55	75
1	K1	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	K3	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	K4	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	K6	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	K7	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	K8	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	KD	343/367 (94%)	336 (98%)	7 (2%)	55	75
1	KE	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	KG	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	KJ	343/367 (94%)	336 (98%)	7 (2%)	55	75
1	KK	343/367 (94%)	336 (98%)	7 (2%)	55	75
1	KL	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	KP	343/367 (94%)	336 (98%)	7 (2%)	55	75
1	KQ	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	KR	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	KS	346/367 (94%)	340 (98%)	6 (2%)	60	78
1	L1	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	L3	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	L4	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	L6	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	L7	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	L8	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	LD	346/367 (94%)	340 (98%)	6 (2%)	60	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	LE	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	LG	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	LJ	346/367 (94%)	340 (98%)	6 (2%)	60 78
1	LK	346/367 (94%)	340 (98%)	6 (2%)	60 78
1	LL	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	LP	346/367 (94%)	340 (98%)	6 (2%)	60 78
1	LQ	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	LR	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	ME	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	NE	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	Q1	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Q3	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Q4	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Q6	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Q7	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Q8	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	QG	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	QL	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	QQ	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	QR	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	R1	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	R3	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	R4	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	R6	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	R7	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	R8	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	RG	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	RL	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	RQ	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	RR	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	S1	344/367 (94%)	338 (98%)	6 (2%)	60 78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S3	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	S4	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	S6	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	S7	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	S8	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	SE	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	SG	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	SL	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	SQ	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	SR	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	T1	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	T3	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	T4	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	T6	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	T7	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	T8	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	TE	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	TG	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	TL	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	TQ	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	TR	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	UE	344/367 (94%)	338 (98%)	6 (2%)	60	78
1	VE	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	X1	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	X4	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	Y1	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	Y3	353/367 (96%)	351 (99%)	2 (1%)	86	92
1	Y4	351/367 (96%)	344 (98%)	7 (2%)	55	75
1	Y6	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	Y7	344/367 (94%)	340 (99%)	4 (1%)	71	84
1	Y8	344/367 (94%)	340 (99%)	4 (1%)	71	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	YG	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	YL	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	YQ	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	YR	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	Z1	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	Z4	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	Z6	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	Z7	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	Z8	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	ZG	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	ZL	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	ZR	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	a1	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	a4	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	a6	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	a7	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	a8	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	aE	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	aG	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	aL	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	aR	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	b3	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	b6	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	b7	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	b8	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	bE	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	bG	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	bL	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	bQ	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	bR	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	cE	344/367 (94%)	338 (98%)	6 (2%)	60 78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	cQ	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	dE	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	dQ	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	eQ	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	f1	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	f4	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	g1	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	g4	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	g6	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	g7	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	g8	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	gG	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	gL	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	gR	344/367 (94%)	340 (99%)	4 (1%)	71 84
1	h1	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	h4	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	h6	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	h7	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	h8	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	hG	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	hR	351/367 (96%)	344 (98%)	7 (2%)	55 75
1	i1	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	i4	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	i6	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	i7	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	i8	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	iG	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	iR	344/367 (94%)	338 (98%)	6 (2%)	60 78
1	j6	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	j7	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	j8	353/367 (96%)	351 (99%)	2 (1%)	86 92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	jG	353/367 (96%)	351 (99%)	2 (1%)	86 92
1	jR	353/367 (96%)	351 (99%)	2 (1%)	86 92
2	DS	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	E1	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	E3	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	E4	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	E6	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	E7	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	E8	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	ED	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	EE	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	EG	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	EJ	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	EK	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	EL	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	EP	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	EQ	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	ER	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	ES	51/56 (91%)	48 (94%)	3 (6%)	19 51
2	F1	50/56 (89%)	50 (100%)	0	100 100
2	F3	50/56 (89%)	50 (100%)	0	100 100
2	F4	50/56 (89%)	50 (100%)	0	100 100
2	F6	50/56 (89%)	50 (100%)	0	100 100
2	F7	50/56 (89%)	50 (100%)	0	100 100
2	F8	50/56 (89%)	50 (100%)	0	100 100
2	FD	51/56 (91%)	48 (94%)	3 (6%)	19 51
2	FG	50/56 (89%)	50 (100%)	0	100 100
2	FJ	51/56 (91%)	48 (94%)	3 (6%)	19 51
2	FK	51/56 (91%)	48 (94%)	3 (6%)	19 51
2	FL	50/56 (89%)	50 (100%)	0	100 100
2	FP	51/56 (91%)	48 (94%)	3 (6%)	19 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	FQ	50/56 (89%)	50 (100%)	0	100 100
2	FR	50/56 (89%)	50 (100%)	0	100 100
2	FS	29/56 (52%)	26 (90%)	3 (10%)	7 31
2	G1	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	G3	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	G4	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	G6	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	G7	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	G8	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GD	29/56 (52%)	26 (90%)	3 (10%)	7 31
2	GE	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GG	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GJ	29/56 (52%)	26 (90%)	3 (10%)	7 31
2	GK	29/56 (52%)	26 (90%)	3 (10%)	7 31
2	GL	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GP	29/56 (52%)	26 (90%)	3 (10%)	7 31
2	GQ	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GR	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	GS	51/56 (91%)	51 (100%)	0	100 100
2	H1	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	H3	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	H4	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	H6	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	H7	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	H8	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	HD	51/56 (91%)	51 (100%)	0	100 100
2	HE	50/56 (89%)	50 (100%)	0	100 100
2	HG	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	HJ	51/56 (91%)	51 (100%)	0	100 100
2	HK	51/56 (91%)	51 (100%)	0	100 100
2	HL	49/56 (88%)	48 (98%)	1 (2%)	55 75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	HP	51/56 (91%)	51 (100%)	0	100	100
2	HQ	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	HR	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	IE	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	JE	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	LS	51/56 (91%)	47 (92%)	4 (8%)	12	42
2	M1	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	M3	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	M4	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	M6	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	M7	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	M8	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	MD	51/56 (91%)	47 (92%)	4 (8%)	12	42
2	MG	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	MJ	51/56 (91%)	47 (92%)	4 (8%)	12	42
2	MK	51/56 (91%)	47 (92%)	4 (8%)	12	42
2	ML	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	MP	51/56 (91%)	47 (92%)	4 (8%)	12	42
2	MQ	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	MR	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	MS	51/56 (91%)	50 (98%)	1 (2%)	55	75
2	N1	50/56 (89%)	50 (100%)	0	100	100
2	N3	50/56 (89%)	50 (100%)	0	100	100
2	N4	50/56 (89%)	50 (100%)	0	100	100
2	N6	50/56 (89%)	50 (100%)	0	100	100
2	N7	50/56 (89%)	50 (100%)	0	100	100
2	N8	50/56 (89%)	50 (100%)	0	100	100
2	ND	51/56 (91%)	50 (98%)	1 (2%)	55	75
2	NG	50/56 (89%)	50 (100%)	0	100	100
2	NJ	51/56 (91%)	50 (98%)	1 (2%)	55	75
2	NK	51/56 (91%)	50 (98%)	1 (2%)	55	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	NL	50/56 (89%)	50 (100%)	0	100 100
2	NP	51/56 (91%)	50 (98%)	1 (2%)	55 75
2	NQ	50/56 (89%)	50 (100%)	0	100 100
2	NR	50/56 (89%)	50 (100%)	0	100 100
2	O1	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	O3	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	O4	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	O6	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	O7	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	O8	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	OE	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	OG	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	OL	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	OQ	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	OR	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	P1	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	P3	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	P4	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	P6	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	P7	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	P8	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	PE	50/56 (89%)	50 (100%)	0	100 100
2	PG	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	PL	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	PQ	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	PR	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	QE	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	RE	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	U1	50/56 (89%)	50 (100%)	0	100 100
2	U3	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	U4	50/56 (89%)	50 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	U6	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	U7	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	U8	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	UG	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	UL	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	UQ	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	UR	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	V1	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	V3	50/56 (89%)	50 (100%)	0	100 100
2	V4	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	V6	50/56 (89%)	50 (100%)	0	100 100
2	V7	50/56 (89%)	50 (100%)	0	100 100
2	V8	50/56 (89%)	50 (100%)	0	100 100
2	VG	50/56 (89%)	50 (100%)	0	100 100
2	VL	50/56 (89%)	50 (100%)	0	100 100
2	VQ	50/56 (89%)	50 (100%)	0	100 100
2	VR	50/56 (89%)	50 (100%)	0	100 100
2	W1	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	W3	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	W4	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	W6	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	W7	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	W8	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	WE	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	WG	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	WL	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	WQ	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	WR	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	X3	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	X6	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	X7	49/56 (88%)	48 (98%)	1 (2%)	55 75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	X8	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	XE	50/56 (89%)	50 (100%)	0	100 100
2	XG	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	XL	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	XQ	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	XR	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	YE	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	Z3	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	ZE	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	ZQ	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	a3	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	aQ	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	b1	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	b4	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	c1	50/56 (89%)	50 (100%)	0	100 100
2	c3	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	c4	50/56 (89%)	50 (100%)	0	100 100
2	c6	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	c7	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	c8	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	cG	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	cL	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	cR	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	d1	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	d3	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	d4	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	d6	50/56 (89%)	50 (100%)	0	100 100
2	d7	50/56 (89%)	50 (100%)	0	100 100
2	d8	50/56 (89%)	50 (100%)	0	100 100
2	dG	50/56 (89%)	50 (100%)	0	100 100
2	dL	50/56 (89%)	50 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	dR	50/56 (89%)	50 (100%)	0	100	100
2	e1	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	e4	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	e6	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	e7	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	e8	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	eE	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	eG	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	eL	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	eR	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	f6	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	f7	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	f8	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	fE	50/56 (89%)	50 (100%)	0	100	100
2	fG	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	fL	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	fQ	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	fR	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	gE	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	gQ	50/56 (89%)	50 (100%)	0	100	100
2	hE	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	hL	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	hQ	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	iL	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	iQ	49/56 (88%)	48 (98%)	1 (2%)	55	75
2	j1	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	j4	50/56 (89%)	50 (100%)	0	100	100
2	k1	50/56 (89%)	50 (100%)	0	100	100
2	k4	25/56 (45%)	23 (92%)	2 (8%)	12	42
2	k6	50/56 (89%)	47 (94%)	3 (6%)	19	50
2	k7	50/56 (89%)	47 (94%)	3 (6%)	19	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	k8	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	kG	50/56 (89%)	47 (94%)	3 (6%)	19 50
2	kR	50/56 (89%)	50 (100%)	0	100 100
2	l1	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	l4	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	l6	50/56 (89%)	50 (100%)	0	100 100
2	l7	50/56 (89%)	50 (100%)	0	100 100
2	l8	50/56 (89%)	50 (100%)	0	100 100
2	lG	50/56 (89%)	50 (100%)	0	100 100
2	lR	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	m1	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	m6	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	m7	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	m8	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	mG	25/56 (45%)	23 (92%)	2 (8%)	12 42
2	mR	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	n6	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	n7	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	n8	49/56 (88%)	48 (98%)	1 (2%)	55 75
2	nG	49/56 (88%)	48 (98%)	1 (2%)	55 75
3	A2	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	A5	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	A9	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AA	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AB	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AC	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AF	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AH	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AI	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AM	258/304 (85%)	256 (99%)	2 (1%)	81 89
3	AN	258/304 (85%)	256 (99%)	2 (1%)	81 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AO	258/304 (85%)	256 (99%)	2 (1%)	81 89
4	B2	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	B5	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	B9	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BA	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BB	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BC	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BF	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BH	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BI	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BM	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BN	193/233 (83%)	192 (100%)	1 (0%)	88 94
4	BO	193/233 (83%)	192 (100%)	1 (0%)	88 94
5	C2	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	C5	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	C9	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CA	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CB	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CC	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CF	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CH	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CI	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CM	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CN	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	CO	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	D2	115/567 (20%)	115 (100%)	0	100 100
5	D5	115/567 (20%)	115 (100%)	0	100 100
5	D9	115/567 (20%)	115 (100%)	0	100 100
5	DA	115/567 (20%)	115 (100%)	0	100 100
5	DB	115/567 (20%)	115 (100%)	0	100 100
5	DC	115/567 (20%)	115 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	DF	115/567 (20%)	115 (100%)	0	100	100
5	DH	115/567 (20%)	115 (100%)	0	100	100
5	DI	115/567 (20%)	115 (100%)	0	100	100
5	DM	115/567 (20%)	115 (100%)	0	100	100
5	DN	115/567 (20%)	115 (100%)	0	100	100
5	DO	115/567 (20%)	115 (100%)	0	100	100
5	E2	126/567 (22%)	126 (100%)	0	100	100
5	E5	126/567 (22%)	126 (100%)	0	100	100
5	E9	126/567 (22%)	126 (100%)	0	100	100
5	EA	126/567 (22%)	126 (100%)	0	100	100
5	EB	126/567 (22%)	126 (100%)	0	100	100
5	EC	126/567 (22%)	126 (100%)	0	100	100
5	EF	126/567 (22%)	126 (100%)	0	100	100
5	EH	126/567 (22%)	126 (100%)	0	100	100
5	EI	126/567 (22%)	126 (100%)	0	100	100
5	EM	126/567 (22%)	126 (100%)	0	100	100
5	EN	126/567 (22%)	126 (100%)	0	100	100
5	EO	126/567 (22%)	126 (100%)	0	100	100
5	F2	97/567 (17%)	97 (100%)	0	100	100
5	F5	97/567 (17%)	97 (100%)	0	100	100
5	F9	97/567 (17%)	97 (100%)	0	100	100
5	FA	97/567 (17%)	97 (100%)	0	100	100
5	FB	97/567 (17%)	97 (100%)	0	100	100
5	FC	97/567 (17%)	97 (100%)	0	100	100
5	FF	97/567 (17%)	97 (100%)	0	100	100
5	FH	97/567 (17%)	97 (100%)	0	100	100
5	FI	97/567 (17%)	97 (100%)	0	100	100
5	FM	97/567 (17%)	97 (100%)	0	100	100
5	FN	97/567 (17%)	97 (100%)	0	100	100
5	FO	97/567 (17%)	97 (100%)	0	100	100
5	N2	432/567 (76%)	431 (100%)	1 (0%)	93	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	N5	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	N9	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NA	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NB	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NC	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NF	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NH	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NI	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NM	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NN	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	NO	432/567 (76%)	431 (100%)	1 (0%)	93 97
5	O2	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	O5	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	O9	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OA	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OB	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OC	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OF	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OH	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OI	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OM	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	ON	431/567 (76%)	430 (100%)	1 (0%)	93 97
5	OO	431/567 (76%)	430 (100%)	1 (0%)	93 97
6	K2	1/132 (1%)	1 (100%)	0	100 100
6	K5	1/132 (1%)	1 (100%)	0	100 100
6	K9	1/132 (1%)	1 (100%)	0	100 100
6	KA	1/132 (1%)	1 (100%)	0	100 100
6	KB	1/132 (1%)	1 (100%)	0	100 100
6	KC	1/132 (1%)	1 (100%)	0	100 100
6	KF	1/132 (1%)	1 (100%)	0	100 100
6	KH	1/132 (1%)	1 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	KI	1/132 (1%)	1 (100%)	0	100	100
6	KM	1/132 (1%)	1 (100%)	0	100	100
6	KN	1/132 (1%)	1 (100%)	0	100	100
6	KO	1/132 (1%)	1 (100%)	0	100	100
All	All	116815/148257 (79%)	115173 (99%)	1642 (1%)	68	81

5 of 1642 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BG	259	PHE
2	FK	22	LYS
1	CS	45	MET
1	LG	98	ASN
1	BG	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 765 such sidechains are listed below:

Mol	Chain	Res	Type
1	SG	150	ASN
1	QL	365	HIS
1	gG	27	HIS
1	RG	348	ASN
1	DJ	143	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	R1	1
1	Y1	1
1	g1	1
1	J6	1
1	R6	1
1	A7	1
1	J7	1
1	R7	1
1	AG	1
1	hG	1
1	AL	1
1	JL	1
1	RL	1
1	ZL	1
1	AQ	1
1	RQ	1
1	cQ	1
1	RR	1
1	ZR	1
1	hR	1
1	A1	1
1	J1	1
1	A3	1
1	J3	1
1	R3	1
1	A4	1
1	J4	1
1	R4	1
1	Y4	1
1	g4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	A6	1
1	Z6	1
1	h6	1
1	Z7	1
1	h7	1
1	A8	1
1	J8	1
1	R8	1
1	Z8	1
1	h8	1
1	BE	1
1	LE	1
1	TE	1
1	bE	1
1	JG	1
1	RG	1
1	ZG	1
1	JQ	1
1	AR	1
1	JR	1

The worst 5 of 50 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R1	20:SER	C	21:ALA	N	3.93
1	Y1	20:SER	C	21:ALA	N	3.93
1	g1	20:SER	C	21:ALA	N	3.93
1	J6	20:SER	C	21:ALA	N	3.93
1	R6	20:SER	C	21:ALA	N	3.93

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4459. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.