wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 04:16 pm GMT

PDB ID	:	5MQ3
EMDB ID	:	EMD-3543
Title	:	Structure of AaLS-neg
Authors	:	Sasaki, E.; Boehringer, D.; Leibundgut, M.; Ban, N.; Hilvert, D.
Deposited on	:	2016-12-20
Resolution	:	5.40 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

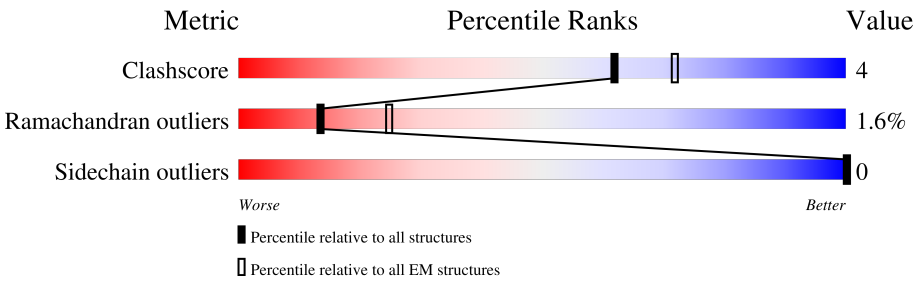
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.40 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)
Clashscore	158937	4297
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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	161	53% 92% 8%
1	AB	161	50% 89% 11% •
1	AC	161	61% 94% 6%
1	AD	161	61% 91% 9%
1	AE	161	62% 94% 6%
1	AF	161	68% 93% 7%
1	AG	161	65% 94% 6%
1	AH	161	54% 90% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AI	161	47% 94% 6%
1	AJ	161	63% 95% 5%
1	AK	161	61% 89% 11%
1	AL	161	64% 90% 10%
1	AM	161	68% 94% 6%
1	AN	161	65% 91% 9%
1	AO	161	48% 92% 8%
1	BA	161	63% 92% 8%
1	BB	161	66% 88% 12%
1	BC	161	60% 94% 6%
1	BD	161	61% 91% 9%
1	BE	161	67% 90% 10%
1	BF	161	65% 93% 7%
1	BG	161	62% 94% 6%
1	BH	161	63% 90% 9%
1	BI	161	57% 93% 7%
1	BJ	161	52% 96%
1	BK	161	54% 89% 11%
1	BL	161	54% 91% 9%
1	BM	161	66% 94% 6%
1	BN	161	66% 92% 8%
1	BO	161	68% 93% 7%
1	CA	161	53% 91% 9%
1	CB	161	56% 89% 11%
1	CC	161	68% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CD	161	60% 91% 9%
1	CE	161	56% 90% 10%
1	CF	161	36% 92% 8%
1	CG	161	35% 94% 6%
1	CH	161	41% 90% 9%
1	CI	161	50% 93% 7%
1	CJ	161	50% 95% 5%
1	CK	161	49% 89% 11%
1	CL	161	56% 90% 10%
1	CM	161	42% 94% 6%
1	CN	161	39% 91% 9%
1	CO	161	47% 92% 8%
1	DA	161	47% 91% 9%
1	DB	161	38% 89% 11%
1	DC	161	34% 94% 6%
1	DD	161	36% 91% 9%
1	DE	161	45% 91% 9%
1	DF	161	50% 93% 7%
1	DG	161	61% 94% 6%
1	DH	161	59% 90% 9%
1	DI	161	47% 94% 6%
1	DJ	161	45% 95% 5%
1	DK	161	42% 89% 11%
1	DL	161	50% 91% 9%
1	DM	161	57% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DN	161	60% 91% 9%
1	DO	161	49% 93% 7%
1	EA	161	58% 91% 9%
1	EB	161	66% 90% 9%
1	EC	161	62% 94% 6%
1	ED	161	62% 91% 9%
1	EE	161	55% 93% 7%
1	EF	161	65% 93% 7%
1	EG	161	55% 94% 6%
1	EH	161	59% 91% 8%
1	EI	161	68% 93% 7%
1	EJ	161	63% 94% 6%
1	EK	161	56% 89% 11%
1	EL	161	59% 91% 9%
1	EM	161	55% 94% 6%
1	EN	161	57% 91% 9%
1	EO	161	63% 92% 8%
1	FA	161	66% 91% 9%
1	FB	161	66% 89% 11%
1	FC	161	70% 94% 6%
1	FD	161	62% 91% 9%
1	FE	161	60% 94% 6%
1	FF	161	47% 93% 7%
1	FG	161	61% 94% 6%
1	FH	161	65% 91% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FI	161	65% 93% 7%
1	FJ	161	63% 95% 5%
1	FK	161	67% 90% 10%
1	FL	161	63% 91% 9%
1	FM	161	48% 94% 6%
1	FN	161	61% 91% 9%
1	FO	161	63% 93% 7%
1	GA	161	68% 92% 8%
1	GB	161	66% 89% 11%
1	GC	161	73% 94% 6%
1	GD	161	55% 91% 9%
1	GE	161	61% 91% 9%
1	GF	161	50% 92% 8%
1	GG	161	60% 94% 6%
1	GH	161	68% 91% 8%
1	GI	161	63% 93% 7%
1	GJ	161	52% 95% 5%
1	GK	161	63% 90% 10%
1	GL	161	58% 93% 7%
1	GM	161	48% 94% 6%
1	GN	161	61% 91% 9%
1	GO	161	67% 92% 8%
1	HA	161	60% 91% 9%
1	HB	161	60% 89% 11%
1	HC	161	61% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	HD	161	66% 91% 9%
1	HE	161	61% 91% 9%
1	HF	161	61% 93% 7%
1	HG	161	58% 94% 6%
1	HH	161	51% 93% 7%
1	HI	161	50% 94% 6%
1	HJ	161	53% 94% 6%
1	HK	161	56% 89% 11%
1	HL	161	59% 91% 9%
1	HM	161	65% 94% 6%
1	HN	161	62% 91% 9%
1	HO	161	68% 93% 7%
1	IA	161	56% 92% 8%
1	IB	161	63% 88% 12%
1	IC	161	64% 94% 6%
1	ID	161	66% 91% 9%
1	IE	161	61% 91% 9%
1	IF	161	64% 93% 7%
1	IG	161	60% 94% 6%
1	IH	161	57% 91% 8%
1	II	161	65% 94% 6%
1	IJ	161	66% 93% 7%
1	IK	161	59% 90% 10%
1	IL	161	58% 90% 10%
1	IM	161	56% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	IN	161	58% 91% 9%
1	IO	161	63% 93% 7%
1	JA	161	32% 92% 8%
1	JB	161	29% 88% 12%
1	JC	161	36% 94% 6%
1	JD	161	39% 91% 9%
1	JE	161	32% 93% 7%
1	JF	161	43% 93% 7%
1	JG	161	56% 94% 6%
1	JH	161	44% 91% 8%
1	JI	161	30% 91% 9%
1	JJ	161	33% 94% 6%
1	JK	161	36% 89% 11%
1	JL	161	48% 90% 10%
1	JM	161	58% 94% 6%
1	JN	161	53% 91% 9%
1	JO	161	39% 94% 6%
1	KA	161	55% 91% 9%
1	KB	161	56% 89% 11%
1	KC	161	68% 94% 6%
1	KD	161	61% 91% 9%
1	KE	161	62% 94% 6%
1	KF	161	50% 93% 7%
1	KG	161	49% 94% 6%
1	KH	161	53% 90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	KI	161	57% 94% 6%
1	KJ	161	53% 95% 5%
1	KK	161	55% 89% 11%
1	KL	161	53% 90% 10%
1	KM	161	42% 94% 6%
1	KN	161	44% 91% 9%
1	KO	161	49% 94% 6%
1	LA	161	61% 91% 9%
1	LB	161	58% 89% 11%
1	LC	161	56% 94% 6%
1	LD	161	56% 91% 9%
1	LE	161	60% 93% 7%
1	LF	161	61% 94% 6%
1	LG	161	63% 94% 6%
1	LH	161	62% 90% 9%
1	LI	161	41% 93% 7%
1	LJ	161	55% 94% 6%
1	LK	161	48% 90% 10%
1	LL	161	61% 91% 9%
1	LM	161	65% 94% 6%
1	LN	161	60% 91% 9%
1	LO	161	47% 93% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 143640 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 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	AA	161	798	476	161	161	0	0
1	AB	161	798	476	161	161	0	0
1	AC	161	798	476	161	161	0	0
1	AD	161	798	476	161	161	0	0
1	AE	161	798	476	161	161	0	0
1	AF	161	798	476	161	161	0	0
1	AG	161	798	476	161	161	0	0
1	AH	161	798	476	161	161	0	0
1	AI	161	798	476	161	161	0	0
1	AJ	161	798	476	161	161	0	0
1	AK	161	798	476	161	161	0	0
1	AL	161	798	476	161	161	0	0
1	AM	161	798	476	161	161	0	0
1	AN	161	798	476	161	161	0	0
1	AO	161	798	476	161	161	0	0
1	BA	161	798	476	161	161	0	0
1	BB	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	BC	161	798	476	161	161	0	0
1	BD	161	798	476	161	161	0	0
1	BE	161	798	476	161	161	0	0
1	BF	161	798	476	161	161	0	0
1	BG	161	798	476	161	161	0	0
1	BH	161	798	476	161	161	0	0
1	BI	161	798	476	161	161	0	0
1	BJ	161	798	476	161	161	0	0
1	BK	161	798	476	161	161	0	0
1	BL	161	798	476	161	161	0	0
1	BM	161	798	476	161	161	0	0
1	BN	161	798	476	161	161	0	0
1	BO	161	798	476	161	161	0	0
1	CA	161	798	476	161	161	0	0
1	CB	161	798	476	161	161	0	0
1	CC	161	798	476	161	161	0	0
1	CD	161	798	476	161	161	0	0
1	CE	161	798	476	161	161	0	0
1	CF	161	798	476	161	161	0	0
1	CG	161	798	476	161	161	0	0
1	CH	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	CI	161	798	476	161	161	0	0
1	CJ	161	798	476	161	161	0	0
1	CK	161	798	476	161	161	0	0
1	CL	161	798	476	161	161	0	0
1	CM	161	798	476	161	161	0	0
1	CN	161	798	476	161	161	0	0
1	CO	161	798	476	161	161	0	0
1	DA	161	798	476	161	161	0	0
1	DB	161	798	476	161	161	0	0
1	DC	161	798	476	161	161	0	0
1	DD	161	798	476	161	161	0	0
1	DE	161	798	476	161	161	0	0
1	DF	161	798	476	161	161	0	0
1	DG	161	798	476	161	161	0	0
1	DH	161	798	476	161	161	0	0
1	DI	161	798	476	161	161	0	0
1	DJ	161	798	476	161	161	0	0
1	DK	161	798	476	161	161	0	0
1	DL	161	798	476	161	161	0	0
1	DM	161	798	476	161	161	0	0
1	DN	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	DO	161	798	476	161	161	0	0
1	EA	161	798	476	161	161	0	0
1	EB	161	798	476	161	161	0	0
1	EC	161	798	476	161	161	0	0
1	ED	161	798	476	161	161	0	0
1	EE	161	798	476	161	161	0	0
1	EF	161	798	476	161	161	0	0
1	EG	161	798	476	161	161	0	0
1	EH	161	798	476	161	161	0	0
1	EI	161	798	476	161	161	0	0
1	EJ	161	798	476	161	161	0	0
1	EK	161	798	476	161	161	0	0
1	EL	161	798	476	161	161	0	0
1	EM	161	798	476	161	161	0	0
1	EN	161	798	476	161	161	0	0
1	EO	161	798	476	161	161	0	0
1	FA	161	798	476	161	161	0	0
1	FB	161	798	476	161	161	0	0
1	FC	161	798	476	161	161	0	0
1	FD	161	798	476	161	161	0	0
1	FE	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	FF	161	798	476	161	161	0	0
1	FG	161	798	476	161	161	0	0
1	FH	161	798	476	161	161	0	0
1	FI	161	798	476	161	161	0	0
1	FJ	161	798	476	161	161	0	0
1	FK	161	798	476	161	161	0	0
1	FL	161	798	476	161	161	0	0
1	FM	161	798	476	161	161	0	0
1	FN	161	798	476	161	161	0	0
1	FO	161	798	476	161	161	0	0
1	GA	161	798	476	161	161	0	0
1	GB	161	798	476	161	161	0	0
1	GC	161	798	476	161	161	0	0
1	GD	161	798	476	161	161	0	0
1	GE	161	798	476	161	161	0	0
1	GF	161	798	476	161	161	0	0
1	GG	161	798	476	161	161	0	0
1	GH	161	798	476	161	161	0	0
1	GI	161	798	476	161	161	0	0
1	GJ	161	798	476	161	161	0	0
1	GK	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	GL	161	798	476	161	161	0	0
1	GM	161	798	476	161	161	0	0
1	GN	161	798	476	161	161	0	0
1	GO	161	798	476	161	161	0	0
1	HA	161	798	476	161	161	0	0
1	HB	161	798	476	161	161	0	0
1	HC	161	798	476	161	161	0	0
1	HD	161	798	476	161	161	0	0
1	HE	161	798	476	161	161	0	0
1	HF	161	798	476	161	161	0	0
1	HG	161	798	476	161	161	0	0
1	HH	161	798	476	161	161	0	0
1	HI	161	798	476	161	161	0	0
1	HJ	161	798	476	161	161	0	0
1	HK	161	798	476	161	161	0	0
1	HL	161	798	476	161	161	0	0
1	HM	161	798	476	161	161	0	0
1	HN	161	798	476	161	161	0	0
1	HO	161	798	476	161	161	0	0
1	IA	161	798	476	161	161	0	0
1	IB	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	IC	161	798	476	161	161	0	0
1	ID	161	798	476	161	161	0	0
1	IE	161	798	476	161	161	0	0
1	IF	161	798	476	161	161	0	0
1	IG	161	798	476	161	161	0	0
1	IH	161	798	476	161	161	0	0
1	II	161	798	476	161	161	0	0
1	IJ	161	798	476	161	161	0	0
1	IK	161	798	476	161	161	0	0
1	IL	161	798	476	161	161	0	0
1	IM	161	798	476	161	161	0	0
1	IN	161	798	476	161	161	0	0
1	IO	161	798	476	161	161	0	0
1	JA	161	798	476	161	161	0	0
1	JB	161	798	476	161	161	0	0
1	JC	161	798	476	161	161	0	0
1	JD	161	798	476	161	161	0	0
1	JE	161	798	476	161	161	0	0
1	JF	161	798	476	161	161	0	0
1	JG	161	798	476	161	161	0	0
1	JH	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	JI	161	798	476	161	161	0	0
1	JJ	161	798	476	161	161	0	0
1	JK	161	798	476	161	161	0	0
1	JL	161	798	476	161	161	0	0
1	JM	161	798	476	161	161	0	0
1	JN	161	798	476	161	161	0	0
1	JO	161	798	476	161	161	0	0
1	KA	161	798	476	161	161	0	0
1	KB	161	798	476	161	161	0	0
1	KC	161	798	476	161	161	0	0
1	KD	161	798	476	161	161	0	0
1	KE	161	798	476	161	161	0	0
1	KF	161	798	476	161	161	0	0
1	KG	161	798	476	161	161	0	0
1	KH	161	798	476	161	161	0	0
1	KI	161	798	476	161	161	0	0
1	KJ	161	798	476	161	161	0	0
1	KK	161	798	476	161	161	0	0
1	KL	161	798	476	161	161	0	0
1	KM	161	798	476	161	161	0	0
1	KN	161	798	476	161	161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	KO	161	798	476	161	161	0	0
1	LA	161	798	476	161	161	0	0
1	LB	161	798	476	161	161	0	0
1	LC	161	798	476	161	161	0	0
1	LD	161	798	476	161	161	0	0
1	LE	161	798	476	161	161	0	0
1	LF	161	798	476	161	161	0	0
1	LG	161	798	476	161	161	0	0
1	LH	161	798	476	161	161	0	0
1	LI	161	798	476	161	161	0	0
1	LJ	161	798	476	161	161	0	0
1	LK	161	798	476	161	161	0	0
1	LL	161	798	476	161	161	0	0
1	LM	161	798	476	161	161	0	0
1	LN	161	798	476	161	161	0	0
1	LO	161	798	476	161	161	0	0

There are 2160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	2	GLU	GLN	conflict	UNP O66529
AA	83	GLU	ARG	conflict	UNP O66529
AA	86	GLU	THR	conflict	UNP O66529
AA	120	GLU	THR	conflict	UNP O66529
AA	123	GLU	GLN	conflict	UNP O66529
AA	155	LEU	-	expression tag	UNP O66529
AA	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AA	157	HIS	-	expression tag	UNP O66529
AA	158	HIS	-	expression tag	UNP O66529
AA	159	HIS	-	expression tag	UNP O66529
AA	160	HIS	-	expression tag	UNP O66529
AA	161	HIS	-	expression tag	UNP O66529
AB	2	GLU	GLN	conflict	UNP O66529
AB	83	GLU	ARG	conflict	UNP O66529
AB	86	GLU	THR	conflict	UNP O66529
AB	120	GLU	THR	conflict	UNP O66529
AB	123	GLU	GLN	conflict	UNP O66529
AB	155	LEU	-	expression tag	UNP O66529
AB	156	GLU	-	expression tag	UNP O66529
AB	157	HIS	-	expression tag	UNP O66529
AB	158	HIS	-	expression tag	UNP O66529
AB	159	HIS	-	expression tag	UNP O66529
AB	160	HIS	-	expression tag	UNP O66529
AB	161	HIS	-	expression tag	UNP O66529
AC	2	GLU	GLN	conflict	UNP O66529
AC	83	GLU	ARG	conflict	UNP O66529
AC	86	GLU	THR	conflict	UNP O66529
AC	120	GLU	THR	conflict	UNP O66529
AC	123	GLU	GLN	conflict	UNP O66529
AC	155	LEU	-	expression tag	UNP O66529
AC	156	GLU	-	expression tag	UNP O66529
AC	157	HIS	-	expression tag	UNP O66529
AC	158	HIS	-	expression tag	UNP O66529
AC	159	HIS	-	expression tag	UNP O66529
AC	160	HIS	-	expression tag	UNP O66529
AC	161	HIS	-	expression tag	UNP O66529
AD	2	GLU	GLN	conflict	UNP O66529
AD	83	GLU	ARG	conflict	UNP O66529
AD	86	GLU	THR	conflict	UNP O66529
AD	120	GLU	THR	conflict	UNP O66529
AD	123	GLU	GLN	conflict	UNP O66529
AD	155	LEU	-	expression tag	UNP O66529
AD	156	GLU	-	expression tag	UNP O66529
AD	157	HIS	-	expression tag	UNP O66529
AD	158	HIS	-	expression tag	UNP O66529
AD	159	HIS	-	expression tag	UNP O66529
AD	160	HIS	-	expression tag	UNP O66529
AD	161	HIS	-	expression tag	UNP O66529
AE	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AE	83	GLU	ARG	conflict	UNP O66529
AE	86	GLU	THR	conflict	UNP O66529
AE	120	GLU	THR	conflict	UNP O66529
AE	123	GLU	GLN	conflict	UNP O66529
AE	155	LEU	-	expression tag	UNP O66529
AE	156	GLU	-	expression tag	UNP O66529
AE	157	HIS	-	expression tag	UNP O66529
AE	158	HIS	-	expression tag	UNP O66529
AE	159	HIS	-	expression tag	UNP O66529
AE	160	HIS	-	expression tag	UNP O66529
AE	161	HIS	-	expression tag	UNP O66529
AF	2	GLU	GLN	conflict	UNP O66529
AF	83	GLU	ARG	conflict	UNP O66529
AF	86	GLU	THR	conflict	UNP O66529
AF	120	GLU	THR	conflict	UNP O66529
AF	123	GLU	GLN	conflict	UNP O66529
AF	155	LEU	-	expression tag	UNP O66529
AF	156	GLU	-	expression tag	UNP O66529
AF	157	HIS	-	expression tag	UNP O66529
AF	158	HIS	-	expression tag	UNP O66529
AF	159	HIS	-	expression tag	UNP O66529
AF	160	HIS	-	expression tag	UNP O66529
AF	161	HIS	-	expression tag	UNP O66529
AG	2	GLU	GLN	conflict	UNP O66529
AG	83	GLU	ARG	conflict	UNP O66529
AG	86	GLU	THR	conflict	UNP O66529
AG	120	GLU	THR	conflict	UNP O66529
AG	123	GLU	GLN	conflict	UNP O66529
AG	155	LEU	-	expression tag	UNP O66529
AG	156	GLU	-	expression tag	UNP O66529
AG	157	HIS	-	expression tag	UNP O66529
AG	158	HIS	-	expression tag	UNP O66529
AG	159	HIS	-	expression tag	UNP O66529
AG	160	HIS	-	expression tag	UNP O66529
AG	161	HIS	-	expression tag	UNP O66529
AH	2	GLU	GLN	conflict	UNP O66529
AH	83	GLU	ARG	conflict	UNP O66529
AH	86	GLU	THR	conflict	UNP O66529
AH	120	GLU	THR	conflict	UNP O66529
AH	123	GLU	GLN	conflict	UNP O66529
AH	155	LEU	-	expression tag	UNP O66529
AH	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AH	157	HIS	-	expression tag	UNP O66529
AH	158	HIS	-	expression tag	UNP O66529
AH	159	HIS	-	expression tag	UNP O66529
AH	160	HIS	-	expression tag	UNP O66529
AH	161	HIS	-	expression tag	UNP O66529
AI	2	GLU	GLN	conflict	UNP O66529
AI	83	GLU	ARG	conflict	UNP O66529
AI	86	GLU	THR	conflict	UNP O66529
AI	120	GLU	THR	conflict	UNP O66529
AI	123	GLU	GLN	conflict	UNP O66529
AI	155	LEU	-	expression tag	UNP O66529
AI	156	GLU	-	expression tag	UNP O66529
AI	157	HIS	-	expression tag	UNP O66529
AI	158	HIS	-	expression tag	UNP O66529
AI	159	HIS	-	expression tag	UNP O66529
AI	160	HIS	-	expression tag	UNP O66529
AI	161	HIS	-	expression tag	UNP O66529
AJ	2	GLU	GLN	conflict	UNP O66529
AJ	83	GLU	ARG	conflict	UNP O66529
AJ	86	GLU	THR	conflict	UNP O66529
AJ	120	GLU	THR	conflict	UNP O66529
AJ	123	GLU	GLN	conflict	UNP O66529
AJ	155	LEU	-	expression tag	UNP O66529
AJ	156	GLU	-	expression tag	UNP O66529
AJ	157	HIS	-	expression tag	UNP O66529
AJ	158	HIS	-	expression tag	UNP O66529
AJ	159	HIS	-	expression tag	UNP O66529
AJ	160	HIS	-	expression tag	UNP O66529
AJ	161	HIS	-	expression tag	UNP O66529
AK	2	GLU	GLN	conflict	UNP O66529
AK	83	GLU	ARG	conflict	UNP O66529
AK	86	GLU	THR	conflict	UNP O66529
AK	120	GLU	THR	conflict	UNP O66529
AK	123	GLU	GLN	conflict	UNP O66529
AK	155	LEU	-	expression tag	UNP O66529
AK	156	GLU	-	expression tag	UNP O66529
AK	157	HIS	-	expression tag	UNP O66529
AK	158	HIS	-	expression tag	UNP O66529
AK	159	HIS	-	expression tag	UNP O66529
AK	160	HIS	-	expression tag	UNP O66529
AK	161	HIS	-	expression tag	UNP O66529
AL	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AL	83	GLU	ARG	conflict	UNP O66529
AL	86	GLU	THR	conflict	UNP O66529
AL	120	GLU	THR	conflict	UNP O66529
AL	123	GLU	GLN	conflict	UNP O66529
AL	155	LEU	-	expression tag	UNP O66529
AL	156	GLU	-	expression tag	UNP O66529
AL	157	HIS	-	expression tag	UNP O66529
AL	158	HIS	-	expression tag	UNP O66529
AL	159	HIS	-	expression tag	UNP O66529
AL	160	HIS	-	expression tag	UNP O66529
AL	161	HIS	-	expression tag	UNP O66529
AM	2	GLU	GLN	conflict	UNP O66529
AM	83	GLU	ARG	conflict	UNP O66529
AM	86	GLU	THR	conflict	UNP O66529
AM	120	GLU	THR	conflict	UNP O66529
AM	123	GLU	GLN	conflict	UNP O66529
AM	155	LEU	-	expression tag	UNP O66529
AM	156	GLU	-	expression tag	UNP O66529
AM	157	HIS	-	expression tag	UNP O66529
AM	158	HIS	-	expression tag	UNP O66529
AM	159	HIS	-	expression tag	UNP O66529
AM	160	HIS	-	expression tag	UNP O66529
AM	161	HIS	-	expression tag	UNP O66529
AN	2	GLU	GLN	conflict	UNP O66529
AN	83	GLU	ARG	conflict	UNP O66529
AN	86	GLU	THR	conflict	UNP O66529
AN	120	GLU	THR	conflict	UNP O66529
AN	123	GLU	GLN	conflict	UNP O66529
AN	155	LEU	-	expression tag	UNP O66529
AN	156	GLU	-	expression tag	UNP O66529
AN	157	HIS	-	expression tag	UNP O66529
AN	158	HIS	-	expression tag	UNP O66529
AN	159	HIS	-	expression tag	UNP O66529
AN	160	HIS	-	expression tag	UNP O66529
AN	161	HIS	-	expression tag	UNP O66529
AO	2	GLU	GLN	conflict	UNP O66529
AO	83	GLU	ARG	conflict	UNP O66529
AO	86	GLU	THR	conflict	UNP O66529
AO	120	GLU	THR	conflict	UNP O66529
AO	123	GLU	GLN	conflict	UNP O66529
AO	155	LEU	-	expression tag	UNP O66529
AO	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AO	157	HIS	-	expression tag	UNP O66529
AO	158	HIS	-	expression tag	UNP O66529
AO	159	HIS	-	expression tag	UNP O66529
AO	160	HIS	-	expression tag	UNP O66529
AO	161	HIS	-	expression tag	UNP O66529
BA	2	GLU	GLN	conflict	UNP O66529
BA	83	GLU	ARG	conflict	UNP O66529
BA	86	GLU	THR	conflict	UNP O66529
BA	120	GLU	THR	conflict	UNP O66529
BA	123	GLU	GLN	conflict	UNP O66529
BA	155	LEU	-	expression tag	UNP O66529
BA	156	GLU	-	expression tag	UNP O66529
BA	157	HIS	-	expression tag	UNP O66529
BA	158	HIS	-	expression tag	UNP O66529
BA	159	HIS	-	expression tag	UNP O66529
BA	160	HIS	-	expression tag	UNP O66529
BA	161	HIS	-	expression tag	UNP O66529
BB	2	GLU	GLN	conflict	UNP O66529
BB	83	GLU	ARG	conflict	UNP O66529
BB	86	GLU	THR	conflict	UNP O66529
BB	120	GLU	THR	conflict	UNP O66529
BB	123	GLU	GLN	conflict	UNP O66529
BB	155	LEU	-	expression tag	UNP O66529
BB	156	GLU	-	expression tag	UNP O66529
BB	157	HIS	-	expression tag	UNP O66529
BB	158	HIS	-	expression tag	UNP O66529
BB	159	HIS	-	expression tag	UNP O66529
BB	160	HIS	-	expression tag	UNP O66529
BB	161	HIS	-	expression tag	UNP O66529
BC	2	GLU	GLN	conflict	UNP O66529
BC	83	GLU	ARG	conflict	UNP O66529
BC	86	GLU	THR	conflict	UNP O66529
BC	120	GLU	THR	conflict	UNP O66529
BC	123	GLU	GLN	conflict	UNP O66529
BC	155	LEU	-	expression tag	UNP O66529
BC	156	GLU	-	expression tag	UNP O66529
BC	157	HIS	-	expression tag	UNP O66529
BC	158	HIS	-	expression tag	UNP O66529
BC	159	HIS	-	expression tag	UNP O66529
BC	160	HIS	-	expression tag	UNP O66529
BC	161	HIS	-	expression tag	UNP O66529
BD	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BD	83	GLU	ARG	conflict	UNP O66529
BD	86	GLU	THR	conflict	UNP O66529
BD	120	GLU	THR	conflict	UNP O66529
BD	123	GLU	GLN	conflict	UNP O66529
BD	155	LEU	-	expression tag	UNP O66529
BD	156	GLU	-	expression tag	UNP O66529
BD	157	HIS	-	expression tag	UNP O66529
BD	158	HIS	-	expression tag	UNP O66529
BD	159	HIS	-	expression tag	UNP O66529
BD	160	HIS	-	expression tag	UNP O66529
BD	161	HIS	-	expression tag	UNP O66529
BE	2	GLU	GLN	conflict	UNP O66529
BE	83	GLU	ARG	conflict	UNP O66529
BE	86	GLU	THR	conflict	UNP O66529
BE	120	GLU	THR	conflict	UNP O66529
BE	123	GLU	GLN	conflict	UNP O66529
BE	155	LEU	-	expression tag	UNP O66529
BE	156	GLU	-	expression tag	UNP O66529
BE	157	HIS	-	expression tag	UNP O66529
BE	158	HIS	-	expression tag	UNP O66529
BE	159	HIS	-	expression tag	UNP O66529
BE	160	HIS	-	expression tag	UNP O66529
BE	161	HIS	-	expression tag	UNP O66529
BF	2	GLU	GLN	conflict	UNP O66529
BF	83	GLU	ARG	conflict	UNP O66529
BF	86	GLU	THR	conflict	UNP O66529
BF	120	GLU	THR	conflict	UNP O66529
BF	123	GLU	GLN	conflict	UNP O66529
BF	155	LEU	-	expression tag	UNP O66529
BF	156	GLU	-	expression tag	UNP O66529
BF	157	HIS	-	expression tag	UNP O66529
BF	158	HIS	-	expression tag	UNP O66529
BF	159	HIS	-	expression tag	UNP O66529
BF	160	HIS	-	expression tag	UNP O66529
BF	161	HIS	-	expression tag	UNP O66529
BG	2	GLU	GLN	conflict	UNP O66529
BG	83	GLU	ARG	conflict	UNP O66529
BG	86	GLU	THR	conflict	UNP O66529
BG	120	GLU	THR	conflict	UNP O66529
BG	123	GLU	GLN	conflict	UNP O66529
BG	155	LEU	-	expression tag	UNP O66529
BG	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BG	157	HIS	-	expression tag	UNP O66529
BG	158	HIS	-	expression tag	UNP O66529
BG	159	HIS	-	expression tag	UNP O66529
BG	160	HIS	-	expression tag	UNP O66529
BG	161	HIS	-	expression tag	UNP O66529
BH	2	GLU	GLN	conflict	UNP O66529
BH	83	GLU	ARG	conflict	UNP O66529
BH	86	GLU	THR	conflict	UNP O66529
BH	120	GLU	THR	conflict	UNP O66529
BH	123	GLU	GLN	conflict	UNP O66529
BH	155	LEU	-	expression tag	UNP O66529
BH	156	GLU	-	expression tag	UNP O66529
BH	157	HIS	-	expression tag	UNP O66529
BH	158	HIS	-	expression tag	UNP O66529
BH	159	HIS	-	expression tag	UNP O66529
BH	160	HIS	-	expression tag	UNP O66529
BH	161	HIS	-	expression tag	UNP O66529
BI	2	GLU	GLN	conflict	UNP O66529
BI	83	GLU	ARG	conflict	UNP O66529
BI	86	GLU	THR	conflict	UNP O66529
BI	120	GLU	THR	conflict	UNP O66529
BI	123	GLU	GLN	conflict	UNP O66529
BI	155	LEU	-	expression tag	UNP O66529
BI	156	GLU	-	expression tag	UNP O66529
BI	157	HIS	-	expression tag	UNP O66529
BI	158	HIS	-	expression tag	UNP O66529
BI	159	HIS	-	expression tag	UNP O66529
BI	160	HIS	-	expression tag	UNP O66529
BI	161	HIS	-	expression tag	UNP O66529
BJ	2	GLU	GLN	conflict	UNP O66529
BJ	83	GLU	ARG	conflict	UNP O66529
BJ	86	GLU	THR	conflict	UNP O66529
BJ	120	GLU	THR	conflict	UNP O66529
BJ	123	GLU	GLN	conflict	UNP O66529
BJ	155	LEU	-	expression tag	UNP O66529
BJ	156	GLU	-	expression tag	UNP O66529
BJ	157	HIS	-	expression tag	UNP O66529
BJ	158	HIS	-	expression tag	UNP O66529
BJ	159	HIS	-	expression tag	UNP O66529
BJ	160	HIS	-	expression tag	UNP O66529
BJ	161	HIS	-	expression tag	UNP O66529
BK	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BK	83	GLU	ARG	conflict	UNP O66529
BK	86	GLU	THR	conflict	UNP O66529
BK	120	GLU	THR	conflict	UNP O66529
BK	123	GLU	GLN	conflict	UNP O66529
BK	155	LEU	-	expression tag	UNP O66529
BK	156	GLU	-	expression tag	UNP O66529
BK	157	HIS	-	expression tag	UNP O66529
BK	158	HIS	-	expression tag	UNP O66529
BK	159	HIS	-	expression tag	UNP O66529
BK	160	HIS	-	expression tag	UNP O66529
BK	161	HIS	-	expression tag	UNP O66529
BL	2	GLU	GLN	conflict	UNP O66529
BL	83	GLU	ARG	conflict	UNP O66529
BL	86	GLU	THR	conflict	UNP O66529
BL	120	GLU	THR	conflict	UNP O66529
BL	123	GLU	GLN	conflict	UNP O66529
BL	155	LEU	-	expression tag	UNP O66529
BL	156	GLU	-	expression tag	UNP O66529
BL	157	HIS	-	expression tag	UNP O66529
BL	158	HIS	-	expression tag	UNP O66529
BL	159	HIS	-	expression tag	UNP O66529
BL	160	HIS	-	expression tag	UNP O66529
BL	161	HIS	-	expression tag	UNP O66529
BM	2	GLU	GLN	conflict	UNP O66529
BM	83	GLU	ARG	conflict	UNP O66529
BM	86	GLU	THR	conflict	UNP O66529
BM	120	GLU	THR	conflict	UNP O66529
BM	123	GLU	GLN	conflict	UNP O66529
BM	155	LEU	-	expression tag	UNP O66529
BM	156	GLU	-	expression tag	UNP O66529
BM	157	HIS	-	expression tag	UNP O66529
BM	158	HIS	-	expression tag	UNP O66529
BM	159	HIS	-	expression tag	UNP O66529
BM	160	HIS	-	expression tag	UNP O66529
BM	161	HIS	-	expression tag	UNP O66529
BN	2	GLU	GLN	conflict	UNP O66529
BN	83	GLU	ARG	conflict	UNP O66529
BN	86	GLU	THR	conflict	UNP O66529
BN	120	GLU	THR	conflict	UNP O66529
BN	123	GLU	GLN	conflict	UNP O66529
BN	155	LEU	-	expression tag	UNP O66529
BN	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BN	157	HIS	-	expression tag	UNP O66529
BN	158	HIS	-	expression tag	UNP O66529
BN	159	HIS	-	expression tag	UNP O66529
BN	160	HIS	-	expression tag	UNP O66529
BN	161	HIS	-	expression tag	UNP O66529
BO	2	GLU	GLN	conflict	UNP O66529
BO	83	GLU	ARG	conflict	UNP O66529
BO	86	GLU	THR	conflict	UNP O66529
BO	120	GLU	THR	conflict	UNP O66529
BO	123	GLU	GLN	conflict	UNP O66529
BO	155	LEU	-	expression tag	UNP O66529
BO	156	GLU	-	expression tag	UNP O66529
BO	157	HIS	-	expression tag	UNP O66529
BO	158	HIS	-	expression tag	UNP O66529
BO	159	HIS	-	expression tag	UNP O66529
BO	160	HIS	-	expression tag	UNP O66529
BO	161	HIS	-	expression tag	UNP O66529
CA	2	GLU	GLN	conflict	UNP O66529
CA	83	GLU	ARG	conflict	UNP O66529
CA	86	GLU	THR	conflict	UNP O66529
CA	120	GLU	THR	conflict	UNP O66529
CA	123	GLU	GLN	conflict	UNP O66529
CA	155	LEU	-	expression tag	UNP O66529
CA	156	GLU	-	expression tag	UNP O66529
CA	157	HIS	-	expression tag	UNP O66529
CA	158	HIS	-	expression tag	UNP O66529
CA	159	HIS	-	expression tag	UNP O66529
CA	160	HIS	-	expression tag	UNP O66529
CA	161	HIS	-	expression tag	UNP O66529
CB	2	GLU	GLN	conflict	UNP O66529
CB	83	GLU	ARG	conflict	UNP O66529
CB	86	GLU	THR	conflict	UNP O66529
CB	120	GLU	THR	conflict	UNP O66529
CB	123	GLU	GLN	conflict	UNP O66529
CB	155	LEU	-	expression tag	UNP O66529
CB	156	GLU	-	expression tag	UNP O66529
CB	157	HIS	-	expression tag	UNP O66529
CB	158	HIS	-	expression tag	UNP O66529
CB	159	HIS	-	expression tag	UNP O66529
CB	160	HIS	-	expression tag	UNP O66529
CB	161	HIS	-	expression tag	UNP O66529
CC	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CC	83	GLU	ARG	conflict	UNP O66529
CC	86	GLU	THR	conflict	UNP O66529
CC	120	GLU	THR	conflict	UNP O66529
CC	123	GLU	GLN	conflict	UNP O66529
CC	155	LEU	-	expression tag	UNP O66529
CC	156	GLU	-	expression tag	UNP O66529
CC	157	HIS	-	expression tag	UNP O66529
CC	158	HIS	-	expression tag	UNP O66529
CC	159	HIS	-	expression tag	UNP O66529
CC	160	HIS	-	expression tag	UNP O66529
CC	161	HIS	-	expression tag	UNP O66529
CD	2	GLU	GLN	conflict	UNP O66529
CD	83	GLU	ARG	conflict	UNP O66529
CD	86	GLU	THR	conflict	UNP O66529
CD	120	GLU	THR	conflict	UNP O66529
CD	123	GLU	GLN	conflict	UNP O66529
CD	155	LEU	-	expression tag	UNP O66529
CD	156	GLU	-	expression tag	UNP O66529
CD	157	HIS	-	expression tag	UNP O66529
CD	158	HIS	-	expression tag	UNP O66529
CD	159	HIS	-	expression tag	UNP O66529
CD	160	HIS	-	expression tag	UNP O66529
CD	161	HIS	-	expression tag	UNP O66529
CE	2	GLU	GLN	conflict	UNP O66529
CE	83	GLU	ARG	conflict	UNP O66529
CE	86	GLU	THR	conflict	UNP O66529
CE	120	GLU	THR	conflict	UNP O66529
CE	123	GLU	GLN	conflict	UNP O66529
CE	155	LEU	-	expression tag	UNP O66529
CE	156	GLU	-	expression tag	UNP O66529
CE	157	HIS	-	expression tag	UNP O66529
CE	158	HIS	-	expression tag	UNP O66529
CE	159	HIS	-	expression tag	UNP O66529
CE	160	HIS	-	expression tag	UNP O66529
CE	161	HIS	-	expression tag	UNP O66529
CF	2	GLU	GLN	conflict	UNP O66529
CF	83	GLU	ARG	conflict	UNP O66529
CF	86	GLU	THR	conflict	UNP O66529
CF	120	GLU	THR	conflict	UNP O66529
CF	123	GLU	GLN	conflict	UNP O66529
CF	155	LEU	-	expression tag	UNP O66529
CF	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CF	157	HIS	-	expression tag	UNP O66529
CF	158	HIS	-	expression tag	UNP O66529
CF	159	HIS	-	expression tag	UNP O66529
CF	160	HIS	-	expression tag	UNP O66529
CF	161	HIS	-	expression tag	UNP O66529
CG	2	GLU	GLN	conflict	UNP O66529
CG	83	GLU	ARG	conflict	UNP O66529
CG	86	GLU	THR	conflict	UNP O66529
CG	120	GLU	THR	conflict	UNP O66529
CG	123	GLU	GLN	conflict	UNP O66529
CG	155	LEU	-	expression tag	UNP O66529
CG	156	GLU	-	expression tag	UNP O66529
CG	157	HIS	-	expression tag	UNP O66529
CG	158	HIS	-	expression tag	UNP O66529
CG	159	HIS	-	expression tag	UNP O66529
CG	160	HIS	-	expression tag	UNP O66529
CG	161	HIS	-	expression tag	UNP O66529
CH	2	GLU	GLN	conflict	UNP O66529
CH	83	GLU	ARG	conflict	UNP O66529
CH	86	GLU	THR	conflict	UNP O66529
CH	120	GLU	THR	conflict	UNP O66529
CH	123	GLU	GLN	conflict	UNP O66529
CH	155	LEU	-	expression tag	UNP O66529
CH	156	GLU	-	expression tag	UNP O66529
CH	157	HIS	-	expression tag	UNP O66529
CH	158	HIS	-	expression tag	UNP O66529
CH	159	HIS	-	expression tag	UNP O66529
CH	160	HIS	-	expression tag	UNP O66529
CH	161	HIS	-	expression tag	UNP O66529
CI	2	GLU	GLN	conflict	UNP O66529
CI	83	GLU	ARG	conflict	UNP O66529
CI	86	GLU	THR	conflict	UNP O66529
CI	120	GLU	THR	conflict	UNP O66529
CI	123	GLU	GLN	conflict	UNP O66529
CI	155	LEU	-	expression tag	UNP O66529
CI	156	GLU	-	expression tag	UNP O66529
CI	157	HIS	-	expression tag	UNP O66529
CI	158	HIS	-	expression tag	UNP O66529
CI	159	HIS	-	expression tag	UNP O66529
CI	160	HIS	-	expression tag	UNP O66529
CI	161	HIS	-	expression tag	UNP O66529
CJ	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	83	GLU	ARG	conflict	UNP O66529
CJ	86	GLU	THR	conflict	UNP O66529
CJ	120	GLU	THR	conflict	UNP O66529
CJ	123	GLU	GLN	conflict	UNP O66529
CJ	155	LEU	-	expression tag	UNP O66529
CJ	156	GLU	-	expression tag	UNP O66529
CJ	157	HIS	-	expression tag	UNP O66529
CJ	158	HIS	-	expression tag	UNP O66529
CJ	159	HIS	-	expression tag	UNP O66529
CJ	160	HIS	-	expression tag	UNP O66529
CJ	161	HIS	-	expression tag	UNP O66529
CK	2	GLU	GLN	conflict	UNP O66529
CK	83	GLU	ARG	conflict	UNP O66529
CK	86	GLU	THR	conflict	UNP O66529
CK	120	GLU	THR	conflict	UNP O66529
CK	123	GLU	GLN	conflict	UNP O66529
CK	155	LEU	-	expression tag	UNP O66529
CK	156	GLU	-	expression tag	UNP O66529
CK	157	HIS	-	expression tag	UNP O66529
CK	158	HIS	-	expression tag	UNP O66529
CK	159	HIS	-	expression tag	UNP O66529
CK	160	HIS	-	expression tag	UNP O66529
CK	161	HIS	-	expression tag	UNP O66529
CL	2	GLU	GLN	conflict	UNP O66529
CL	83	GLU	ARG	conflict	UNP O66529
CL	86	GLU	THR	conflict	UNP O66529
CL	120	GLU	THR	conflict	UNP O66529
CL	123	GLU	GLN	conflict	UNP O66529
CL	155	LEU	-	expression tag	UNP O66529
CL	156	GLU	-	expression tag	UNP O66529
CL	157	HIS	-	expression tag	UNP O66529
CL	158	HIS	-	expression tag	UNP O66529
CL	159	HIS	-	expression tag	UNP O66529
CL	160	HIS	-	expression tag	UNP O66529
CL	161	HIS	-	expression tag	UNP O66529
CM	2	GLU	GLN	conflict	UNP O66529
CM	83	GLU	ARG	conflict	UNP O66529
CM	86	GLU	THR	conflict	UNP O66529
CM	120	GLU	THR	conflict	UNP O66529
CM	123	GLU	GLN	conflict	UNP O66529
CM	155	LEU	-	expression tag	UNP O66529
CM	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CM	157	HIS	-	expression tag	UNP O66529
CM	158	HIS	-	expression tag	UNP O66529
CM	159	HIS	-	expression tag	UNP O66529
CM	160	HIS	-	expression tag	UNP O66529
CM	161	HIS	-	expression tag	UNP O66529
CN	2	GLU	GLN	conflict	UNP O66529
CN	83	GLU	ARG	conflict	UNP O66529
CN	86	GLU	THR	conflict	UNP O66529
CN	120	GLU	THR	conflict	UNP O66529
CN	123	GLU	GLN	conflict	UNP O66529
CN	155	LEU	-	expression tag	UNP O66529
CN	156	GLU	-	expression tag	UNP O66529
CN	157	HIS	-	expression tag	UNP O66529
CN	158	HIS	-	expression tag	UNP O66529
CN	159	HIS	-	expression tag	UNP O66529
CN	160	HIS	-	expression tag	UNP O66529
CN	161	HIS	-	expression tag	UNP O66529
CO	2	GLU	GLN	conflict	UNP O66529
CO	83	GLU	ARG	conflict	UNP O66529
CO	86	GLU	THR	conflict	UNP O66529
CO	120	GLU	THR	conflict	UNP O66529
CO	123	GLU	GLN	conflict	UNP O66529
CO	155	LEU	-	expression tag	UNP O66529
CO	156	GLU	-	expression tag	UNP O66529
CO	157	HIS	-	expression tag	UNP O66529
CO	158	HIS	-	expression tag	UNP O66529
CO	159	HIS	-	expression tag	UNP O66529
CO	160	HIS	-	expression tag	UNP O66529
CO	161	HIS	-	expression tag	UNP O66529
DA	2	GLU	GLN	conflict	UNP O66529
DA	83	GLU	ARG	conflict	UNP O66529
DA	86	GLU	THR	conflict	UNP O66529
DA	120	GLU	THR	conflict	UNP O66529
DA	123	GLU	GLN	conflict	UNP O66529
DA	155	LEU	-	expression tag	UNP O66529
DA	156	GLU	-	expression tag	UNP O66529
DA	157	HIS	-	expression tag	UNP O66529
DA	158	HIS	-	expression tag	UNP O66529
DA	159	HIS	-	expression tag	UNP O66529
DA	160	HIS	-	expression tag	UNP O66529
DA	161	HIS	-	expression tag	UNP O66529
DB	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DB	83	GLU	ARG	conflict	UNP O66529
DB	86	GLU	THR	conflict	UNP O66529
DB	120	GLU	THR	conflict	UNP O66529
DB	123	GLU	GLN	conflict	UNP O66529
DB	155	LEU	-	expression tag	UNP O66529
DB	156	GLU	-	expression tag	UNP O66529
DB	157	HIS	-	expression tag	UNP O66529
DB	158	HIS	-	expression tag	UNP O66529
DB	159	HIS	-	expression tag	UNP O66529
DB	160	HIS	-	expression tag	UNP O66529
DB	161	HIS	-	expression tag	UNP O66529
DC	2	GLU	GLN	conflict	UNP O66529
DC	83	GLU	ARG	conflict	UNP O66529
DC	86	GLU	THR	conflict	UNP O66529
DC	120	GLU	THR	conflict	UNP O66529
DC	123	GLU	GLN	conflict	UNP O66529
DC	155	LEU	-	expression tag	UNP O66529
DC	156	GLU	-	expression tag	UNP O66529
DC	157	HIS	-	expression tag	UNP O66529
DC	158	HIS	-	expression tag	UNP O66529
DC	159	HIS	-	expression tag	UNP O66529
DC	160	HIS	-	expression tag	UNP O66529
DC	161	HIS	-	expression tag	UNP O66529
DD	2	GLU	GLN	conflict	UNP O66529
DD	83	GLU	ARG	conflict	UNP O66529
DD	86	GLU	THR	conflict	UNP O66529
DD	120	GLU	THR	conflict	UNP O66529
DD	123	GLU	GLN	conflict	UNP O66529
DD	155	LEU	-	expression tag	UNP O66529
DD	156	GLU	-	expression tag	UNP O66529
DD	157	HIS	-	expression tag	UNP O66529
DD	158	HIS	-	expression tag	UNP O66529
DD	159	HIS	-	expression tag	UNP O66529
DD	160	HIS	-	expression tag	UNP O66529
DD	161	HIS	-	expression tag	UNP O66529
DE	2	GLU	GLN	conflict	UNP O66529
DE	83	GLU	ARG	conflict	UNP O66529
DE	86	GLU	THR	conflict	UNP O66529
DE	120	GLU	THR	conflict	UNP O66529
DE	123	GLU	GLN	conflict	UNP O66529
DE	155	LEU	-	expression tag	UNP O66529
DE	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DE	157	HIS	-	expression tag	UNP O66529
DE	158	HIS	-	expression tag	UNP O66529
DE	159	HIS	-	expression tag	UNP O66529
DE	160	HIS	-	expression tag	UNP O66529
DE	161	HIS	-	expression tag	UNP O66529
DF	2	GLU	GLN	conflict	UNP O66529
DF	83	GLU	ARG	conflict	UNP O66529
DF	86	GLU	THR	conflict	UNP O66529
DF	120	GLU	THR	conflict	UNP O66529
DF	123	GLU	GLN	conflict	UNP O66529
DF	155	LEU	-	expression tag	UNP O66529
DF	156	GLU	-	expression tag	UNP O66529
DF	157	HIS	-	expression tag	UNP O66529
DF	158	HIS	-	expression tag	UNP O66529
DF	159	HIS	-	expression tag	UNP O66529
DF	160	HIS	-	expression tag	UNP O66529
DF	161	HIS	-	expression tag	UNP O66529
DG	2	GLU	GLN	conflict	UNP O66529
DG	83	GLU	ARG	conflict	UNP O66529
DG	86	GLU	THR	conflict	UNP O66529
DG	120	GLU	THR	conflict	UNP O66529
DG	123	GLU	GLN	conflict	UNP O66529
DG	155	LEU	-	expression tag	UNP O66529
DG	156	GLU	-	expression tag	UNP O66529
DG	157	HIS	-	expression tag	UNP O66529
DG	158	HIS	-	expression tag	UNP O66529
DG	159	HIS	-	expression tag	UNP O66529
DG	160	HIS	-	expression tag	UNP O66529
DG	161	HIS	-	expression tag	UNP O66529
DH	2	GLU	GLN	conflict	UNP O66529
DH	83	GLU	ARG	conflict	UNP O66529
DH	86	GLU	THR	conflict	UNP O66529
DH	120	GLU	THR	conflict	UNP O66529
DH	123	GLU	GLN	conflict	UNP O66529
DH	155	LEU	-	expression tag	UNP O66529
DH	156	GLU	-	expression tag	UNP O66529
DH	157	HIS	-	expression tag	UNP O66529
DH	158	HIS	-	expression tag	UNP O66529
DH	159	HIS	-	expression tag	UNP O66529
DH	160	HIS	-	expression tag	UNP O66529
DH	161	HIS	-	expression tag	UNP O66529
DI	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DI	83	GLU	ARG	conflict	UNP O66529
DI	86	GLU	THR	conflict	UNP O66529
DI	120	GLU	THR	conflict	UNP O66529
DI	123	GLU	GLN	conflict	UNP O66529
DI	155	LEU	-	expression tag	UNP O66529
DI	156	GLU	-	expression tag	UNP O66529
DI	157	HIS	-	expression tag	UNP O66529
DI	158	HIS	-	expression tag	UNP O66529
DI	159	HIS	-	expression tag	UNP O66529
DI	160	HIS	-	expression tag	UNP O66529
DI	161	HIS	-	expression tag	UNP O66529
DJ	2	GLU	GLN	conflict	UNP O66529
DJ	83	GLU	ARG	conflict	UNP O66529
DJ	86	GLU	THR	conflict	UNP O66529
DJ	120	GLU	THR	conflict	UNP O66529
DJ	123	GLU	GLN	conflict	UNP O66529
DJ	155	LEU	-	expression tag	UNP O66529
DJ	156	GLU	-	expression tag	UNP O66529
DJ	157	HIS	-	expression tag	UNP O66529
DJ	158	HIS	-	expression tag	UNP O66529
DJ	159	HIS	-	expression tag	UNP O66529
DJ	160	HIS	-	expression tag	UNP O66529
DJ	161	HIS	-	expression tag	UNP O66529
DK	2	GLU	GLN	conflict	UNP O66529
DK	83	GLU	ARG	conflict	UNP O66529
DK	86	GLU	THR	conflict	UNP O66529
DK	120	GLU	THR	conflict	UNP O66529
DK	123	GLU	GLN	conflict	UNP O66529
DK	155	LEU	-	expression tag	UNP O66529
DK	156	GLU	-	expression tag	UNP O66529
DK	157	HIS	-	expression tag	UNP O66529
DK	158	HIS	-	expression tag	UNP O66529
DK	159	HIS	-	expression tag	UNP O66529
DK	160	HIS	-	expression tag	UNP O66529
DK	161	HIS	-	expression tag	UNP O66529
DL	2	GLU	GLN	conflict	UNP O66529
DL	83	GLU	ARG	conflict	UNP O66529
DL	86	GLU	THR	conflict	UNP O66529
DL	120	GLU	THR	conflict	UNP O66529
DL	123	GLU	GLN	conflict	UNP O66529
DL	155	LEU	-	expression tag	UNP O66529
DL	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DL	157	HIS	-	expression tag	UNP O66529
DL	158	HIS	-	expression tag	UNP O66529
DL	159	HIS	-	expression tag	UNP O66529
DL	160	HIS	-	expression tag	UNP O66529
DL	161	HIS	-	expression tag	UNP O66529
DM	2	GLU	GLN	conflict	UNP O66529
DM	83	GLU	ARG	conflict	UNP O66529
DM	86	GLU	THR	conflict	UNP O66529
DM	120	GLU	THR	conflict	UNP O66529
DM	123	GLU	GLN	conflict	UNP O66529
DM	155	LEU	-	expression tag	UNP O66529
DM	156	GLU	-	expression tag	UNP O66529
DM	157	HIS	-	expression tag	UNP O66529
DM	158	HIS	-	expression tag	UNP O66529
DM	159	HIS	-	expression tag	UNP O66529
DM	160	HIS	-	expression tag	UNP O66529
DM	161	HIS	-	expression tag	UNP O66529
DN	2	GLU	GLN	conflict	UNP O66529
DN	83	GLU	ARG	conflict	UNP O66529
DN	86	GLU	THR	conflict	UNP O66529
DN	120	GLU	THR	conflict	UNP O66529
DN	123	GLU	GLN	conflict	UNP O66529
DN	155	LEU	-	expression tag	UNP O66529
DN	156	GLU	-	expression tag	UNP O66529
DN	157	HIS	-	expression tag	UNP O66529
DN	158	HIS	-	expression tag	UNP O66529
DN	159	HIS	-	expression tag	UNP O66529
DN	160	HIS	-	expression tag	UNP O66529
DN	161	HIS	-	expression tag	UNP O66529
DO	2	GLU	GLN	conflict	UNP O66529
DO	83	GLU	ARG	conflict	UNP O66529
DO	86	GLU	THR	conflict	UNP O66529
DO	120	GLU	THR	conflict	UNP O66529
DO	123	GLU	GLN	conflict	UNP O66529
DO	155	LEU	-	expression tag	UNP O66529
DO	156	GLU	-	expression tag	UNP O66529
DO	157	HIS	-	expression tag	UNP O66529
DO	158	HIS	-	expression tag	UNP O66529
DO	159	HIS	-	expression tag	UNP O66529
DO	160	HIS	-	expression tag	UNP O66529
DO	161	HIS	-	expression tag	UNP O66529
EA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EA	83	GLU	ARG	conflict	UNP O66529
EA	86	GLU	THR	conflict	UNP O66529
EA	120	GLU	THR	conflict	UNP O66529
EA	123	GLU	GLN	conflict	UNP O66529
EA	155	LEU	-	expression tag	UNP O66529
EA	156	GLU	-	expression tag	UNP O66529
EA	157	HIS	-	expression tag	UNP O66529
EA	158	HIS	-	expression tag	UNP O66529
EA	159	HIS	-	expression tag	UNP O66529
EA	160	HIS	-	expression tag	UNP O66529
EA	161	HIS	-	expression tag	UNP O66529
EB	2	GLU	GLN	conflict	UNP O66529
EB	83	GLU	ARG	conflict	UNP O66529
EB	86	GLU	THR	conflict	UNP O66529
EB	120	GLU	THR	conflict	UNP O66529
EB	123	GLU	GLN	conflict	UNP O66529
EB	155	LEU	-	expression tag	UNP O66529
EB	156	GLU	-	expression tag	UNP O66529
EB	157	HIS	-	expression tag	UNP O66529
EB	158	HIS	-	expression tag	UNP O66529
EB	159	HIS	-	expression tag	UNP O66529
EB	160	HIS	-	expression tag	UNP O66529
EB	161	HIS	-	expression tag	UNP O66529
EC	2	GLU	GLN	conflict	UNP O66529
EC	83	GLU	ARG	conflict	UNP O66529
EC	86	GLU	THR	conflict	UNP O66529
EC	120	GLU	THR	conflict	UNP O66529
EC	123	GLU	GLN	conflict	UNP O66529
EC	155	LEU	-	expression tag	UNP O66529
EC	156	GLU	-	expression tag	UNP O66529
EC	157	HIS	-	expression tag	UNP O66529
EC	158	HIS	-	expression tag	UNP O66529
EC	159	HIS	-	expression tag	UNP O66529
EC	160	HIS	-	expression tag	UNP O66529
EC	161	HIS	-	expression tag	UNP O66529
ED	2	GLU	GLN	conflict	UNP O66529
ED	83	GLU	ARG	conflict	UNP O66529
ED	86	GLU	THR	conflict	UNP O66529
ED	120	GLU	THR	conflict	UNP O66529
ED	123	GLU	GLN	conflict	UNP O66529
ED	155	LEU	-	expression tag	UNP O66529
ED	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ED	157	HIS	-	expression tag	UNP O66529
ED	158	HIS	-	expression tag	UNP O66529
ED	159	HIS	-	expression tag	UNP O66529
ED	160	HIS	-	expression tag	UNP O66529
ED	161	HIS	-	expression tag	UNP O66529
EE	2	GLU	GLN	conflict	UNP O66529
EE	83	GLU	ARG	conflict	UNP O66529
EE	86	GLU	THR	conflict	UNP O66529
EE	120	GLU	THR	conflict	UNP O66529
EE	123	GLU	GLN	conflict	UNP O66529
EE	155	LEU	-	expression tag	UNP O66529
EE	156	GLU	-	expression tag	UNP O66529
EE	157	HIS	-	expression tag	UNP O66529
EE	158	HIS	-	expression tag	UNP O66529
EE	159	HIS	-	expression tag	UNP O66529
EE	160	HIS	-	expression tag	UNP O66529
EE	161	HIS	-	expression tag	UNP O66529
EF	2	GLU	GLN	conflict	UNP O66529
EF	83	GLU	ARG	conflict	UNP O66529
EF	86	GLU	THR	conflict	UNP O66529
EF	120	GLU	THR	conflict	UNP O66529
EF	123	GLU	GLN	conflict	UNP O66529
EF	155	LEU	-	expression tag	UNP O66529
EF	156	GLU	-	expression tag	UNP O66529
EF	157	HIS	-	expression tag	UNP O66529
EF	158	HIS	-	expression tag	UNP O66529
EF	159	HIS	-	expression tag	UNP O66529
EF	160	HIS	-	expression tag	UNP O66529
EF	161	HIS	-	expression tag	UNP O66529
EG	2	GLU	GLN	conflict	UNP O66529
EG	83	GLU	ARG	conflict	UNP O66529
EG	86	GLU	THR	conflict	UNP O66529
EG	120	GLU	THR	conflict	UNP O66529
EG	123	GLU	GLN	conflict	UNP O66529
EG	155	LEU	-	expression tag	UNP O66529
EG	156	GLU	-	expression tag	UNP O66529
EG	157	HIS	-	expression tag	UNP O66529
EG	158	HIS	-	expression tag	UNP O66529
EG	159	HIS	-	expression tag	UNP O66529
EG	160	HIS	-	expression tag	UNP O66529
EG	161	HIS	-	expression tag	UNP O66529
EH	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EH	83	GLU	ARG	conflict	UNP O66529
EH	86	GLU	THR	conflict	UNP O66529
EH	120	GLU	THR	conflict	UNP O66529
EH	123	GLU	GLN	conflict	UNP O66529
EH	155	LEU	-	expression tag	UNP O66529
EH	156	GLU	-	expression tag	UNP O66529
EH	157	HIS	-	expression tag	UNP O66529
EH	158	HIS	-	expression tag	UNP O66529
EH	159	HIS	-	expression tag	UNP O66529
EH	160	HIS	-	expression tag	UNP O66529
EH	161	HIS	-	expression tag	UNP O66529
EI	2	GLU	GLN	conflict	UNP O66529
EI	83	GLU	ARG	conflict	UNP O66529
EI	86	GLU	THR	conflict	UNP O66529
EI	120	GLU	THR	conflict	UNP O66529
EI	123	GLU	GLN	conflict	UNP O66529
EI	155	LEU	-	expression tag	UNP O66529
EI	156	GLU	-	expression tag	UNP O66529
EI	157	HIS	-	expression tag	UNP O66529
EI	158	HIS	-	expression tag	UNP O66529
EI	159	HIS	-	expression tag	UNP O66529
EI	160	HIS	-	expression tag	UNP O66529
EI	161	HIS	-	expression tag	UNP O66529
EJ	2	GLU	GLN	conflict	UNP O66529
EJ	83	GLU	ARG	conflict	UNP O66529
EJ	86	GLU	THR	conflict	UNP O66529
EJ	120	GLU	THR	conflict	UNP O66529
EJ	123	GLU	GLN	conflict	UNP O66529
EJ	155	LEU	-	expression tag	UNP O66529
EJ	156	GLU	-	expression tag	UNP O66529
EJ	157	HIS	-	expression tag	UNP O66529
EJ	158	HIS	-	expression tag	UNP O66529
EJ	159	HIS	-	expression tag	UNP O66529
EJ	160	HIS	-	expression tag	UNP O66529
EJ	161	HIS	-	expression tag	UNP O66529
EK	2	GLU	GLN	conflict	UNP O66529
EK	83	GLU	ARG	conflict	UNP O66529
EK	86	GLU	THR	conflict	UNP O66529
EK	120	GLU	THR	conflict	UNP O66529
EK	123	GLU	GLN	conflict	UNP O66529
EK	155	LEU	-	expression tag	UNP O66529
EK	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EK	157	HIS	-	expression tag	UNP O66529
EK	158	HIS	-	expression tag	UNP O66529
EK	159	HIS	-	expression tag	UNP O66529
EK	160	HIS	-	expression tag	UNP O66529
EK	161	HIS	-	expression tag	UNP O66529
EL	2	GLU	GLN	conflict	UNP O66529
EL	83	GLU	ARG	conflict	UNP O66529
EL	86	GLU	THR	conflict	UNP O66529
EL	120	GLU	THR	conflict	UNP O66529
EL	123	GLU	GLN	conflict	UNP O66529
EL	155	LEU	-	expression tag	UNP O66529
EL	156	GLU	-	expression tag	UNP O66529
EL	157	HIS	-	expression tag	UNP O66529
EL	158	HIS	-	expression tag	UNP O66529
EL	159	HIS	-	expression tag	UNP O66529
EL	160	HIS	-	expression tag	UNP O66529
EL	161	HIS	-	expression tag	UNP O66529
EM	2	GLU	GLN	conflict	UNP O66529
EM	83	GLU	ARG	conflict	UNP O66529
EM	86	GLU	THR	conflict	UNP O66529
EM	120	GLU	THR	conflict	UNP O66529
EM	123	GLU	GLN	conflict	UNP O66529
EM	155	LEU	-	expression tag	UNP O66529
EM	156	GLU	-	expression tag	UNP O66529
EM	157	HIS	-	expression tag	UNP O66529
EM	158	HIS	-	expression tag	UNP O66529
EM	159	HIS	-	expression tag	UNP O66529
EM	160	HIS	-	expression tag	UNP O66529
EM	161	HIS	-	expression tag	UNP O66529
EN	2	GLU	GLN	conflict	UNP O66529
EN	83	GLU	ARG	conflict	UNP O66529
EN	86	GLU	THR	conflict	UNP O66529
EN	120	GLU	THR	conflict	UNP O66529
EN	123	GLU	GLN	conflict	UNP O66529
EN	155	LEU	-	expression tag	UNP O66529
EN	156	GLU	-	expression tag	UNP O66529
EN	157	HIS	-	expression tag	UNP O66529
EN	158	HIS	-	expression tag	UNP O66529
EN	159	HIS	-	expression tag	UNP O66529
EN	160	HIS	-	expression tag	UNP O66529
EN	161	HIS	-	expression tag	UNP O66529
EO	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EO	83	GLU	ARG	conflict	UNP O66529
EO	86	GLU	THR	conflict	UNP O66529
EO	120	GLU	THR	conflict	UNP O66529
EO	123	GLU	GLN	conflict	UNP O66529
EO	155	LEU	-	expression tag	UNP O66529
EO	156	GLU	-	expression tag	UNP O66529
EO	157	HIS	-	expression tag	UNP O66529
EO	158	HIS	-	expression tag	UNP O66529
EO	159	HIS	-	expression tag	UNP O66529
EO	160	HIS	-	expression tag	UNP O66529
EO	161	HIS	-	expression tag	UNP O66529
FA	2	GLU	GLN	conflict	UNP O66529
FA	83	GLU	ARG	conflict	UNP O66529
FA	86	GLU	THR	conflict	UNP O66529
FA	120	GLU	THR	conflict	UNP O66529
FA	123	GLU	GLN	conflict	UNP O66529
FA	155	LEU	-	expression tag	UNP O66529
FA	156	GLU	-	expression tag	UNP O66529
FA	157	HIS	-	expression tag	UNP O66529
FA	158	HIS	-	expression tag	UNP O66529
FA	159	HIS	-	expression tag	UNP O66529
FA	160	HIS	-	expression tag	UNP O66529
FA	161	HIS	-	expression tag	UNP O66529
FB	2	GLU	GLN	conflict	UNP O66529
FB	83	GLU	ARG	conflict	UNP O66529
FB	86	GLU	THR	conflict	UNP O66529
FB	120	GLU	THR	conflict	UNP O66529
FB	123	GLU	GLN	conflict	UNP O66529
FB	155	LEU	-	expression tag	UNP O66529
FB	156	GLU	-	expression tag	UNP O66529
FB	157	HIS	-	expression tag	UNP O66529
FB	158	HIS	-	expression tag	UNP O66529
FB	159	HIS	-	expression tag	UNP O66529
FB	160	HIS	-	expression tag	UNP O66529
FB	161	HIS	-	expression tag	UNP O66529
FC	2	GLU	GLN	conflict	UNP O66529
FC	83	GLU	ARG	conflict	UNP O66529
FC	86	GLU	THR	conflict	UNP O66529
FC	120	GLU	THR	conflict	UNP O66529
FC	123	GLU	GLN	conflict	UNP O66529
FC	155	LEU	-	expression tag	UNP O66529
FC	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FC	157	HIS	-	expression tag	UNP O66529
FC	158	HIS	-	expression tag	UNP O66529
FC	159	HIS	-	expression tag	UNP O66529
FC	160	HIS	-	expression tag	UNP O66529
FC	161	HIS	-	expression tag	UNP O66529
FD	2	GLU	GLN	conflict	UNP O66529
FD	83	GLU	ARG	conflict	UNP O66529
FD	86	GLU	THR	conflict	UNP O66529
FD	120	GLU	THR	conflict	UNP O66529
FD	123	GLU	GLN	conflict	UNP O66529
FD	155	LEU	-	expression tag	UNP O66529
FD	156	GLU	-	expression tag	UNP O66529
FD	157	HIS	-	expression tag	UNP O66529
FD	158	HIS	-	expression tag	UNP O66529
FD	159	HIS	-	expression tag	UNP O66529
FD	160	HIS	-	expression tag	UNP O66529
FD	161	HIS	-	expression tag	UNP O66529
FE	2	GLU	GLN	conflict	UNP O66529
FE	83	GLU	ARG	conflict	UNP O66529
FE	86	GLU	THR	conflict	UNP O66529
FE	120	GLU	THR	conflict	UNP O66529
FE	123	GLU	GLN	conflict	UNP O66529
FE	155	LEU	-	expression tag	UNP O66529
FE	156	GLU	-	expression tag	UNP O66529
FE	157	HIS	-	expression tag	UNP O66529
FE	158	HIS	-	expression tag	UNP O66529
FE	159	HIS	-	expression tag	UNP O66529
FE	160	HIS	-	expression tag	UNP O66529
FE	161	HIS	-	expression tag	UNP O66529
FF	2	GLU	GLN	conflict	UNP O66529
FF	83	GLU	ARG	conflict	UNP O66529
FF	86	GLU	THR	conflict	UNP O66529
FF	120	GLU	THR	conflict	UNP O66529
FF	123	GLU	GLN	conflict	UNP O66529
FF	155	LEU	-	expression tag	UNP O66529
FF	156	GLU	-	expression tag	UNP O66529
FF	157	HIS	-	expression tag	UNP O66529
FF	158	HIS	-	expression tag	UNP O66529
FF	159	HIS	-	expression tag	UNP O66529
FF	160	HIS	-	expression tag	UNP O66529
FF	161	HIS	-	expression tag	UNP O66529
FG	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FG	83	GLU	ARG	conflict	UNP O66529
FG	86	GLU	THR	conflict	UNP O66529
FG	120	GLU	THR	conflict	UNP O66529
FG	123	GLU	GLN	conflict	UNP O66529
FG	155	LEU	-	expression tag	UNP O66529
FG	156	GLU	-	expression tag	UNP O66529
FG	157	HIS	-	expression tag	UNP O66529
FG	158	HIS	-	expression tag	UNP O66529
FG	159	HIS	-	expression tag	UNP O66529
FG	160	HIS	-	expression tag	UNP O66529
FG	161	HIS	-	expression tag	UNP O66529
FH	2	GLU	GLN	conflict	UNP O66529
FH	83	GLU	ARG	conflict	UNP O66529
FH	86	GLU	THR	conflict	UNP O66529
FH	120	GLU	THR	conflict	UNP O66529
FH	123	GLU	GLN	conflict	UNP O66529
FH	155	LEU	-	expression tag	UNP O66529
FH	156	GLU	-	expression tag	UNP O66529
FH	157	HIS	-	expression tag	UNP O66529
FH	158	HIS	-	expression tag	UNP O66529
FH	159	HIS	-	expression tag	UNP O66529
FH	160	HIS	-	expression tag	UNP O66529
FH	161	HIS	-	expression tag	UNP O66529
FI	2	GLU	GLN	conflict	UNP O66529
FI	83	GLU	ARG	conflict	UNP O66529
FI	86	GLU	THR	conflict	UNP O66529
FI	120	GLU	THR	conflict	UNP O66529
FI	123	GLU	GLN	conflict	UNP O66529
FI	155	LEU	-	expression tag	UNP O66529
FI	156	GLU	-	expression tag	UNP O66529
FI	157	HIS	-	expression tag	UNP O66529
FI	158	HIS	-	expression tag	UNP O66529
FI	159	HIS	-	expression tag	UNP O66529
FI	160	HIS	-	expression tag	UNP O66529
FI	161	HIS	-	expression tag	UNP O66529
FJ	2	GLU	GLN	conflict	UNP O66529
FJ	83	GLU	ARG	conflict	UNP O66529
FJ	86	GLU	THR	conflict	UNP O66529
FJ	120	GLU	THR	conflict	UNP O66529
FJ	123	GLU	GLN	conflict	UNP O66529
FJ	155	LEU	-	expression tag	UNP O66529
FJ	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FJ	157	HIS	-	expression tag	UNP O66529
FJ	158	HIS	-	expression tag	UNP O66529
FJ	159	HIS	-	expression tag	UNP O66529
FJ	160	HIS	-	expression tag	UNP O66529
FJ	161	HIS	-	expression tag	UNP O66529
FK	2	GLU	GLN	conflict	UNP O66529
FK	83	GLU	ARG	conflict	UNP O66529
FK	86	GLU	THR	conflict	UNP O66529
FK	120	GLU	THR	conflict	UNP O66529
FK	123	GLU	GLN	conflict	UNP O66529
FK	155	LEU	-	expression tag	UNP O66529
FK	156	GLU	-	expression tag	UNP O66529
FK	157	HIS	-	expression tag	UNP O66529
FK	158	HIS	-	expression tag	UNP O66529
FK	159	HIS	-	expression tag	UNP O66529
FK	160	HIS	-	expression tag	UNP O66529
FK	161	HIS	-	expression tag	UNP O66529
FL	2	GLU	GLN	conflict	UNP O66529
FL	83	GLU	ARG	conflict	UNP O66529
FL	86	GLU	THR	conflict	UNP O66529
FL	120	GLU	THR	conflict	UNP O66529
FL	123	GLU	GLN	conflict	UNP O66529
FL	155	LEU	-	expression tag	UNP O66529
FL	156	GLU	-	expression tag	UNP O66529
FL	157	HIS	-	expression tag	UNP O66529
FL	158	HIS	-	expression tag	UNP O66529
FL	159	HIS	-	expression tag	UNP O66529
FL	160	HIS	-	expression tag	UNP O66529
FL	161	HIS	-	expression tag	UNP O66529
FM	2	GLU	GLN	conflict	UNP O66529
FM	83	GLU	ARG	conflict	UNP O66529
FM	86	GLU	THR	conflict	UNP O66529
FM	120	GLU	THR	conflict	UNP O66529
FM	123	GLU	GLN	conflict	UNP O66529
FM	155	LEU	-	expression tag	UNP O66529
FM	156	GLU	-	expression tag	UNP O66529
FM	157	HIS	-	expression tag	UNP O66529
FM	158	HIS	-	expression tag	UNP O66529
FM	159	HIS	-	expression tag	UNP O66529
FM	160	HIS	-	expression tag	UNP O66529
FM	161	HIS	-	expression tag	UNP O66529
FN	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FN	83	GLU	ARG	conflict	UNP O66529
FN	86	GLU	THR	conflict	UNP O66529
FN	120	GLU	THR	conflict	UNP O66529
FN	123	GLU	GLN	conflict	UNP O66529
FN	155	LEU	-	expression tag	UNP O66529
FN	156	GLU	-	expression tag	UNP O66529
FN	157	HIS	-	expression tag	UNP O66529
FN	158	HIS	-	expression tag	UNP O66529
FN	159	HIS	-	expression tag	UNP O66529
FN	160	HIS	-	expression tag	UNP O66529
FN	161	HIS	-	expression tag	UNP O66529
FO	2	GLU	GLN	conflict	UNP O66529
FO	83	GLU	ARG	conflict	UNP O66529
FO	86	GLU	THR	conflict	UNP O66529
FO	120	GLU	THR	conflict	UNP O66529
FO	123	GLU	GLN	conflict	UNP O66529
FO	155	LEU	-	expression tag	UNP O66529
FO	156	GLU	-	expression tag	UNP O66529
FO	157	HIS	-	expression tag	UNP O66529
FO	158	HIS	-	expression tag	UNP O66529
FO	159	HIS	-	expression tag	UNP O66529
FO	160	HIS	-	expression tag	UNP O66529
FO	161	HIS	-	expression tag	UNP O66529
GA	2	GLU	GLN	conflict	UNP O66529
GA	83	GLU	ARG	conflict	UNP O66529
GA	86	GLU	THR	conflict	UNP O66529
GA	120	GLU	THR	conflict	UNP O66529
GA	123	GLU	GLN	conflict	UNP O66529
GA	155	LEU	-	expression tag	UNP O66529
GA	156	GLU	-	expression tag	UNP O66529
GA	157	HIS	-	expression tag	UNP O66529
GA	158	HIS	-	expression tag	UNP O66529
GA	159	HIS	-	expression tag	UNP O66529
GA	160	HIS	-	expression tag	UNP O66529
GA	161	HIS	-	expression tag	UNP O66529
GB	2	GLU	GLN	conflict	UNP O66529
GB	83	GLU	ARG	conflict	UNP O66529
GB	86	GLU	THR	conflict	UNP O66529
GB	120	GLU	THR	conflict	UNP O66529
GB	123	GLU	GLN	conflict	UNP O66529
GB	155	LEU	-	expression tag	UNP O66529
GB	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GB	157	HIS	-	expression tag	UNP O66529
GB	158	HIS	-	expression tag	UNP O66529
GB	159	HIS	-	expression tag	UNP O66529
GB	160	HIS	-	expression tag	UNP O66529
GB	161	HIS	-	expression tag	UNP O66529
GC	2	GLU	GLN	conflict	UNP O66529
GC	83	GLU	ARG	conflict	UNP O66529
GC	86	GLU	THR	conflict	UNP O66529
GC	120	GLU	THR	conflict	UNP O66529
GC	123	GLU	GLN	conflict	UNP O66529
GC	155	LEU	-	expression tag	UNP O66529
GC	156	GLU	-	expression tag	UNP O66529
GC	157	HIS	-	expression tag	UNP O66529
GC	158	HIS	-	expression tag	UNP O66529
GC	159	HIS	-	expression tag	UNP O66529
GC	160	HIS	-	expression tag	UNP O66529
GC	161	HIS	-	expression tag	UNP O66529
GD	2	GLU	GLN	conflict	UNP O66529
GD	83	GLU	ARG	conflict	UNP O66529
GD	86	GLU	THR	conflict	UNP O66529
GD	120	GLU	THR	conflict	UNP O66529
GD	123	GLU	GLN	conflict	UNP O66529
GD	155	LEU	-	expression tag	UNP O66529
GD	156	GLU	-	expression tag	UNP O66529
GD	157	HIS	-	expression tag	UNP O66529
GD	158	HIS	-	expression tag	UNP O66529
GD	159	HIS	-	expression tag	UNP O66529
GD	160	HIS	-	expression tag	UNP O66529
GD	161	HIS	-	expression tag	UNP O66529
GE	2	GLU	GLN	conflict	UNP O66529
GE	83	GLU	ARG	conflict	UNP O66529
GE	86	GLU	THR	conflict	UNP O66529
GE	120	GLU	THR	conflict	UNP O66529
GE	123	GLU	GLN	conflict	UNP O66529
GE	155	LEU	-	expression tag	UNP O66529
GE	156	GLU	-	expression tag	UNP O66529
GE	157	HIS	-	expression tag	UNP O66529
GE	158	HIS	-	expression tag	UNP O66529
GE	159	HIS	-	expression tag	UNP O66529
GE	160	HIS	-	expression tag	UNP O66529
GE	161	HIS	-	expression tag	UNP O66529
GF	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GF	83	GLU	ARG	conflict	UNP O66529
GF	86	GLU	THR	conflict	UNP O66529
GF	120	GLU	THR	conflict	UNP O66529
GF	123	GLU	GLN	conflict	UNP O66529
GF	155	LEU	-	expression tag	UNP O66529
GF	156	GLU	-	expression tag	UNP O66529
GF	157	HIS	-	expression tag	UNP O66529
GF	158	HIS	-	expression tag	UNP O66529
GF	159	HIS	-	expression tag	UNP O66529
GF	160	HIS	-	expression tag	UNP O66529
GF	161	HIS	-	expression tag	UNP O66529
GG	2	GLU	GLN	conflict	UNP O66529
GG	83	GLU	ARG	conflict	UNP O66529
GG	86	GLU	THR	conflict	UNP O66529
GG	120	GLU	THR	conflict	UNP O66529
GG	123	GLU	GLN	conflict	UNP O66529
GG	155	LEU	-	expression tag	UNP O66529
GG	156	GLU	-	expression tag	UNP O66529
GG	157	HIS	-	expression tag	UNP O66529
GG	158	HIS	-	expression tag	UNP O66529
GG	159	HIS	-	expression tag	UNP O66529
GG	160	HIS	-	expression tag	UNP O66529
GG	161	HIS	-	expression tag	UNP O66529
GH	2	GLU	GLN	conflict	UNP O66529
GH	83	GLU	ARG	conflict	UNP O66529
GH	86	GLU	THR	conflict	UNP O66529
GH	120	GLU	THR	conflict	UNP O66529
GH	123	GLU	GLN	conflict	UNP O66529
GH	155	LEU	-	expression tag	UNP O66529
GH	156	GLU	-	expression tag	UNP O66529
GH	157	HIS	-	expression tag	UNP O66529
GH	158	HIS	-	expression tag	UNP O66529
GH	159	HIS	-	expression tag	UNP O66529
GH	160	HIS	-	expression tag	UNP O66529
GH	161	HIS	-	expression tag	UNP O66529
GI	2	GLU	GLN	conflict	UNP O66529
GI	83	GLU	ARG	conflict	UNP O66529
GI	86	GLU	THR	conflict	UNP O66529
GI	120	GLU	THR	conflict	UNP O66529
GI	123	GLU	GLN	conflict	UNP O66529
GI	155	LEU	-	expression tag	UNP O66529
GI	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GI	157	HIS	-	expression tag	UNP O66529
GI	158	HIS	-	expression tag	UNP O66529
GI	159	HIS	-	expression tag	UNP O66529
GI	160	HIS	-	expression tag	UNP O66529
GI	161	HIS	-	expression tag	UNP O66529
GJ	2	GLU	GLN	conflict	UNP O66529
GJ	83	GLU	ARG	conflict	UNP O66529
GJ	86	GLU	THR	conflict	UNP O66529
GJ	120	GLU	THR	conflict	UNP O66529
GJ	123	GLU	GLN	conflict	UNP O66529
GJ	155	LEU	-	expression tag	UNP O66529
GJ	156	GLU	-	expression tag	UNP O66529
GJ	157	HIS	-	expression tag	UNP O66529
GJ	158	HIS	-	expression tag	UNP O66529
GJ	159	HIS	-	expression tag	UNP O66529
GJ	160	HIS	-	expression tag	UNP O66529
GJ	161	HIS	-	expression tag	UNP O66529
GK	2	GLU	GLN	conflict	UNP O66529
GK	83	GLU	ARG	conflict	UNP O66529
GK	86	GLU	THR	conflict	UNP O66529
GK	120	GLU	THR	conflict	UNP O66529
GK	123	GLU	GLN	conflict	UNP O66529
GK	155	LEU	-	expression tag	UNP O66529
GK	156	GLU	-	expression tag	UNP O66529
GK	157	HIS	-	expression tag	UNP O66529
GK	158	HIS	-	expression tag	UNP O66529
GK	159	HIS	-	expression tag	UNP O66529
GK	160	HIS	-	expression tag	UNP O66529
GK	161	HIS	-	expression tag	UNP O66529
GL	2	GLU	GLN	conflict	UNP O66529
GL	83	GLU	ARG	conflict	UNP O66529
GL	86	GLU	THR	conflict	UNP O66529
GL	120	GLU	THR	conflict	UNP O66529
GL	123	GLU	GLN	conflict	UNP O66529
GL	155	LEU	-	expression tag	UNP O66529
GL	156	GLU	-	expression tag	UNP O66529
GL	157	HIS	-	expression tag	UNP O66529
GL	158	HIS	-	expression tag	UNP O66529
GL	159	HIS	-	expression tag	UNP O66529
GL	160	HIS	-	expression tag	UNP O66529
GL	161	HIS	-	expression tag	UNP O66529
GM	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GM	83	GLU	ARG	conflict	UNP O66529
GM	86	GLU	THR	conflict	UNP O66529
GM	120	GLU	THR	conflict	UNP O66529
GM	123	GLU	GLN	conflict	UNP O66529
GM	155	LEU	-	expression tag	UNP O66529
GM	156	GLU	-	expression tag	UNP O66529
GM	157	HIS	-	expression tag	UNP O66529
GM	158	HIS	-	expression tag	UNP O66529
GM	159	HIS	-	expression tag	UNP O66529
GM	160	HIS	-	expression tag	UNP O66529
GM	161	HIS	-	expression tag	UNP O66529
GN	2	GLU	GLN	conflict	UNP O66529
GN	83	GLU	ARG	conflict	UNP O66529
GN	86	GLU	THR	conflict	UNP O66529
GN	120	GLU	THR	conflict	UNP O66529
GN	123	GLU	GLN	conflict	UNP O66529
GN	155	LEU	-	expression tag	UNP O66529
GN	156	GLU	-	expression tag	UNP O66529
GN	157	HIS	-	expression tag	UNP O66529
GN	158	HIS	-	expression tag	UNP O66529
GN	159	HIS	-	expression tag	UNP O66529
GN	160	HIS	-	expression tag	UNP O66529
GN	161	HIS	-	expression tag	UNP O66529
GO	2	GLU	GLN	conflict	UNP O66529
GO	83	GLU	ARG	conflict	UNP O66529
GO	86	GLU	THR	conflict	UNP O66529
GO	120	GLU	THR	conflict	UNP O66529
GO	123	GLU	GLN	conflict	UNP O66529
GO	155	LEU	-	expression tag	UNP O66529
GO	156	GLU	-	expression tag	UNP O66529
GO	157	HIS	-	expression tag	UNP O66529
GO	158	HIS	-	expression tag	UNP O66529
GO	159	HIS	-	expression tag	UNP O66529
GO	160	HIS	-	expression tag	UNP O66529
GO	161	HIS	-	expression tag	UNP O66529
HA	2	GLU	GLN	conflict	UNP O66529
HA	83	GLU	ARG	conflict	UNP O66529
HA	86	GLU	THR	conflict	UNP O66529
HA	120	GLU	THR	conflict	UNP O66529
HA	123	GLU	GLN	conflict	UNP O66529
HA	155	LEU	-	expression tag	UNP O66529
HA	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HA	157	HIS	-	expression tag	UNP O66529
HA	158	HIS	-	expression tag	UNP O66529
HA	159	HIS	-	expression tag	UNP O66529
HA	160	HIS	-	expression tag	UNP O66529
HA	161	HIS	-	expression tag	UNP O66529
HB	2	GLU	GLN	conflict	UNP O66529
HB	83	GLU	ARG	conflict	UNP O66529
HB	86	GLU	THR	conflict	UNP O66529
HB	120	GLU	THR	conflict	UNP O66529
HB	123	GLU	GLN	conflict	UNP O66529
HB	155	LEU	-	expression tag	UNP O66529
HB	156	GLU	-	expression tag	UNP O66529
HB	157	HIS	-	expression tag	UNP O66529
HB	158	HIS	-	expression tag	UNP O66529
HB	159	HIS	-	expression tag	UNP O66529
HB	160	HIS	-	expression tag	UNP O66529
HB	161	HIS	-	expression tag	UNP O66529
HC	2	GLU	GLN	conflict	UNP O66529
HC	83	GLU	ARG	conflict	UNP O66529
HC	86	GLU	THR	conflict	UNP O66529
HC	120	GLU	THR	conflict	UNP O66529
HC	123	GLU	GLN	conflict	UNP O66529
HC	155	LEU	-	expression tag	UNP O66529
HC	156	GLU	-	expression tag	UNP O66529
HC	157	HIS	-	expression tag	UNP O66529
HC	158	HIS	-	expression tag	UNP O66529
HC	159	HIS	-	expression tag	UNP O66529
HC	160	HIS	-	expression tag	UNP O66529
HC	161	HIS	-	expression tag	UNP O66529
HD	2	GLU	GLN	conflict	UNP O66529
HD	83	GLU	ARG	conflict	UNP O66529
HD	86	GLU	THR	conflict	UNP O66529
HD	120	GLU	THR	conflict	UNP O66529
HD	123	GLU	GLN	conflict	UNP O66529
HD	155	LEU	-	expression tag	UNP O66529
HD	156	GLU	-	expression tag	UNP O66529
HD	157	HIS	-	expression tag	UNP O66529
HD	158	HIS	-	expression tag	UNP O66529
HD	159	HIS	-	expression tag	UNP O66529
HD	160	HIS	-	expression tag	UNP O66529
HD	161	HIS	-	expression tag	UNP O66529
HE	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HE	83	GLU	ARG	conflict	UNP O66529
HE	86	GLU	THR	conflict	UNP O66529
HE	120	GLU	THR	conflict	UNP O66529
HE	123	GLU	GLN	conflict	UNP O66529
HE	155	LEU	-	expression tag	UNP O66529
HE	156	GLU	-	expression tag	UNP O66529
HE	157	HIS	-	expression tag	UNP O66529
HE	158	HIS	-	expression tag	UNP O66529
HE	159	HIS	-	expression tag	UNP O66529
HE	160	HIS	-	expression tag	UNP O66529
HE	161	HIS	-	expression tag	UNP O66529
HF	2	GLU	GLN	conflict	UNP O66529
HF	83	GLU	ARG	conflict	UNP O66529
HF	86	GLU	THR	conflict	UNP O66529
HF	120	GLU	THR	conflict	UNP O66529
HF	123	GLU	GLN	conflict	UNP O66529
HF	155	LEU	-	expression tag	UNP O66529
HF	156	GLU	-	expression tag	UNP O66529
HF	157	HIS	-	expression tag	UNP O66529
HF	158	HIS	-	expression tag	UNP O66529
HF	159	HIS	-	expression tag	UNP O66529
HF	160	HIS	-	expression tag	UNP O66529
HF	161	HIS	-	expression tag	UNP O66529
HG	2	GLU	GLN	conflict	UNP O66529
HG	83	GLU	ARG	conflict	UNP O66529
HG	86	GLU	THR	conflict	UNP O66529
HG	120	GLU	THR	conflict	UNP O66529
HG	123	GLU	GLN	conflict	UNP O66529
HG	155	LEU	-	expression tag	UNP O66529
HG	156	GLU	-	expression tag	UNP O66529
HG	157	HIS	-	expression tag	UNP O66529
HG	158	HIS	-	expression tag	UNP O66529
HG	159	HIS	-	expression tag	UNP O66529
HG	160	HIS	-	expression tag	UNP O66529
HG	161	HIS	-	expression tag	UNP O66529
HH	2	GLU	GLN	conflict	UNP O66529
HH	83	GLU	ARG	conflict	UNP O66529
HH	86	GLU	THR	conflict	UNP O66529
HH	120	GLU	THR	conflict	UNP O66529
HH	123	GLU	GLN	conflict	UNP O66529
HH	155	LEU	-	expression tag	UNP O66529
HH	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HH	157	HIS	-	expression tag	UNP O66529
HH	158	HIS	-	expression tag	UNP O66529
HH	159	HIS	-	expression tag	UNP O66529
HH	160	HIS	-	expression tag	UNP O66529
HH	161	HIS	-	expression tag	UNP O66529
HI	2	GLU	GLN	conflict	UNP O66529
HI	83	GLU	ARG	conflict	UNP O66529
HI	86	GLU	THR	conflict	UNP O66529
HI	120	GLU	THR	conflict	UNP O66529
HI	123	GLU	GLN	conflict	UNP O66529
HI	155	LEU	-	expression tag	UNP O66529
HI	156	GLU	-	expression tag	UNP O66529
HI	157	HIS	-	expression tag	UNP O66529
HI	158	HIS	-	expression tag	UNP O66529
HI	159	HIS	-	expression tag	UNP O66529
HI	160	HIS	-	expression tag	UNP O66529
HI	161	HIS	-	expression tag	UNP O66529
HJ	2	GLU	GLN	conflict	UNP O66529
HJ	83	GLU	ARG	conflict	UNP O66529
HJ	86	GLU	THR	conflict	UNP O66529
HJ	120	GLU	THR	conflict	UNP O66529
HJ	123	GLU	GLN	conflict	UNP O66529
HJ	155	LEU	-	expression tag	UNP O66529
HJ	156	GLU	-	expression tag	UNP O66529
HJ	157	HIS	-	expression tag	UNP O66529
HJ	158	HIS	-	expression tag	UNP O66529
HJ	159	HIS	-	expression tag	UNP O66529
HJ	160	HIS	-	expression tag	UNP O66529
HJ	161	HIS	-	expression tag	UNP O66529
HK	2	GLU	GLN	conflict	UNP O66529
HK	83	GLU	ARG	conflict	UNP O66529
HK	86	GLU	THR	conflict	UNP O66529
HK	120	GLU	THR	conflict	UNP O66529
HK	123	GLU	GLN	conflict	UNP O66529
HK	155	LEU	-	expression tag	UNP O66529
HK	156	GLU	-	expression tag	UNP O66529
HK	157	HIS	-	expression tag	UNP O66529
HK	158	HIS	-	expression tag	UNP O66529
HK	159	HIS	-	expression tag	UNP O66529
HK	160	HIS	-	expression tag	UNP O66529
HK	161	HIS	-	expression tag	UNP O66529
HL	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HL	83	GLU	ARG	conflict	UNP O66529
HL	86	GLU	THR	conflict	UNP O66529
HL	120	GLU	THR	conflict	UNP O66529
HL	123	GLU	GLN	conflict	UNP O66529
HL	155	LEU	-	expression tag	UNP O66529
HL	156	GLU	-	expression tag	UNP O66529
HL	157	HIS	-	expression tag	UNP O66529
HL	158	HIS	-	expression tag	UNP O66529
HL	159	HIS	-	expression tag	UNP O66529
HL	160	HIS	-	expression tag	UNP O66529
HL	161	HIS	-	expression tag	UNP O66529
HM	2	GLU	GLN	conflict	UNP O66529
HM	83	GLU	ARG	conflict	UNP O66529
HM	86	GLU	THR	conflict	UNP O66529
HM	120	GLU	THR	conflict	UNP O66529
HM	123	GLU	GLN	conflict	UNP O66529
HM	155	LEU	-	expression tag	UNP O66529
HM	156	GLU	-	expression tag	UNP O66529
HM	157	HIS	-	expression tag	UNP O66529
HM	158	HIS	-	expression tag	UNP O66529
HM	159	HIS	-	expression tag	UNP O66529
HM	160	HIS	-	expression tag	UNP O66529
HM	161	HIS	-	expression tag	UNP O66529
HN	2	GLU	GLN	conflict	UNP O66529
HN	83	GLU	ARG	conflict	UNP O66529
HN	86	GLU	THR	conflict	UNP O66529
HN	120	GLU	THR	conflict	UNP O66529
HN	123	GLU	GLN	conflict	UNP O66529
HN	155	LEU	-	expression tag	UNP O66529
HN	156	GLU	-	expression tag	UNP O66529
HN	157	HIS	-	expression tag	UNP O66529
HN	158	HIS	-	expression tag	UNP O66529
HN	159	HIS	-	expression tag	UNP O66529
HN	160	HIS	-	expression tag	UNP O66529
HN	161	HIS	-	expression tag	UNP O66529
HO	2	GLU	GLN	conflict	UNP O66529
HO	83	GLU	ARG	conflict	UNP O66529
HO	86	GLU	THR	conflict	UNP O66529
HO	120	GLU	THR	conflict	UNP O66529
HO	123	GLU	GLN	conflict	UNP O66529
HO	155	LEU	-	expression tag	UNP O66529
HO	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HO	157	HIS	-	expression tag	UNP O66529
HO	158	HIS	-	expression tag	UNP O66529
HO	159	HIS	-	expression tag	UNP O66529
HO	160	HIS	-	expression tag	UNP O66529
HO	161	HIS	-	expression tag	UNP O66529
IA	2	GLU	GLN	conflict	UNP O66529
IA	83	GLU	ARG	conflict	UNP O66529
IA	86	GLU	THR	conflict	UNP O66529
IA	120	GLU	THR	conflict	UNP O66529
IA	123	GLU	GLN	conflict	UNP O66529
IA	155	LEU	-	expression tag	UNP O66529
IA	156	GLU	-	expression tag	UNP O66529
IA	157	HIS	-	expression tag	UNP O66529
IA	158	HIS	-	expression tag	UNP O66529
IA	159	HIS	-	expression tag	UNP O66529
IA	160	HIS	-	expression tag	UNP O66529
IA	161	HIS	-	expression tag	UNP O66529
IB	2	GLU	GLN	conflict	UNP O66529
IB	83	GLU	ARG	conflict	UNP O66529
IB	86	GLU	THR	conflict	UNP O66529
IB	120	GLU	THR	conflict	UNP O66529
IB	123	GLU	GLN	conflict	UNP O66529
IB	155	LEU	-	expression tag	UNP O66529
IB	156	GLU	-	expression tag	UNP O66529
IB	157	HIS	-	expression tag	UNP O66529
IB	158	HIS	-	expression tag	UNP O66529
IB	159	HIS	-	expression tag	UNP O66529
IB	160	HIS	-	expression tag	UNP O66529
IB	161	HIS	-	expression tag	UNP O66529
IC	2	GLU	GLN	conflict	UNP O66529
IC	83	GLU	ARG	conflict	UNP O66529
IC	86	GLU	THR	conflict	UNP O66529
IC	120	GLU	THR	conflict	UNP O66529
IC	123	GLU	GLN	conflict	UNP O66529
IC	155	LEU	-	expression tag	UNP O66529
IC	156	GLU	-	expression tag	UNP O66529
IC	157	HIS	-	expression tag	UNP O66529
IC	158	HIS	-	expression tag	UNP O66529
IC	159	HIS	-	expression tag	UNP O66529
IC	160	HIS	-	expression tag	UNP O66529
IC	161	HIS	-	expression tag	UNP O66529
ID	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ID	83	GLU	ARG	conflict	UNP O66529
ID	86	GLU	THR	conflict	UNP O66529
ID	120	GLU	THR	conflict	UNP O66529
ID	123	GLU	GLN	conflict	UNP O66529
ID	155	LEU	-	expression tag	UNP O66529
ID	156	GLU	-	expression tag	UNP O66529
ID	157	HIS	-	expression tag	UNP O66529
ID	158	HIS	-	expression tag	UNP O66529
ID	159	HIS	-	expression tag	UNP O66529
ID	160	HIS	-	expression tag	UNP O66529
ID	161	HIS	-	expression tag	UNP O66529
IE	2	GLU	GLN	conflict	UNP O66529
IE	83	GLU	ARG	conflict	UNP O66529
IE	86	GLU	THR	conflict	UNP O66529
IE	120	GLU	THR	conflict	UNP O66529
IE	123	GLU	GLN	conflict	UNP O66529
IE	155	LEU	-	expression tag	UNP O66529
IE	156	GLU	-	expression tag	UNP O66529
IE	157	HIS	-	expression tag	UNP O66529
IE	158	HIS	-	expression tag	UNP O66529
IE	159	HIS	-	expression tag	UNP O66529
IE	160	HIS	-	expression tag	UNP O66529
IE	161	HIS	-	expression tag	UNP O66529
IF	2	GLU	GLN	conflict	UNP O66529
IF	83	GLU	ARG	conflict	UNP O66529
IF	86	GLU	THR	conflict	UNP O66529
IF	120	GLU	THR	conflict	UNP O66529
IF	123	GLU	GLN	conflict	UNP O66529
IF	155	LEU	-	expression tag	UNP O66529
IF	156	GLU	-	expression tag	UNP O66529
IF	157	HIS	-	expression tag	UNP O66529
IF	158	HIS	-	expression tag	UNP O66529
IF	159	HIS	-	expression tag	UNP O66529
IF	160	HIS	-	expression tag	UNP O66529
IF	161	HIS	-	expression tag	UNP O66529
IG	2	GLU	GLN	conflict	UNP O66529
IG	83	GLU	ARG	conflict	UNP O66529
IG	86	GLU	THR	conflict	UNP O66529
IG	120	GLU	THR	conflict	UNP O66529
IG	123	GLU	GLN	conflict	UNP O66529
IG	155	LEU	-	expression tag	UNP O66529
IG	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
IG	157	HIS	-	expression tag	UNP O66529
IG	158	HIS	-	expression tag	UNP O66529
IG	159	HIS	-	expression tag	UNP O66529
IG	160	HIS	-	expression tag	UNP O66529
IG	161	HIS	-	expression tag	UNP O66529
IH	2	GLU	GLN	conflict	UNP O66529
IH	83	GLU	ARG	conflict	UNP O66529
IH	86	GLU	THR	conflict	UNP O66529
IH	120	GLU	THR	conflict	UNP O66529
IH	123	GLU	GLN	conflict	UNP O66529
IH	155	LEU	-	expression tag	UNP O66529
IH	156	GLU	-	expression tag	UNP O66529
IH	157	HIS	-	expression tag	UNP O66529
IH	158	HIS	-	expression tag	UNP O66529
IH	159	HIS	-	expression tag	UNP O66529
IH	160	HIS	-	expression tag	UNP O66529
IH	161	HIS	-	expression tag	UNP O66529
II	2	GLU	GLN	conflict	UNP O66529
II	83	GLU	ARG	conflict	UNP O66529
II	86	GLU	THR	conflict	UNP O66529
II	120	GLU	THR	conflict	UNP O66529
II	123	GLU	GLN	conflict	UNP O66529
II	155	LEU	-	expression tag	UNP O66529
II	156	GLU	-	expression tag	UNP O66529
II	157	HIS	-	expression tag	UNP O66529
II	158	HIS	-	expression tag	UNP O66529
II	159	HIS	-	expression tag	UNP O66529
II	160	HIS	-	expression tag	UNP O66529
II	161	HIS	-	expression tag	UNP O66529
IJ	2	GLU	GLN	conflict	UNP O66529
IJ	83	GLU	ARG	conflict	UNP O66529
IJ	86	GLU	THR	conflict	UNP O66529
IJ	120	GLU	THR	conflict	UNP O66529
IJ	123	GLU	GLN	conflict	UNP O66529
IJ	155	LEU	-	expression tag	UNP O66529
IJ	156	GLU	-	expression tag	UNP O66529
IJ	157	HIS	-	expression tag	UNP O66529
IJ	158	HIS	-	expression tag	UNP O66529
IJ	159	HIS	-	expression tag	UNP O66529
IJ	160	HIS	-	expression tag	UNP O66529
IJ	161	HIS	-	expression tag	UNP O66529
IK	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
IK	83	GLU	ARG	conflict	UNP O66529
IK	86	GLU	THR	conflict	UNP O66529
IK	120	GLU	THR	conflict	UNP O66529
IK	123	GLU	GLN	conflict	UNP O66529
IK	155	LEU	-	expression tag	UNP O66529
IK	156	GLU	-	expression tag	UNP O66529
IK	157	HIS	-	expression tag	UNP O66529
IK	158	HIS	-	expression tag	UNP O66529
IK	159	HIS	-	expression tag	UNP O66529
IK	160	HIS	-	expression tag	UNP O66529
IK	161	HIS	-	expression tag	UNP O66529
IL	2	GLU	GLN	conflict	UNP O66529
IL	83	GLU	ARG	conflict	UNP O66529
IL	86	GLU	THR	conflict	UNP O66529
IL	120	GLU	THR	conflict	UNP O66529
IL	123	GLU	GLN	conflict	UNP O66529
IL	155	LEU	-	expression tag	UNP O66529
IL	156	GLU	-	expression tag	UNP O66529
IL	157	HIS	-	expression tag	UNP O66529
IL	158	HIS	-	expression tag	UNP O66529
IL	159	HIS	-	expression tag	UNP O66529
IL	160	HIS	-	expression tag	UNP O66529
IL	161	HIS	-	expression tag	UNP O66529
IM	2	GLU	GLN	conflict	UNP O66529
IM	83	GLU	ARG	conflict	UNP O66529
IM	86	GLU	THR	conflict	UNP O66529
IM	120	GLU	THR	conflict	UNP O66529
IM	123	GLU	GLN	conflict	UNP O66529
IM	155	LEU	-	expression tag	UNP O66529
IM	156	GLU	-	expression tag	UNP O66529
IM	157	HIS	-	expression tag	UNP O66529
IM	158	HIS	-	expression tag	UNP O66529
IM	159	HIS	-	expression tag	UNP O66529
IM	160	HIS	-	expression tag	UNP O66529
IM	161	HIS	-	expression tag	UNP O66529
IN	2	GLU	GLN	conflict	UNP O66529
IN	83	GLU	ARG	conflict	UNP O66529
IN	86	GLU	THR	conflict	UNP O66529
IN	120	GLU	THR	conflict	UNP O66529
IN	123	GLU	GLN	conflict	UNP O66529
IN	155	LEU	-	expression tag	UNP O66529
IN	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
IN	157	HIS	-	expression tag	UNP O66529
IN	158	HIS	-	expression tag	UNP O66529
IN	159	HIS	-	expression tag	UNP O66529
IN	160	HIS	-	expression tag	UNP O66529
IN	161	HIS	-	expression tag	UNP O66529
IO	2	GLU	GLN	conflict	UNP O66529
IO	83	GLU	ARG	conflict	UNP O66529
IO	86	GLU	THR	conflict	UNP O66529
IO	120	GLU	THR	conflict	UNP O66529
IO	123	GLU	GLN	conflict	UNP O66529
IO	155	LEU	-	expression tag	UNP O66529
IO	156	GLU	-	expression tag	UNP O66529
IO	157	HIS	-	expression tag	UNP O66529
IO	158	HIS	-	expression tag	UNP O66529
IO	159	HIS	-	expression tag	UNP O66529
IO	160	HIS	-	expression tag	UNP O66529
IO	161	HIS	-	expression tag	UNP O66529
JA	2	GLU	GLN	conflict	UNP O66529
JA	83	GLU	ARG	conflict	UNP O66529
JA	86	GLU	THR	conflict	UNP O66529
JA	120	GLU	THR	conflict	UNP O66529
JA	123	GLU	GLN	conflict	UNP O66529
JA	155	LEU	-	expression tag	UNP O66529
JA	156	GLU	-	expression tag	UNP O66529
JA	157	HIS	-	expression tag	UNP O66529
JA	158	HIS	-	expression tag	UNP O66529
JA	159	HIS	-	expression tag	UNP O66529
JA	160	HIS	-	expression tag	UNP O66529
JA	161	HIS	-	expression tag	UNP O66529
JB	2	GLU	GLN	conflict	UNP O66529
JB	83	GLU	ARG	conflict	UNP O66529
JB	86	GLU	THR	conflict	UNP O66529
JB	120	GLU	THR	conflict	UNP O66529
JB	123	GLU	GLN	conflict	UNP O66529
JB	155	LEU	-	expression tag	UNP O66529
JB	156	GLU	-	expression tag	UNP O66529
JB	157	HIS	-	expression tag	UNP O66529
JB	158	HIS	-	expression tag	UNP O66529
JB	159	HIS	-	expression tag	UNP O66529
JB	160	HIS	-	expression tag	UNP O66529
JB	161	HIS	-	expression tag	UNP O66529
JC	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JC	83	GLU	ARG	conflict	UNP O66529
JC	86	GLU	THR	conflict	UNP O66529
JC	120	GLU	THR	conflict	UNP O66529
JC	123	GLU	GLN	conflict	UNP O66529
JC	155	LEU	-	expression tag	UNP O66529
JC	156	GLU	-	expression tag	UNP O66529
JC	157	HIS	-	expression tag	UNP O66529
JC	158	HIS	-	expression tag	UNP O66529
JC	159	HIS	-	expression tag	UNP O66529
JC	160	HIS	-	expression tag	UNP O66529
JC	161	HIS	-	expression tag	UNP O66529
JD	2	GLU	GLN	conflict	UNP O66529
JD	83	GLU	ARG	conflict	UNP O66529
JD	86	GLU	THR	conflict	UNP O66529
JD	120	GLU	THR	conflict	UNP O66529
JD	123	GLU	GLN	conflict	UNP O66529
JD	155	LEU	-	expression tag	UNP O66529
JD	156	GLU	-	expression tag	UNP O66529
JD	157	HIS	-	expression tag	UNP O66529
JD	158	HIS	-	expression tag	UNP O66529
JD	159	HIS	-	expression tag	UNP O66529
JD	160	HIS	-	expression tag	UNP O66529
JD	161	HIS	-	expression tag	UNP O66529
JE	2	GLU	GLN	conflict	UNP O66529
JE	83	GLU	ARG	conflict	UNP O66529
JE	86	GLU	THR	conflict	UNP O66529
JE	120	GLU	THR	conflict	UNP O66529
JE	123	GLU	GLN	conflict	UNP O66529
JE	155	LEU	-	expression tag	UNP O66529
JE	156	GLU	-	expression tag	UNP O66529
JE	157	HIS	-	expression tag	UNP O66529
JE	158	HIS	-	expression tag	UNP O66529
JE	159	HIS	-	expression tag	UNP O66529
JE	160	HIS	-	expression tag	UNP O66529
JE	161	HIS	-	expression tag	UNP O66529
JF	2	GLU	GLN	conflict	UNP O66529
JF	83	GLU	ARG	conflict	UNP O66529
JF	86	GLU	THR	conflict	UNP O66529
JF	120	GLU	THR	conflict	UNP O66529
JF	123	GLU	GLN	conflict	UNP O66529
JF	155	LEU	-	expression tag	UNP O66529
JF	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JF	157	HIS	-	expression tag	UNP O66529
JF	158	HIS	-	expression tag	UNP O66529
JF	159	HIS	-	expression tag	UNP O66529
JF	160	HIS	-	expression tag	UNP O66529
JF	161	HIS	-	expression tag	UNP O66529
JG	2	GLU	GLN	conflict	UNP O66529
JG	83	GLU	ARG	conflict	UNP O66529
JG	86	GLU	THR	conflict	UNP O66529
JG	120	GLU	THR	conflict	UNP O66529
JG	123	GLU	GLN	conflict	UNP O66529
JG	155	LEU	-	expression tag	UNP O66529
JG	156	GLU	-	expression tag	UNP O66529
JG	157	HIS	-	expression tag	UNP O66529
JG	158	HIS	-	expression tag	UNP O66529
JG	159	HIS	-	expression tag	UNP O66529
JG	160	HIS	-	expression tag	UNP O66529
JG	161	HIS	-	expression tag	UNP O66529
JH	2	GLU	GLN	conflict	UNP O66529
JH	83	GLU	ARG	conflict	UNP O66529
JH	86	GLU	THR	conflict	UNP O66529
JH	120	GLU	THR	conflict	UNP O66529
JH	123	GLU	GLN	conflict	UNP O66529
JH	155	LEU	-	expression tag	UNP O66529
JH	156	GLU	-	expression tag	UNP O66529
JH	157	HIS	-	expression tag	UNP O66529
JH	158	HIS	-	expression tag	UNP O66529
JH	159	HIS	-	expression tag	UNP O66529
JH	160	HIS	-	expression tag	UNP O66529
JH	161	HIS	-	expression tag	UNP O66529
JI	2	GLU	GLN	conflict	UNP O66529
JI	83	GLU	ARG	conflict	UNP O66529
JI	86	GLU	THR	conflict	UNP O66529
JI	120	GLU	THR	conflict	UNP O66529
JI	123	GLU	GLN	conflict	UNP O66529
JI	155	LEU	-	expression tag	UNP O66529
JI	156	GLU	-	expression tag	UNP O66529
JI	157	HIS	-	expression tag	UNP O66529
JI	158	HIS	-	expression tag	UNP O66529
JI	159	HIS	-	expression tag	UNP O66529
JI	160	HIS	-	expression tag	UNP O66529
JI	161	HIS	-	expression tag	UNP O66529
JJ	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JJ	83	GLU	ARG	conflict	UNP O66529
JJ	86	GLU	THR	conflict	UNP O66529
JJ	120	GLU	THR	conflict	UNP O66529
JJ	123	GLU	GLN	conflict	UNP O66529
JJ	155	LEU	-	expression tag	UNP O66529
JJ	156	GLU	-	expression tag	UNP O66529
JJ	157	HIS	-	expression tag	UNP O66529
JJ	158	HIS	-	expression tag	UNP O66529
JJ	159	HIS	-	expression tag	UNP O66529
JJ	160	HIS	-	expression tag	UNP O66529
JJ	161	HIS	-	expression tag	UNP O66529
JK	2	GLU	GLN	conflict	UNP O66529
JK	83	GLU	ARG	conflict	UNP O66529
JK	86	GLU	THR	conflict	UNP O66529
JK	120	GLU	THR	conflict	UNP O66529
JK	123	GLU	GLN	conflict	UNP O66529
JK	155	LEU	-	expression tag	UNP O66529
JK	156	GLU	-	expression tag	UNP O66529
JK	157	HIS	-	expression tag	UNP O66529
JK	158	HIS	-	expression tag	UNP O66529
JK	159	HIS	-	expression tag	UNP O66529
JK	160	HIS	-	expression tag	UNP O66529
JK	161	HIS	-	expression tag	UNP O66529
JL	2	GLU	GLN	conflict	UNP O66529
JL	83	GLU	ARG	conflict	UNP O66529
JL	86	GLU	THR	conflict	UNP O66529
JL	120	GLU	THR	conflict	UNP O66529
JL	123	GLU	GLN	conflict	UNP O66529
JL	155	LEU	-	expression tag	UNP O66529
JL	156	GLU	-	expression tag	UNP O66529
JL	157	HIS	-	expression tag	UNP O66529
JL	158	HIS	-	expression tag	UNP O66529
JL	159	HIS	-	expression tag	UNP O66529
JL	160	HIS	-	expression tag	UNP O66529
JL	161	HIS	-	expression tag	UNP O66529
JM	2	GLU	GLN	conflict	UNP O66529
JM	83	GLU	ARG	conflict	UNP O66529
JM	86	GLU	THR	conflict	UNP O66529
JM	120	GLU	THR	conflict	UNP O66529
JM	123	GLU	GLN	conflict	UNP O66529
JM	155	LEU	-	expression tag	UNP O66529
JM	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JM	157	HIS	-	expression tag	UNP O66529
JM	158	HIS	-	expression tag	UNP O66529
JM	159	HIS	-	expression tag	UNP O66529
JM	160	HIS	-	expression tag	UNP O66529
JM	161	HIS	-	expression tag	UNP O66529
JN	2	GLU	GLN	conflict	UNP O66529
JN	83	GLU	ARG	conflict	UNP O66529
JN	86	GLU	THR	conflict	UNP O66529
JN	120	GLU	THR	conflict	UNP O66529
JN	123	GLU	GLN	conflict	UNP O66529
JN	155	LEU	-	expression tag	UNP O66529
JN	156	GLU	-	expression tag	UNP O66529
JN	157	HIS	-	expression tag	UNP O66529
JN	158	HIS	-	expression tag	UNP O66529
JN	159	HIS	-	expression tag	UNP O66529
JN	160	HIS	-	expression tag	UNP O66529
JN	161	HIS	-	expression tag	UNP O66529
JO	2	GLU	GLN	conflict	UNP O66529
JO	83	GLU	ARG	conflict	UNP O66529
JO	86	GLU	THR	conflict	UNP O66529
JO	120	GLU	THR	conflict	UNP O66529
JO	123	GLU	GLN	conflict	UNP O66529
JO	155	LEU	-	expression tag	UNP O66529
JO	156	GLU	-	expression tag	UNP O66529
JO	157	HIS	-	expression tag	UNP O66529
JO	158	HIS	-	expression tag	UNP O66529
JO	159	HIS	-	expression tag	UNP O66529
JO	160	HIS	-	expression tag	UNP O66529
JO	161	HIS	-	expression tag	UNP O66529
KA	2	GLU	GLN	conflict	UNP O66529
KA	83	GLU	ARG	conflict	UNP O66529
KA	86	GLU	THR	conflict	UNP O66529
KA	120	GLU	THR	conflict	UNP O66529
KA	123	GLU	GLN	conflict	UNP O66529
KA	155	LEU	-	expression tag	UNP O66529
KA	156	GLU	-	expression tag	UNP O66529
KA	157	HIS	-	expression tag	UNP O66529
KA	158	HIS	-	expression tag	UNP O66529
KA	159	HIS	-	expression tag	UNP O66529
KA	160	HIS	-	expression tag	UNP O66529
KA	161	HIS	-	expression tag	UNP O66529
KB	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KB	83	GLU	ARG	conflict	UNP O66529
KB	86	GLU	THR	conflict	UNP O66529
KB	120	GLU	THR	conflict	UNP O66529
KB	123	GLU	GLN	conflict	UNP O66529
KB	155	LEU	-	expression tag	UNP O66529
KB	156	GLU	-	expression tag	UNP O66529
KB	157	HIS	-	expression tag	UNP O66529
KB	158	HIS	-	expression tag	UNP O66529
KB	159	HIS	-	expression tag	UNP O66529
KB	160	HIS	-	expression tag	UNP O66529
KB	161	HIS	-	expression tag	UNP O66529
KC	2	GLU	GLN	conflict	UNP O66529
KC	83	GLU	ARG	conflict	UNP O66529
KC	86	GLU	THR	conflict	UNP O66529
KC	120	GLU	THR	conflict	UNP O66529
KC	123	GLU	GLN	conflict	UNP O66529
KC	155	LEU	-	expression tag	UNP O66529
KC	156	GLU	-	expression tag	UNP O66529
KC	157	HIS	-	expression tag	UNP O66529
KC	158	HIS	-	expression tag	UNP O66529
KC	159	HIS	-	expression tag	UNP O66529
KC	160	HIS	-	expression tag	UNP O66529
KC	161	HIS	-	expression tag	UNP O66529
KD	2	GLU	GLN	conflict	UNP O66529
KD	83	GLU	ARG	conflict	UNP O66529
KD	86	GLU	THR	conflict	UNP O66529
KD	120	GLU	THR	conflict	UNP O66529
KD	123	GLU	GLN	conflict	UNP O66529
KD	155	LEU	-	expression tag	UNP O66529
KD	156	GLU	-	expression tag	UNP O66529
KD	157	HIS	-	expression tag	UNP O66529
KD	158	HIS	-	expression tag	UNP O66529
KD	159	HIS	-	expression tag	UNP O66529
KD	160	HIS	-	expression tag	UNP O66529
KD	161	HIS	-	expression tag	UNP O66529
KE	2	GLU	GLN	conflict	UNP O66529
KE	83	GLU	ARG	conflict	UNP O66529
KE	86	GLU	THR	conflict	UNP O66529
KE	120	GLU	THR	conflict	UNP O66529
KE	123	GLU	GLN	conflict	UNP O66529
KE	155	LEU	-	expression tag	UNP O66529
KE	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KE	157	HIS	-	expression tag	UNP O66529
KE	158	HIS	-	expression tag	UNP O66529
KE	159	HIS	-	expression tag	UNP O66529
KE	160	HIS	-	expression tag	UNP O66529
KE	161	HIS	-	expression tag	UNP O66529
KF	2	GLU	GLN	conflict	UNP O66529
KF	83	GLU	ARG	conflict	UNP O66529
KF	86	GLU	THR	conflict	UNP O66529
KF	120	GLU	THR	conflict	UNP O66529
KF	123	GLU	GLN	conflict	UNP O66529
KF	155	LEU	-	expression tag	UNP O66529
KF	156	GLU	-	expression tag	UNP O66529
KF	157	HIS	-	expression tag	UNP O66529
KF	158	HIS	-	expression tag	UNP O66529
KF	159	HIS	-	expression tag	UNP O66529
KF	160	HIS	-	expression tag	UNP O66529
KF	161	HIS	-	expression tag	UNP O66529
KG	2	GLU	GLN	conflict	UNP O66529
KG	83	GLU	ARG	conflict	UNP O66529
KG	86	GLU	THR	conflict	UNP O66529
KG	120	GLU	THR	conflict	UNP O66529
KG	123	GLU	GLN	conflict	UNP O66529
KG	155	LEU	-	expression tag	UNP O66529
KG	156	GLU	-	expression tag	UNP O66529
KG	157	HIS	-	expression tag	UNP O66529
KG	158	HIS	-	expression tag	UNP O66529
KG	159	HIS	-	expression tag	UNP O66529
KG	160	HIS	-	expression tag	UNP O66529
KG	161	HIS	-	expression tag	UNP O66529
KH	2	GLU	GLN	conflict	UNP O66529
KH	83	GLU	ARG	conflict	UNP O66529
KH	86	GLU	THR	conflict	UNP O66529
KH	120	GLU	THR	conflict	UNP O66529
KH	123	GLU	GLN	conflict	UNP O66529
KH	155	LEU	-	expression tag	UNP O66529
KH	156	GLU	-	expression tag	UNP O66529
KH	157	HIS	-	expression tag	UNP O66529
KH	158	HIS	-	expression tag	UNP O66529
KH	159	HIS	-	expression tag	UNP O66529
KH	160	HIS	-	expression tag	UNP O66529
KH	161	HIS	-	expression tag	UNP O66529
KI	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KI	83	GLU	ARG	conflict	UNP O66529
KI	86	GLU	THR	conflict	UNP O66529
KI	120	GLU	THR	conflict	UNP O66529
KI	123	GLU	GLN	conflict	UNP O66529
KI	155	LEU	-	expression tag	UNP O66529
KI	156	GLU	-	expression tag	UNP O66529
KI	157	HIS	-	expression tag	UNP O66529
KI	158	HIS	-	expression tag	UNP O66529
KI	159	HIS	-	expression tag	UNP O66529
KI	160	HIS	-	expression tag	UNP O66529
KI	161	HIS	-	expression tag	UNP O66529
KJ	2	GLU	GLN	conflict	UNP O66529
KJ	83	GLU	ARG	conflict	UNP O66529
KJ	86	GLU	THR	conflict	UNP O66529
KJ	120	GLU	THR	conflict	UNP O66529
KJ	123	GLU	GLN	conflict	UNP O66529
KJ	155	LEU	-	expression tag	UNP O66529
KJ	156	GLU	-	expression tag	UNP O66529
KJ	157	HIS	-	expression tag	UNP O66529
KJ	158	HIS	-	expression tag	UNP O66529
KJ	159	HIS	-	expression tag	UNP O66529
KJ	160	HIS	-	expression tag	UNP O66529
KJ	161	HIS	-	expression tag	UNP O66529
KK	2	GLU	GLN	conflict	UNP O66529
KK	83	GLU	ARG	conflict	UNP O66529
KK	86	GLU	THR	conflict	UNP O66529
KK	120	GLU	THR	conflict	UNP O66529
KK	123	GLU	GLN	conflict	UNP O66529
KK	155	LEU	-	expression tag	UNP O66529
KK	156	GLU	-	expression tag	UNP O66529
KK	157	HIS	-	expression tag	UNP O66529
KK	158	HIS	-	expression tag	UNP O66529
KK	159	HIS	-	expression tag	UNP O66529
KK	160	HIS	-	expression tag	UNP O66529
KK	161	HIS	-	expression tag	UNP O66529
KL	2	GLU	GLN	conflict	UNP O66529
KL	83	GLU	ARG	conflict	UNP O66529
KL	86	GLU	THR	conflict	UNP O66529
KL	120	GLU	THR	conflict	UNP O66529
KL	123	GLU	GLN	conflict	UNP O66529
KL	155	LEU	-	expression tag	UNP O66529
KL	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KL	157	HIS	-	expression tag	UNP O66529
KL	158	HIS	-	expression tag	UNP O66529
KL	159	HIS	-	expression tag	UNP O66529
KL	160	HIS	-	expression tag	UNP O66529
KL	161	HIS	-	expression tag	UNP O66529
KM	2	GLU	GLN	conflict	UNP O66529
KM	83	GLU	ARG	conflict	UNP O66529
KM	86	GLU	THR	conflict	UNP O66529
KM	120	GLU	THR	conflict	UNP O66529
KM	123	GLU	GLN	conflict	UNP O66529
KM	155	LEU	-	expression tag	UNP O66529
KM	156	GLU	-	expression tag	UNP O66529
KM	157	HIS	-	expression tag	UNP O66529
KM	158	HIS	-	expression tag	UNP O66529
KM	159	HIS	-	expression tag	UNP O66529
KM	160	HIS	-	expression tag	UNP O66529
KM	161	HIS	-	expression tag	UNP O66529
KN	2	GLU	GLN	conflict	UNP O66529
KN	83	GLU	ARG	conflict	UNP O66529
KN	86	GLU	THR	conflict	UNP O66529
KN	120	GLU	THR	conflict	UNP O66529
KN	123	GLU	GLN	conflict	UNP O66529
KN	155	LEU	-	expression tag	UNP O66529
KN	156	GLU	-	expression tag	UNP O66529
KN	157	HIS	-	expression tag	UNP O66529
KN	158	HIS	-	expression tag	UNP O66529
KN	159	HIS	-	expression tag	UNP O66529
KN	160	HIS	-	expression tag	UNP O66529
KN	161	HIS	-	expression tag	UNP O66529
KO	2	GLU	GLN	conflict	UNP O66529
KO	83	GLU	ARG	conflict	UNP O66529
KO	86	GLU	THR	conflict	UNP O66529
KO	120	GLU	THR	conflict	UNP O66529
KO	123	GLU	GLN	conflict	UNP O66529
KO	155	LEU	-	expression tag	UNP O66529
KO	156	GLU	-	expression tag	UNP O66529
KO	157	HIS	-	expression tag	UNP O66529
KO	158	HIS	-	expression tag	UNP O66529
KO	159	HIS	-	expression tag	UNP O66529
KO	160	HIS	-	expression tag	UNP O66529
KO	161	HIS	-	expression tag	UNP O66529
LA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LA	83	GLU	ARG	conflict	UNP O66529
LA	86	GLU	THR	conflict	UNP O66529
LA	120	GLU	THR	conflict	UNP O66529
LA	123	GLU	GLN	conflict	UNP O66529
LA	155	LEU	-	expression tag	UNP O66529
LA	156	GLU	-	expression tag	UNP O66529
LA	157	HIS	-	expression tag	UNP O66529
LA	158	HIS	-	expression tag	UNP O66529
LA	159	HIS	-	expression tag	UNP O66529
LA	160	HIS	-	expression tag	UNP O66529
LA	161	HIS	-	expression tag	UNP O66529
LB	2	GLU	GLN	conflict	UNP O66529
LB	83	GLU	ARG	conflict	UNP O66529
LB	86	GLU	THR	conflict	UNP O66529
LB	120	GLU	THR	conflict	UNP O66529
LB	123	GLU	GLN	conflict	UNP O66529
LB	155	LEU	-	expression tag	UNP O66529
LB	156	GLU	-	expression tag	UNP O66529
LB	157	HIS	-	expression tag	UNP O66529
LB	158	HIS	-	expression tag	UNP O66529
LB	159	HIS	-	expression tag	UNP O66529
LB	160	HIS	-	expression tag	UNP O66529
LB	161	HIS	-	expression tag	UNP O66529
LC	2	GLU	GLN	conflict	UNP O66529
LC	83	GLU	ARG	conflict	UNP O66529
LC	86	GLU	THR	conflict	UNP O66529
LC	120	GLU	THR	conflict	UNP O66529
LC	123	GLU	GLN	conflict	UNP O66529
LC	155	LEU	-	expression tag	UNP O66529
LC	156	GLU	-	expression tag	UNP O66529
LC	157	HIS	-	expression tag	UNP O66529
LC	158	HIS	-	expression tag	UNP O66529
LC	159	HIS	-	expression tag	UNP O66529
LC	160	HIS	-	expression tag	UNP O66529
LC	161	HIS	-	expression tag	UNP O66529
LD	2	GLU	GLN	conflict	UNP O66529
LD	83	GLU	ARG	conflict	UNP O66529
LD	86	GLU	THR	conflict	UNP O66529
LD	120	GLU	THR	conflict	UNP O66529
LD	123	GLU	GLN	conflict	UNP O66529
LD	155	LEU	-	expression tag	UNP O66529
LD	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LD	157	HIS	-	expression tag	UNP O66529
LD	158	HIS	-	expression tag	UNP O66529
LD	159	HIS	-	expression tag	UNP O66529
LD	160	HIS	-	expression tag	UNP O66529
LD	161	HIS	-	expression tag	UNP O66529
LE	2	GLU	GLN	conflict	UNP O66529
LE	83	GLU	ARG	conflict	UNP O66529
LE	86	GLU	THR	conflict	UNP O66529
LE	120	GLU	THR	conflict	UNP O66529
LE	123	GLU	GLN	conflict	UNP O66529
LE	155	LEU	-	expression tag	UNP O66529
LE	156	GLU	-	expression tag	UNP O66529
LE	157	HIS	-	expression tag	UNP O66529
LE	158	HIS	-	expression tag	UNP O66529
LE	159	HIS	-	expression tag	UNP O66529
LE	160	HIS	-	expression tag	UNP O66529
LE	161	HIS	-	expression tag	UNP O66529
LF	2	GLU	GLN	conflict	UNP O66529
LF	83	GLU	ARG	conflict	UNP O66529
LF	86	GLU	THR	conflict	UNP O66529
LF	120	GLU	THR	conflict	UNP O66529
LF	123	GLU	GLN	conflict	UNP O66529
LF	155	LEU	-	expression tag	UNP O66529
LF	156	GLU	-	expression tag	UNP O66529
LF	157	HIS	-	expression tag	UNP O66529
LF	158	HIS	-	expression tag	UNP O66529
LF	159	HIS	-	expression tag	UNP O66529
LF	160	HIS	-	expression tag	UNP O66529
LF	161	HIS	-	expression tag	UNP O66529
LG	2	GLU	GLN	conflict	UNP O66529
LG	83	GLU	ARG	conflict	UNP O66529
LG	86	GLU	THR	conflict	UNP O66529
LG	120	GLU	THR	conflict	UNP O66529
LG	123	GLU	GLN	conflict	UNP O66529
LG	155	LEU	-	expression tag	UNP O66529
LG	156	GLU	-	expression tag	UNP O66529
LG	157	HIS	-	expression tag	UNP O66529
LG	158	HIS	-	expression tag	UNP O66529
LG	159	HIS	-	expression tag	UNP O66529
LG	160	HIS	-	expression tag	UNP O66529
LG	161	HIS	-	expression tag	UNP O66529
LH	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LH	83	GLU	ARG	conflict	UNP O66529
LH	86	GLU	THR	conflict	UNP O66529
LH	120	GLU	THR	conflict	UNP O66529
LH	123	GLU	GLN	conflict	UNP O66529
LH	155	LEU	-	expression tag	UNP O66529
LH	156	GLU	-	expression tag	UNP O66529
LH	157	HIS	-	expression tag	UNP O66529
LH	158	HIS	-	expression tag	UNP O66529
LH	159	HIS	-	expression tag	UNP O66529
LH	160	HIS	-	expression tag	UNP O66529
LH	161	HIS	-	expression tag	UNP O66529
LI	2	GLU	GLN	conflict	UNP O66529
LI	83	GLU	ARG	conflict	UNP O66529
LI	86	GLU	THR	conflict	UNP O66529
LI	120	GLU	THR	conflict	UNP O66529
LI	123	GLU	GLN	conflict	UNP O66529
LI	155	LEU	-	expression tag	UNP O66529
LI	156	GLU	-	expression tag	UNP O66529
LI	157	HIS	-	expression tag	UNP O66529
LI	158	HIS	-	expression tag	UNP O66529
LI	159	HIS	-	expression tag	UNP O66529
LI	160	HIS	-	expression tag	UNP O66529
LI	161	HIS	-	expression tag	UNP O66529
LJ	2	GLU	GLN	conflict	UNP O66529
LJ	83	GLU	ARG	conflict	UNP O66529
LJ	86	GLU	THR	conflict	UNP O66529
LJ	120	GLU	THR	conflict	UNP O66529
LJ	123	GLU	GLN	conflict	UNP O66529
LJ	155	LEU	-	expression tag	UNP O66529
LJ	156	GLU	-	expression tag	UNP O66529
LJ	157	HIS	-	expression tag	UNP O66529
LJ	158	HIS	-	expression tag	UNP O66529
LJ	159	HIS	-	expression tag	UNP O66529
LJ	160	HIS	-	expression tag	UNP O66529
LJ	161	HIS	-	expression tag	UNP O66529
LK	2	GLU	GLN	conflict	UNP O66529
LK	83	GLU	ARG	conflict	UNP O66529
LK	86	GLU	THR	conflict	UNP O66529
LK	120	GLU	THR	conflict	UNP O66529
LK	123	GLU	GLN	conflict	UNP O66529
LK	155	LEU	-	expression tag	UNP O66529
LK	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LK	157	HIS	-	expression tag	UNP O66529
LK	158	HIS	-	expression tag	UNP O66529
LK	159	HIS	-	expression tag	UNP O66529
LK	160	HIS	-	expression tag	UNP O66529
LK	161	HIS	-	expression tag	UNP O66529
LL	2	GLU	GLN	conflict	UNP O66529
LL	83	GLU	ARG	conflict	UNP O66529
LL	86	GLU	THR	conflict	UNP O66529
LL	120	GLU	THR	conflict	UNP O66529
LL	123	GLU	GLN	conflict	UNP O66529
LL	155	LEU	-	expression tag	UNP O66529
LL	156	GLU	-	expression tag	UNP O66529
LL	157	HIS	-	expression tag	UNP O66529
LL	158	HIS	-	expression tag	UNP O66529
LL	159	HIS	-	expression tag	UNP O66529
LL	160	HIS	-	expression tag	UNP O66529
LL	161	HIS	-	expression tag	UNP O66529
LM	2	GLU	GLN	conflict	UNP O66529
LM	83	GLU	ARG	conflict	UNP O66529
LM	86	GLU	THR	conflict	UNP O66529
LM	120	GLU	THR	conflict	UNP O66529
LM	123	GLU	GLN	conflict	UNP O66529
LM	155	LEU	-	expression tag	UNP O66529
LM	156	GLU	-	expression tag	UNP O66529
LM	157	HIS	-	expression tag	UNP O66529
LM	158	HIS	-	expression tag	UNP O66529
LM	159	HIS	-	expression tag	UNP O66529
LM	160	HIS	-	expression tag	UNP O66529
LM	161	HIS	-	expression tag	UNP O66529
LN	2	GLU	GLN	conflict	UNP O66529
LN	83	GLU	ARG	conflict	UNP O66529
LN	86	GLU	THR	conflict	UNP O66529
LN	120	GLU	THR	conflict	UNP O66529
LN	123	GLU	GLN	conflict	UNP O66529
LN	155	LEU	-	expression tag	UNP O66529
LN	156	GLU	-	expression tag	UNP O66529
LN	157	HIS	-	expression tag	UNP O66529
LN	158	HIS	-	expression tag	UNP O66529
LN	159	HIS	-	expression tag	UNP O66529
LN	160	HIS	-	expression tag	UNP O66529
LN	161	HIS	-	expression tag	UNP O66529
LO	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

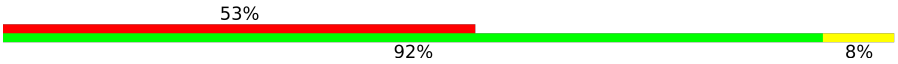
Chain	Residue	Modelled	Actual	Comment	Reference
LO	83	GLU	ARG	conflict	UNP O66529
LO	86	GLU	THR	conflict	UNP O66529
LO	120	GLU	THR	conflict	UNP O66529
LO	123	GLU	GLN	conflict	UNP O66529
LO	155	LEU	-	expression tag	UNP O66529
LO	156	GLU	-	expression tag	UNP O66529
LO	157	HIS	-	expression tag	UNP O66529
LO	158	HIS	-	expression tag	UNP O66529
LO	159	HIS	-	expression tag	UNP O66529
LO	160	HIS	-	expression tag	UNP O66529
LO	161	HIS	-	expression tag	UNP O66529

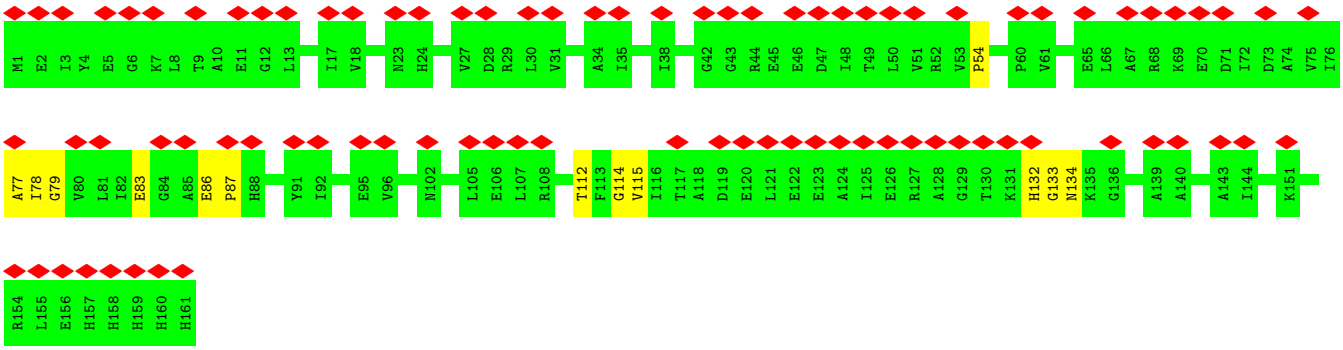
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

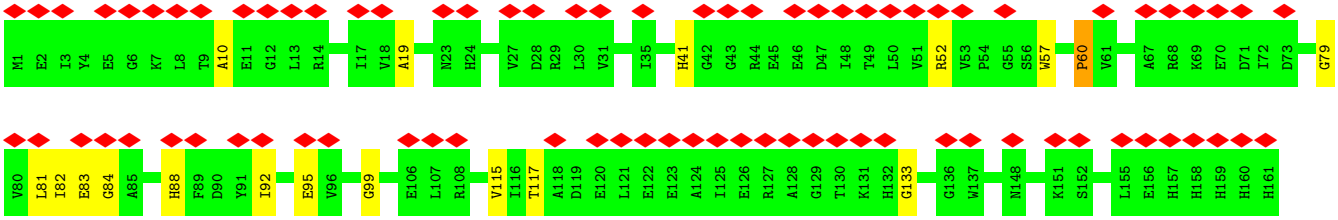
Chain AA:





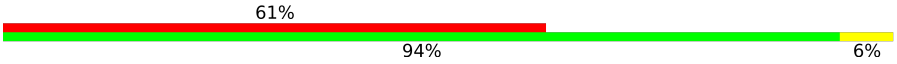
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

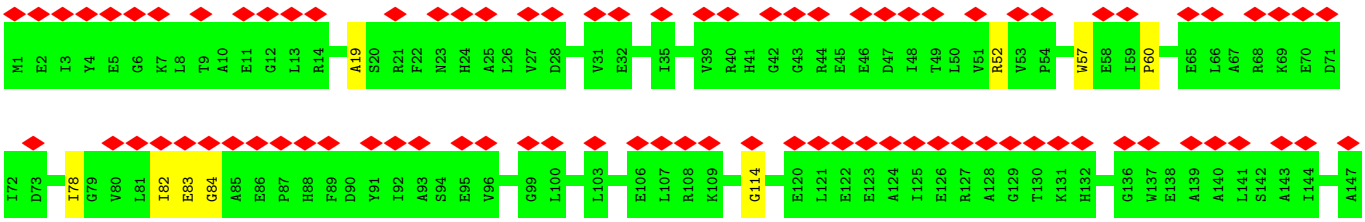
Chain AB:

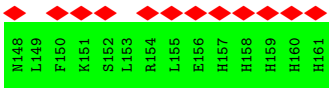


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AC:

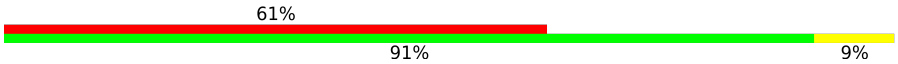


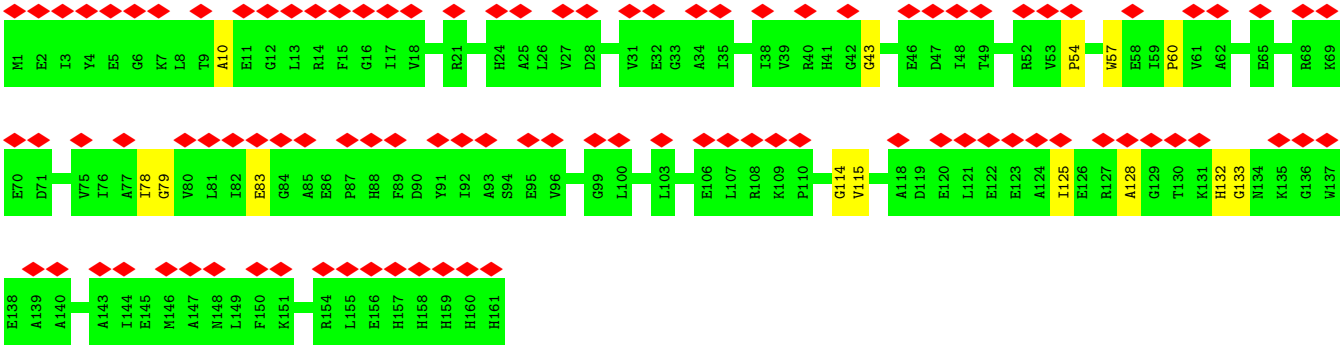




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

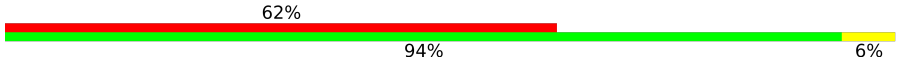
Chain AD:

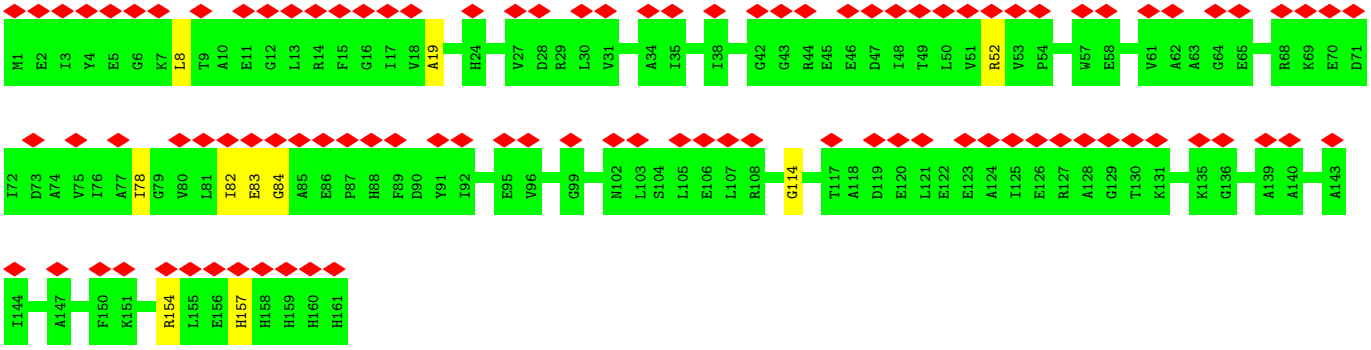




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

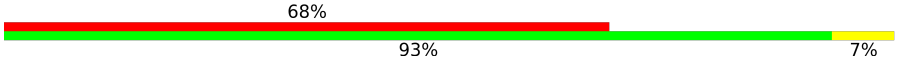
Chain AE:

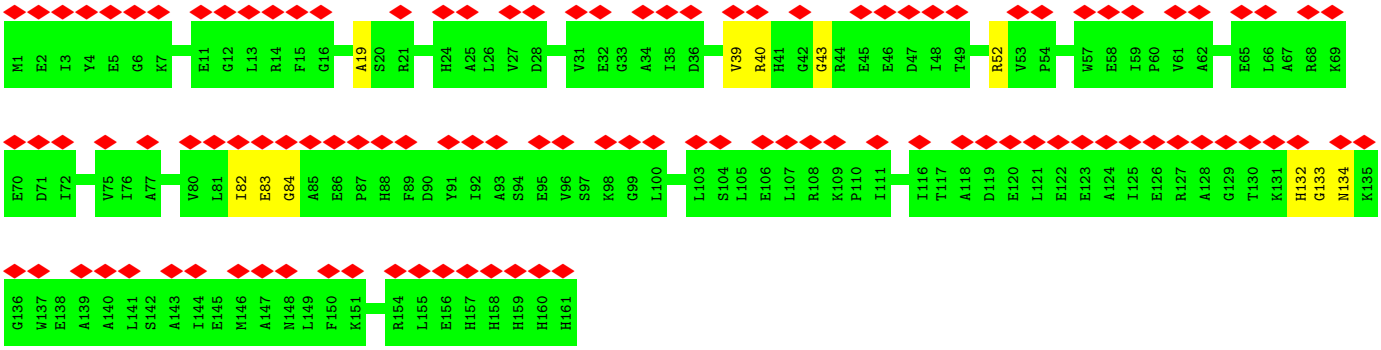




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

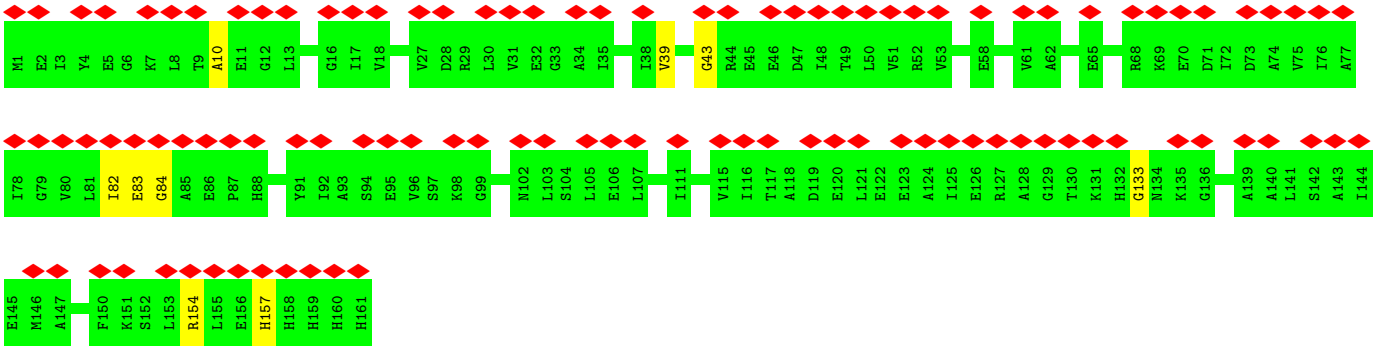
Chain AF:





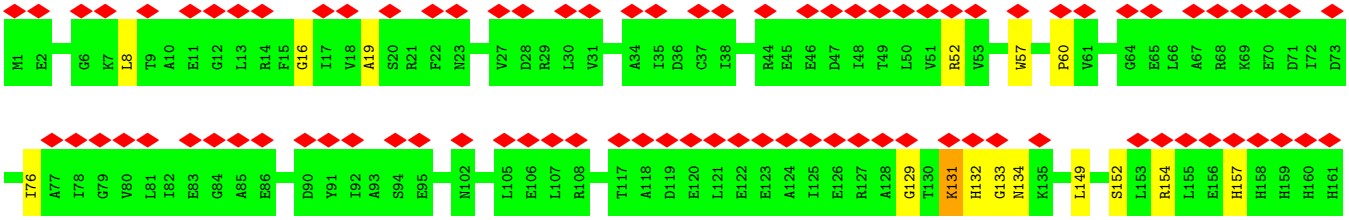
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AG: 65% 94% 6%



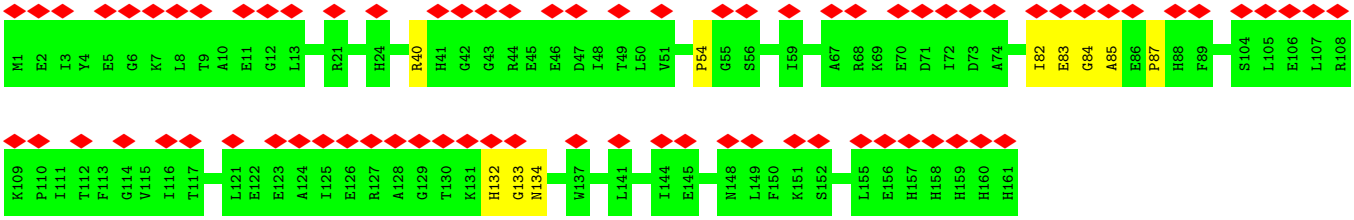
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AH: 54% 90% 9%



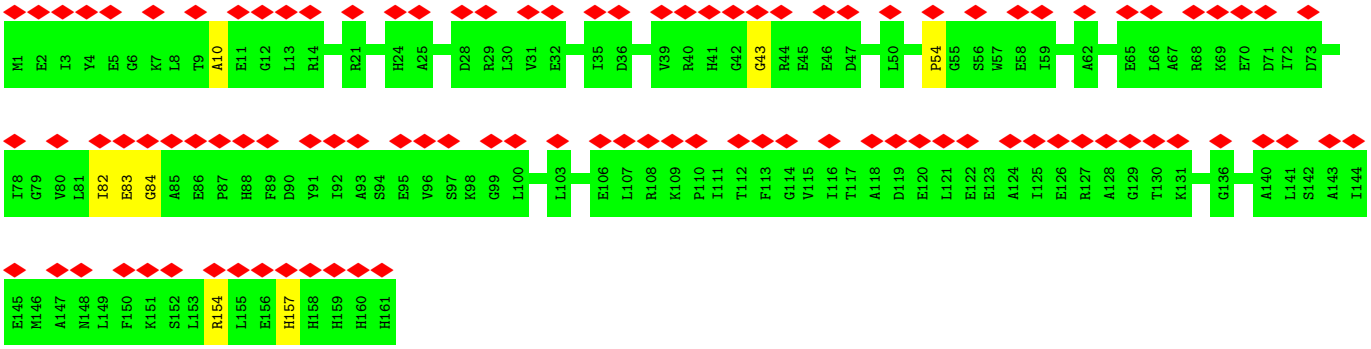
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AI: 47% 94% 6%



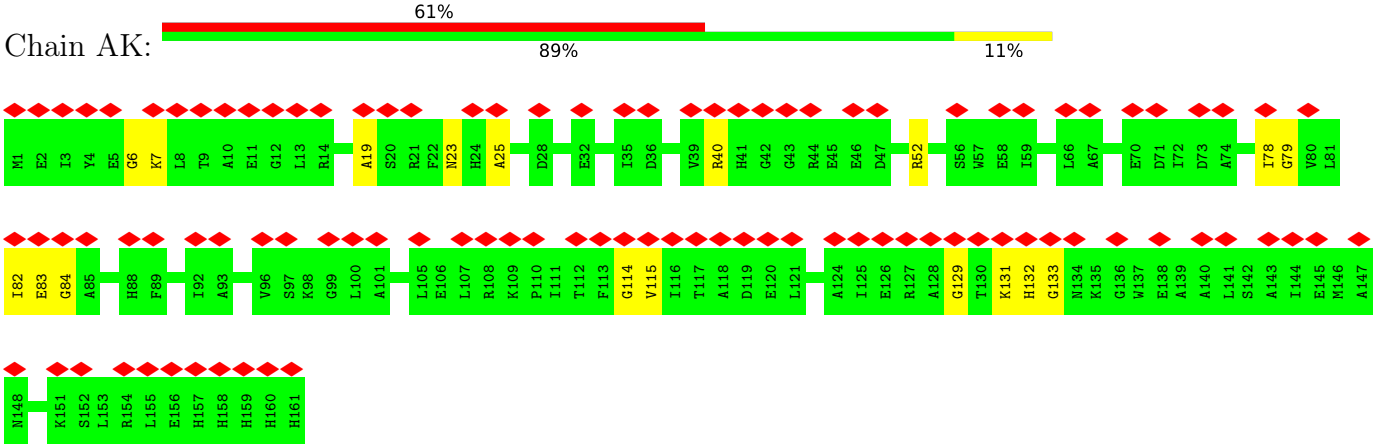
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AJ: 63% 95% 5%



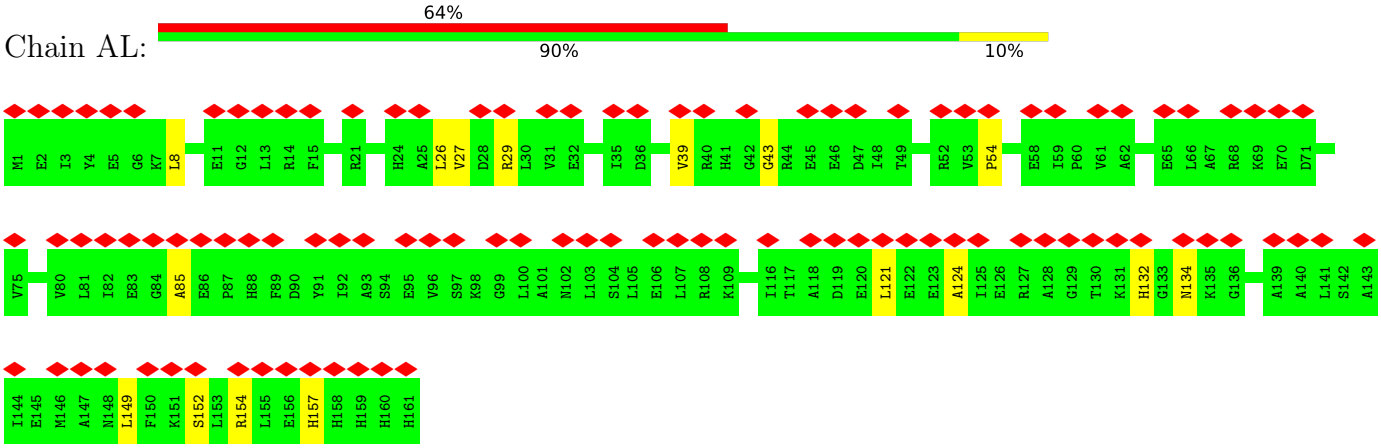
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AK:



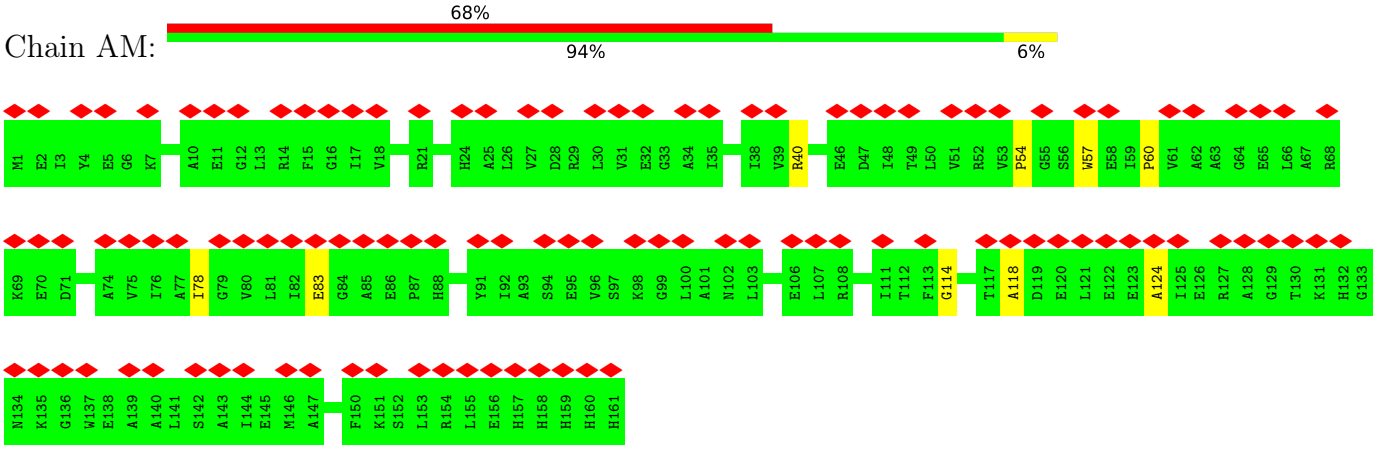
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AL:



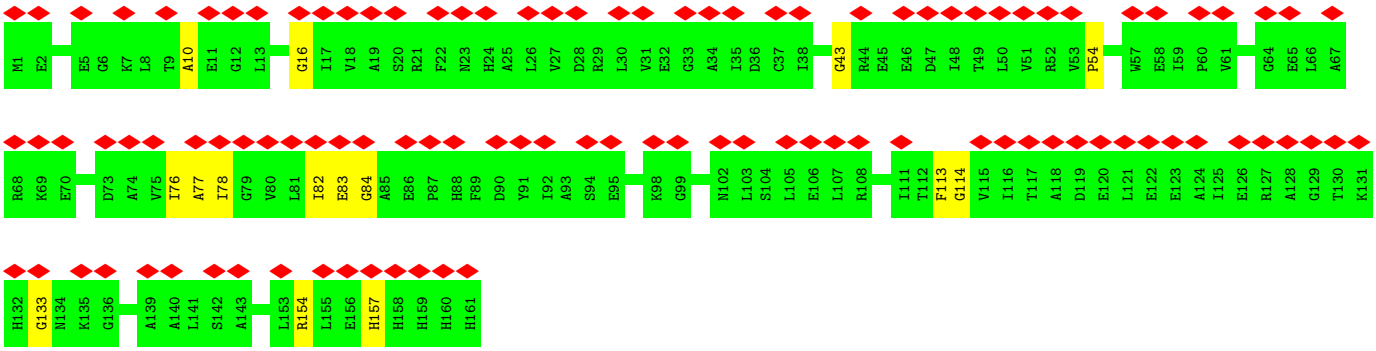
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AM:



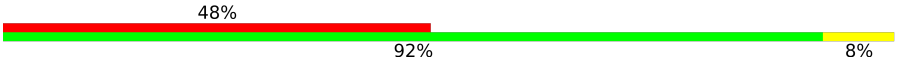
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

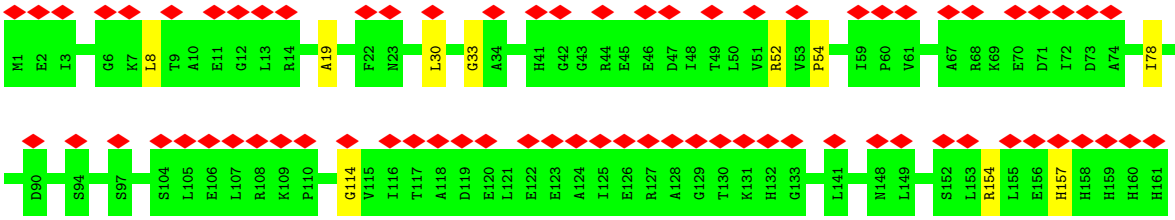
Chain AN:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

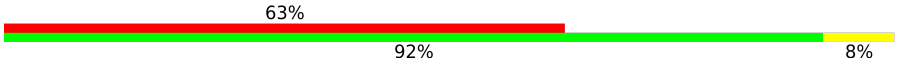
Chain AO:

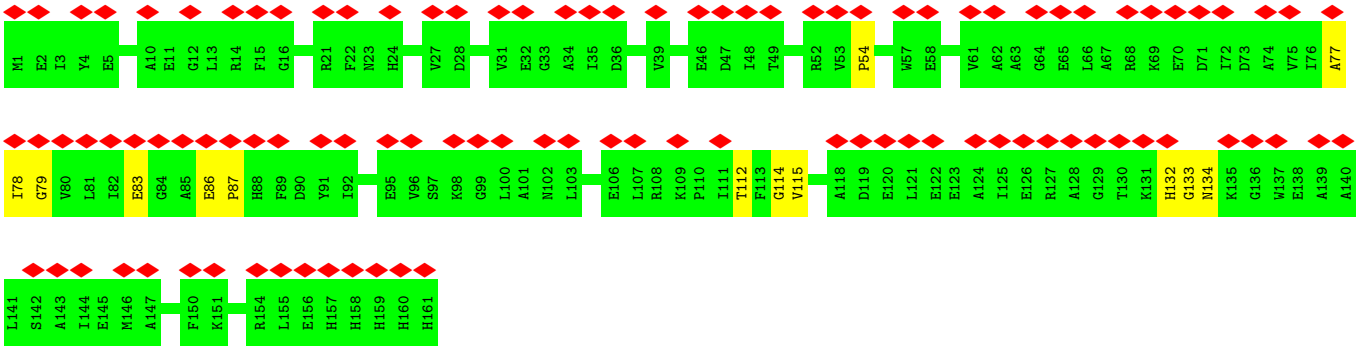




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

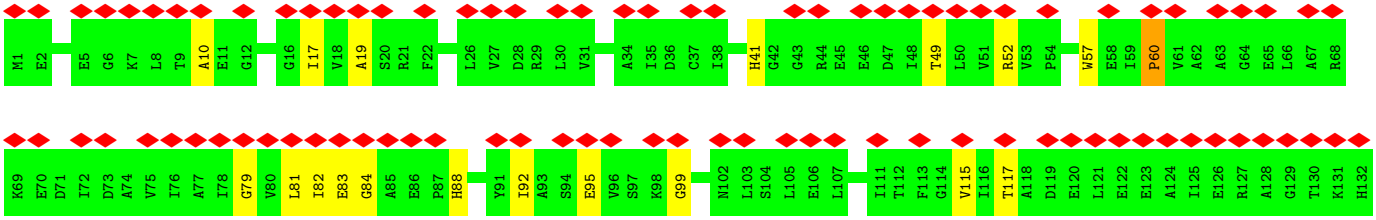
Chain BA:

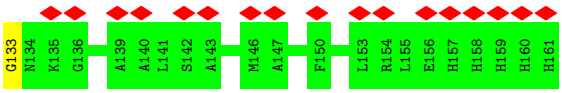




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

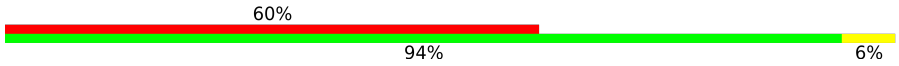
Chain BB:

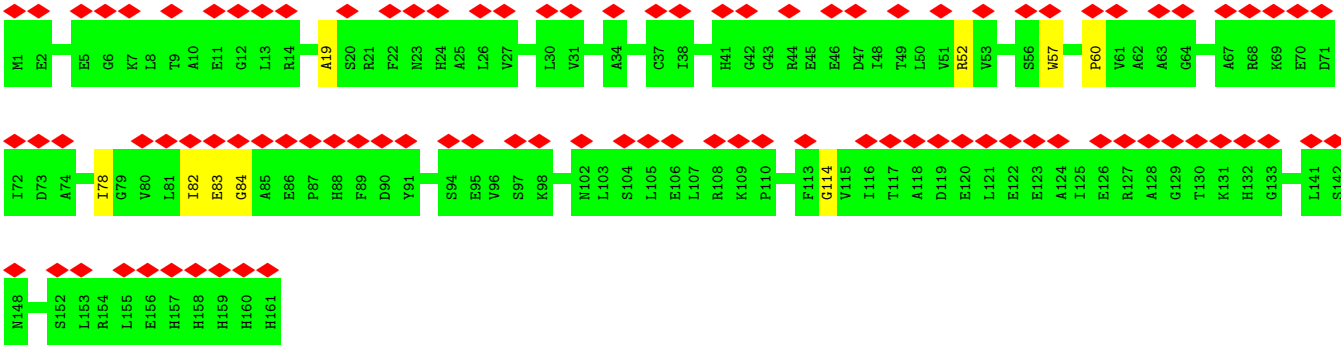




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

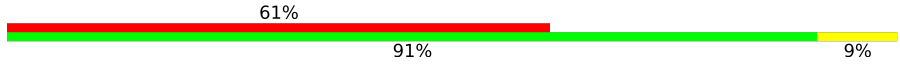
Chain BC:

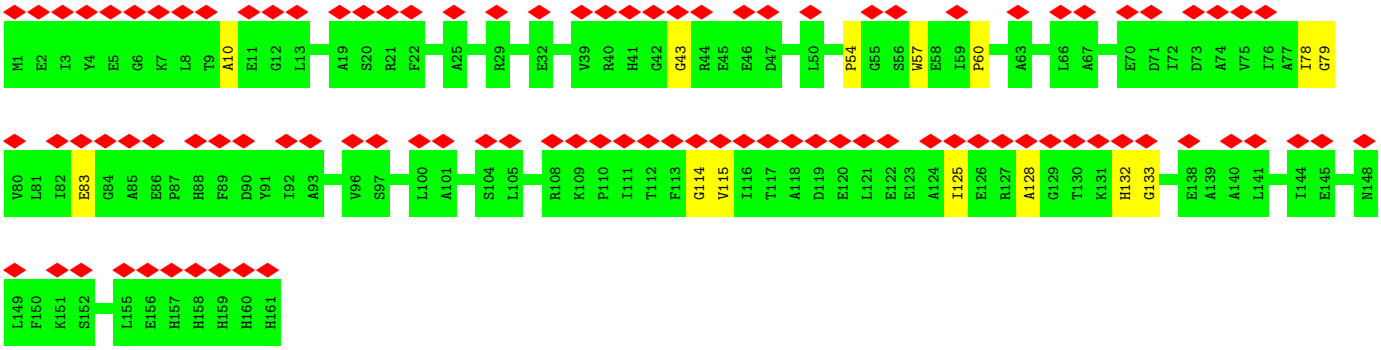




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

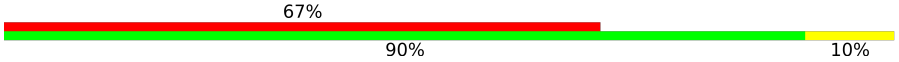
Chain BD:

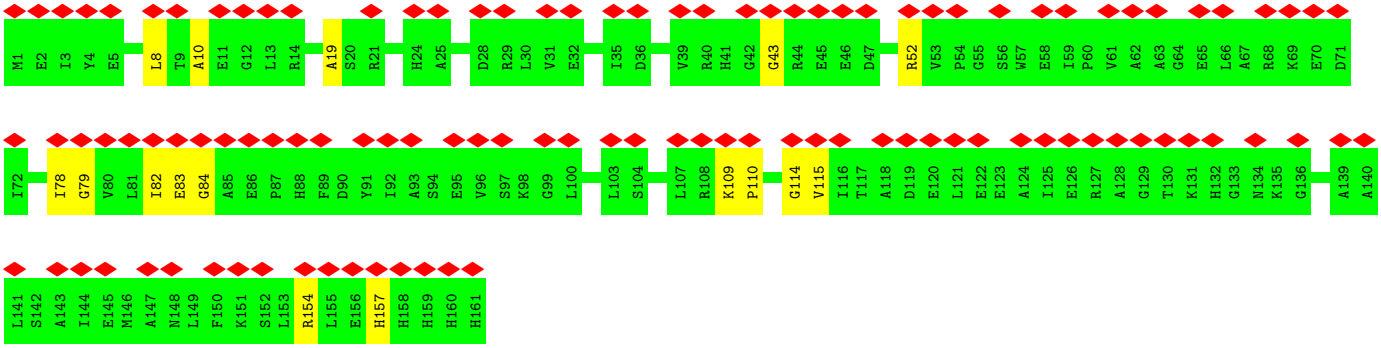




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

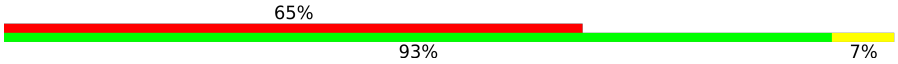
Chain BE:

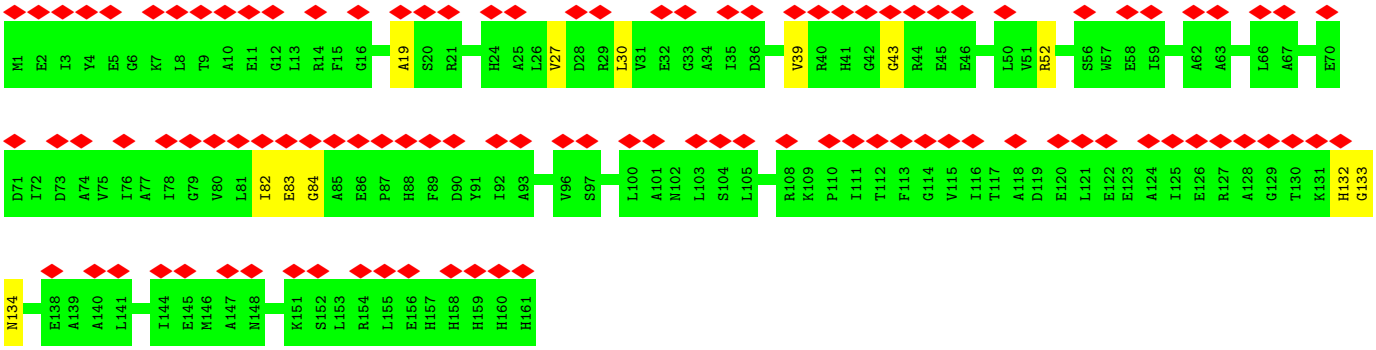




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

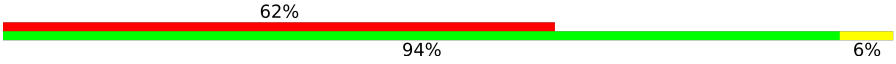
Chain BF:

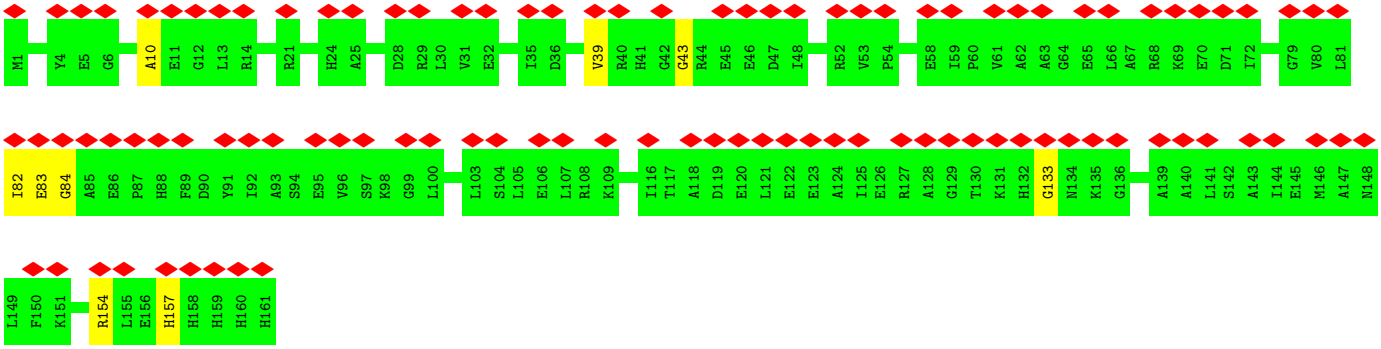




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

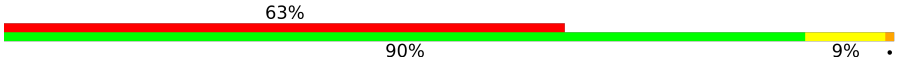
Chain BG:

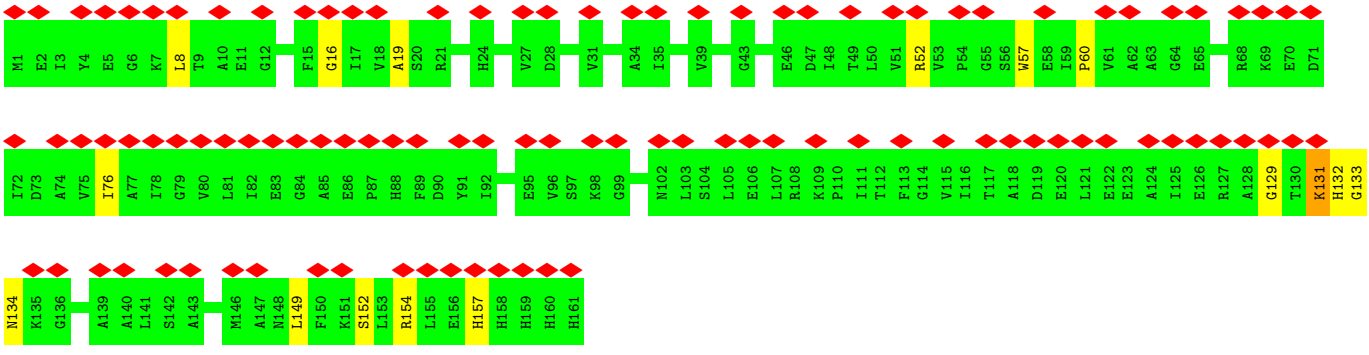




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

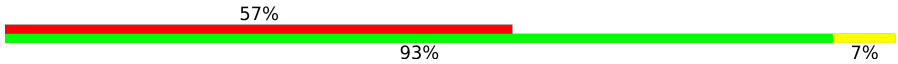
Chain BH:

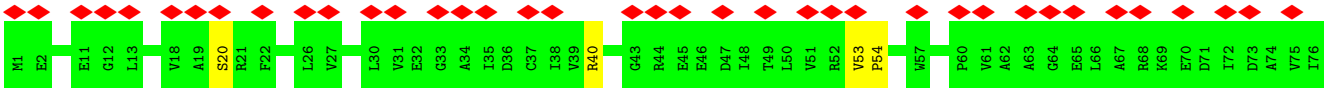


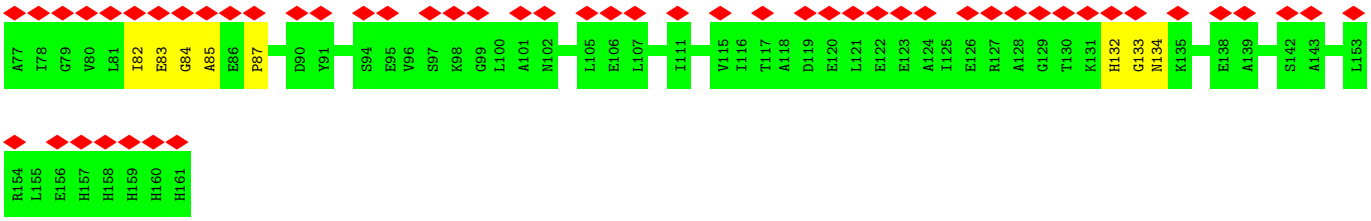


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BI:

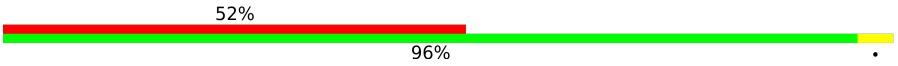


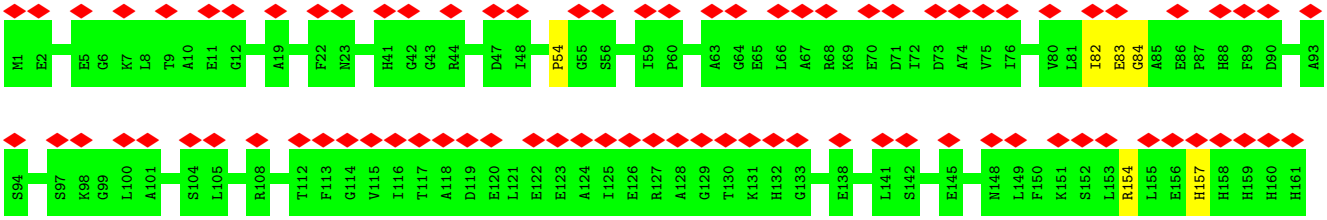




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

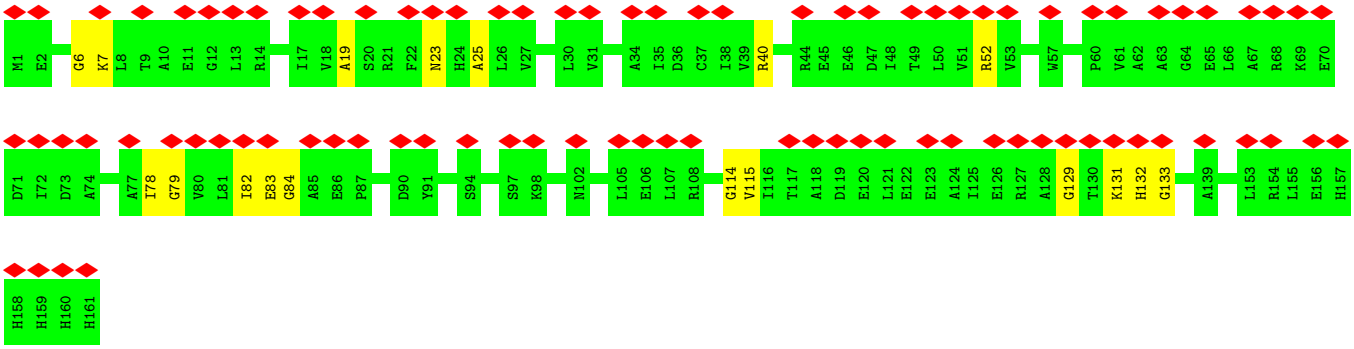
Chain BJ:





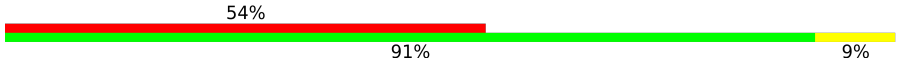
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

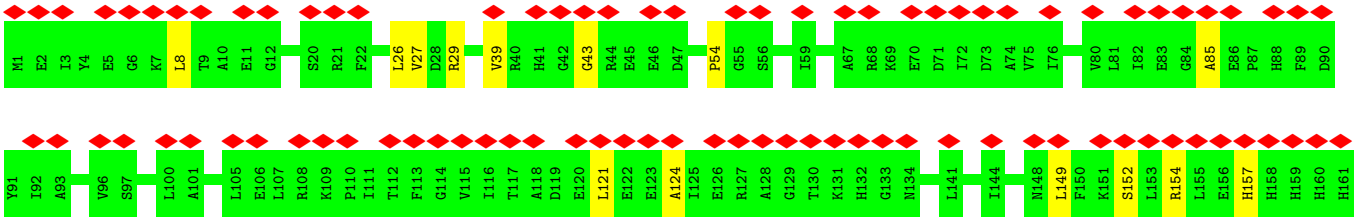
Chain BK:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

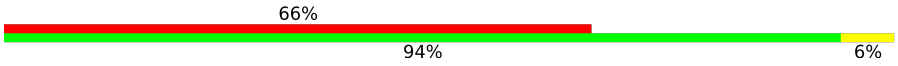
Chain BL:

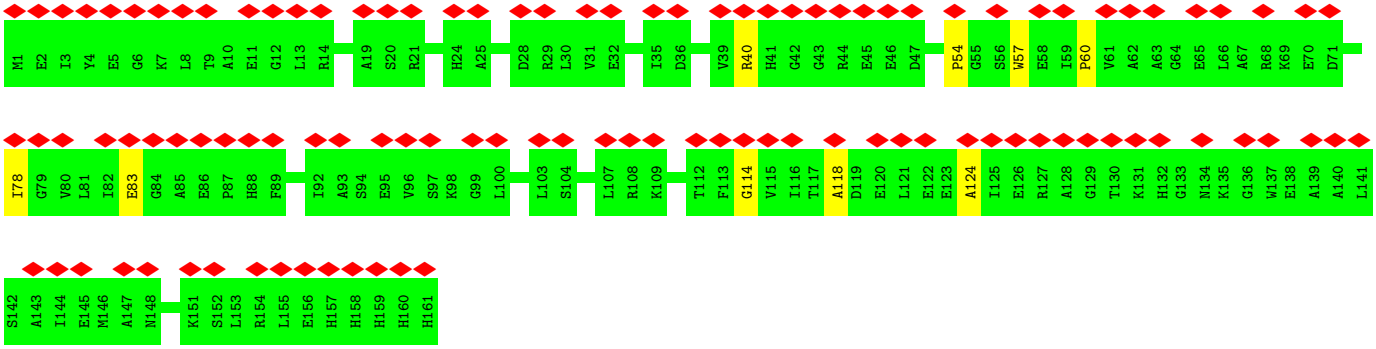




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

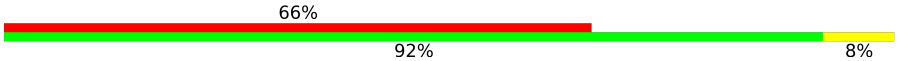
Chain BM:

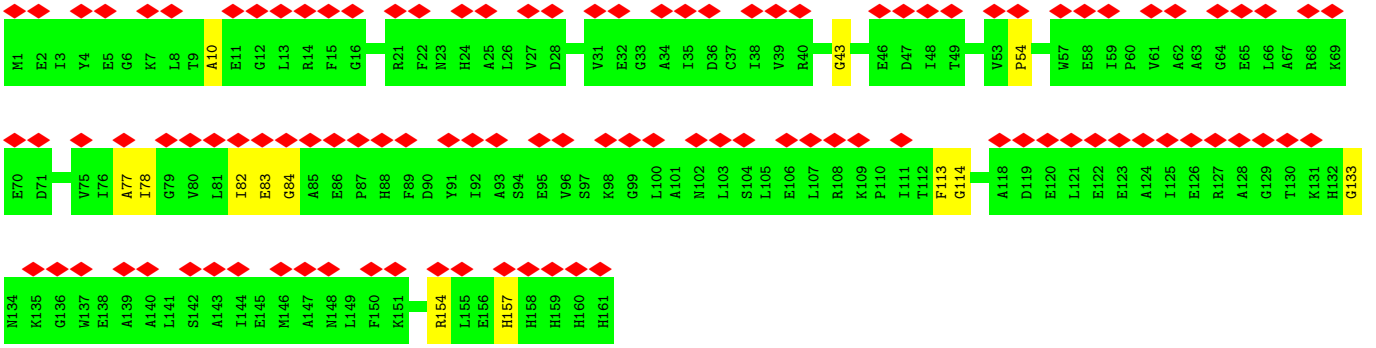




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

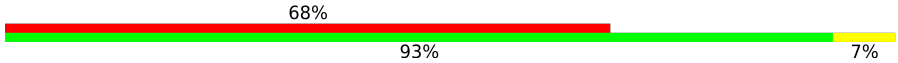
Chain BN:

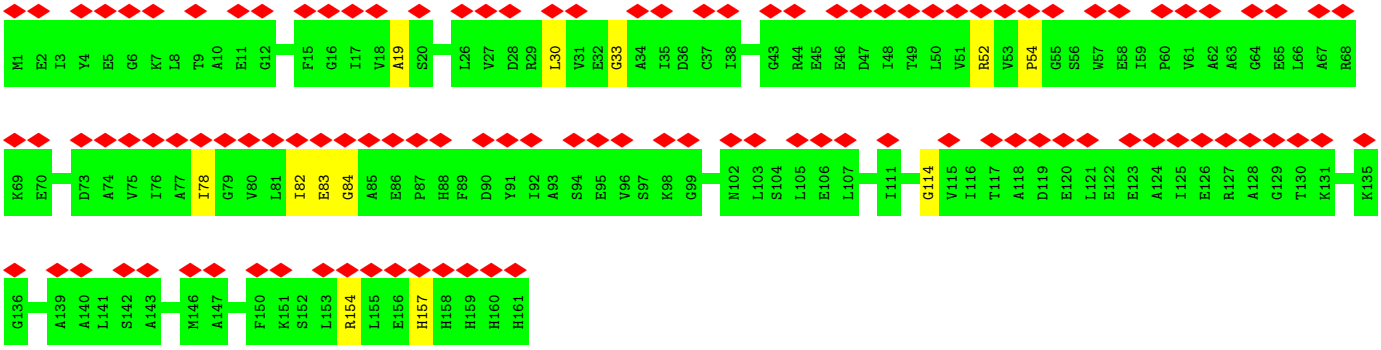




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

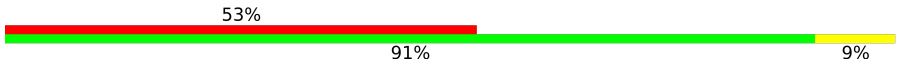
Chain BO:

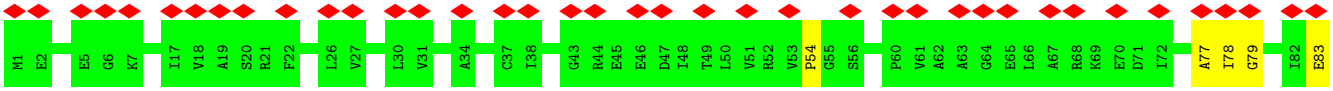


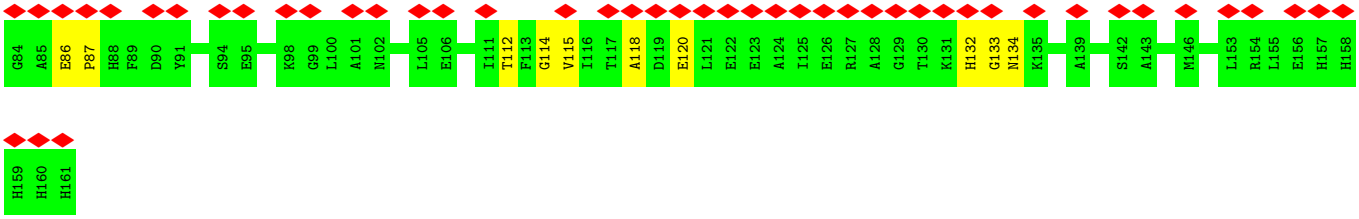


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA:

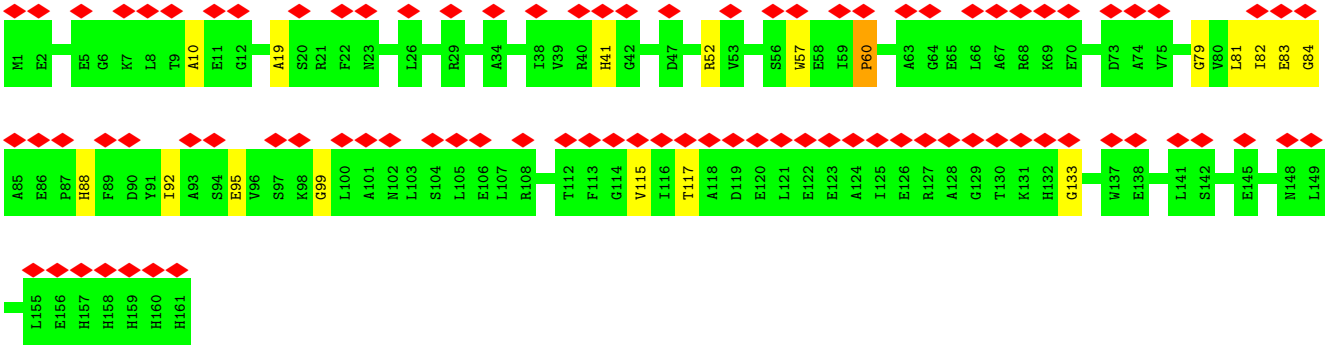






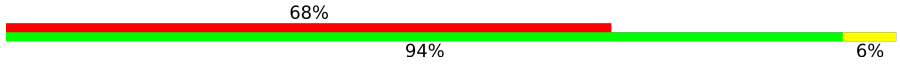
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

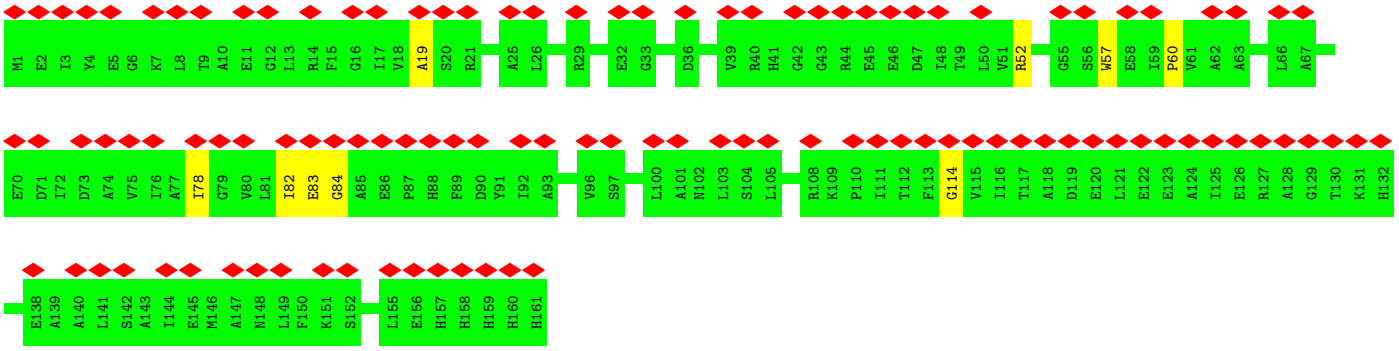
Chain CB:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

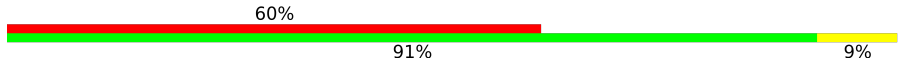
Chain CC:

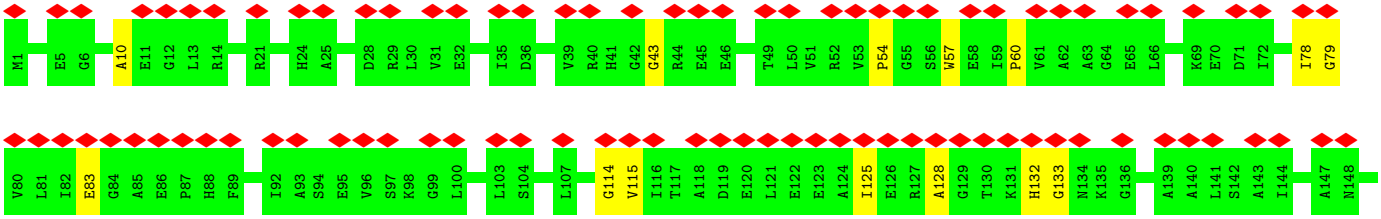


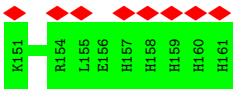


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CD:

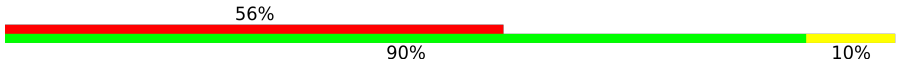


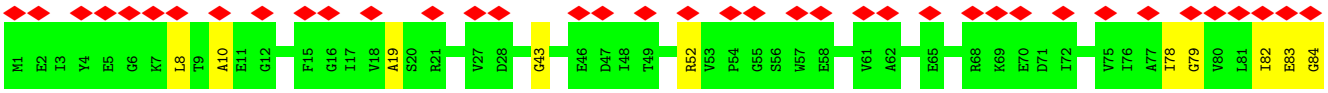


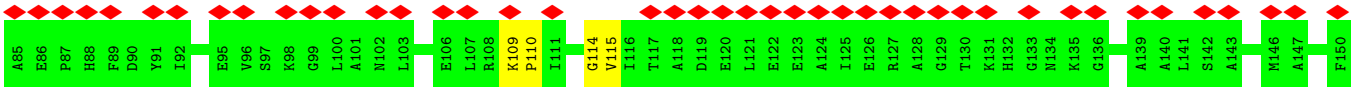


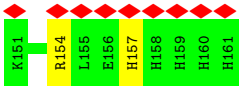
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CE:



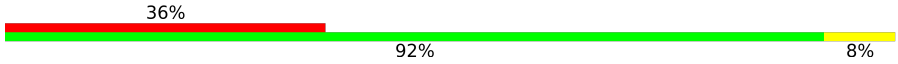


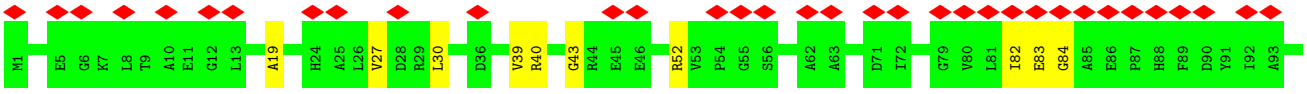


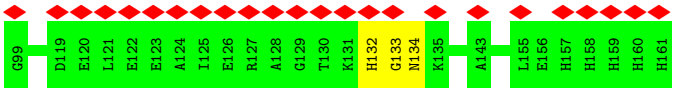


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CF:

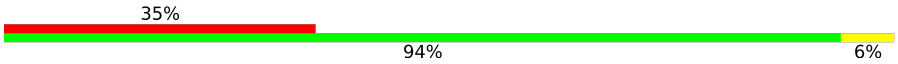


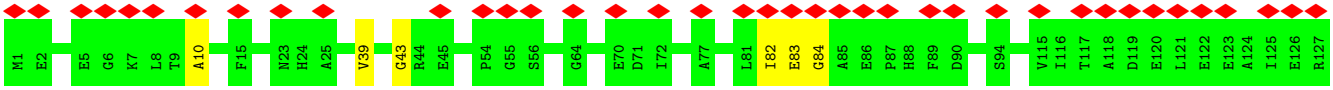


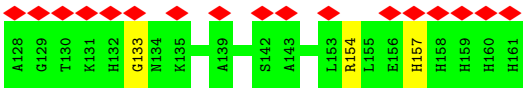


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CG:

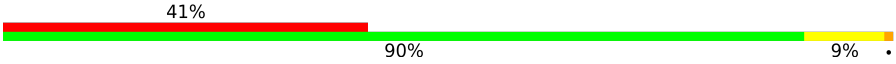


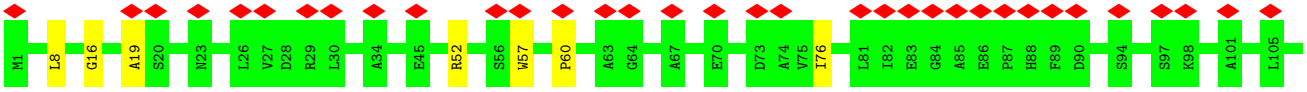


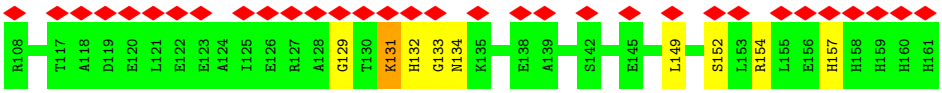


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CH:

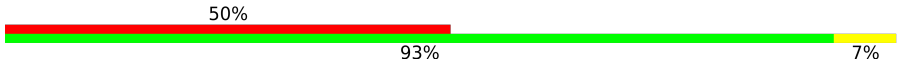


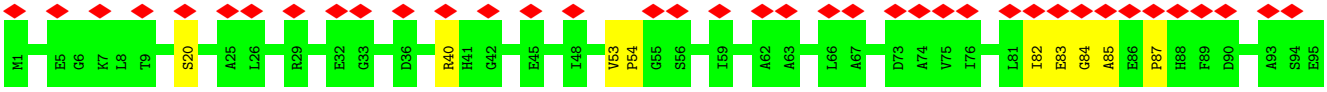


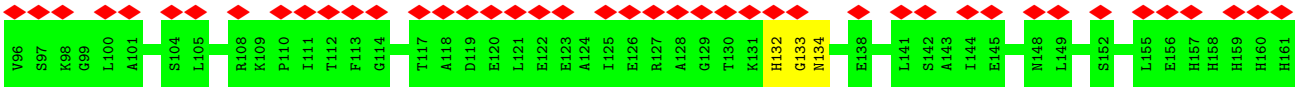


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CI:

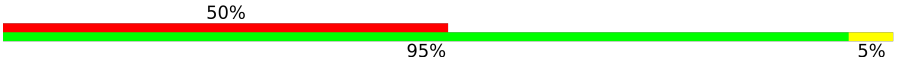


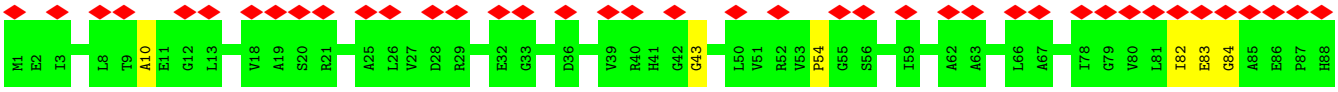


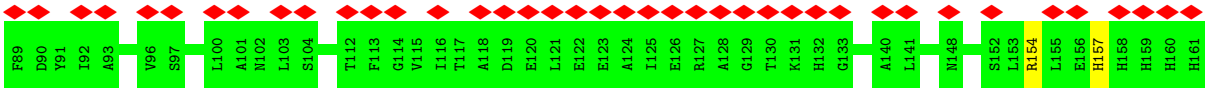


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CJ:

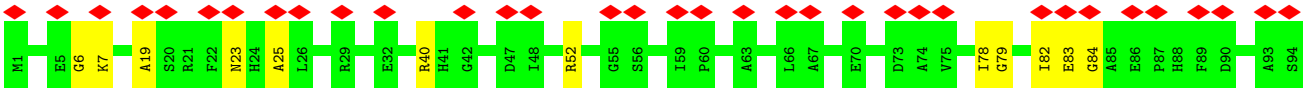


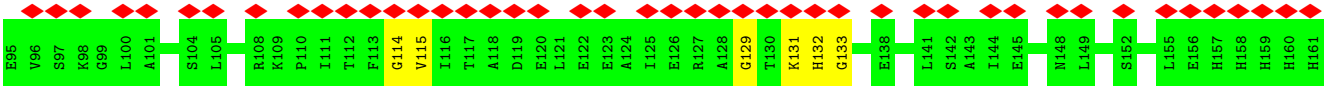




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

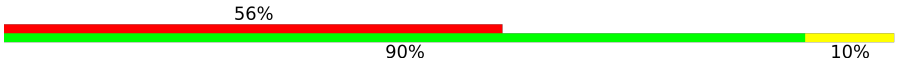
Chain CK:

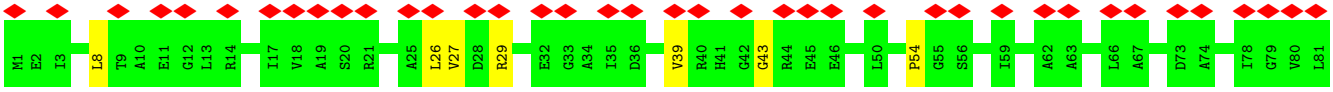


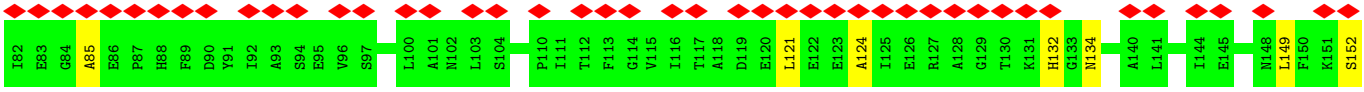


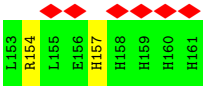
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CL:



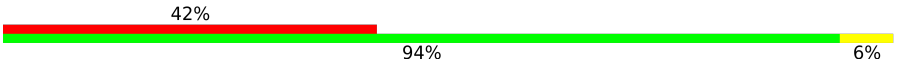


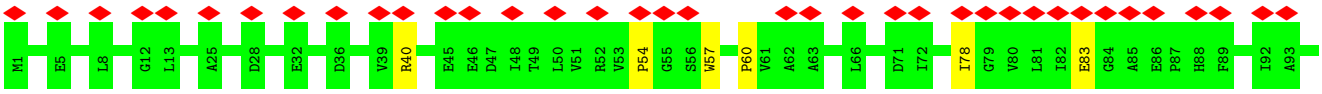


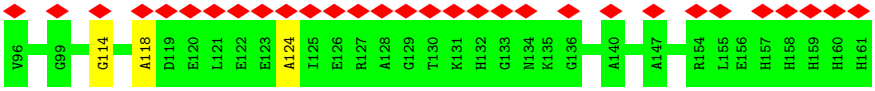


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CM:

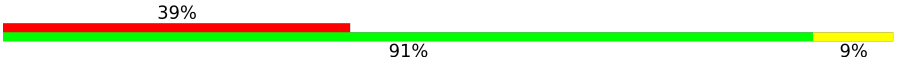


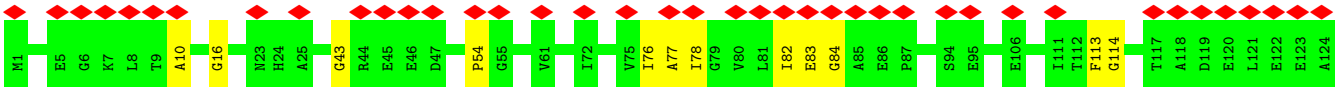


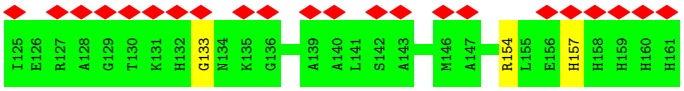


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CN:

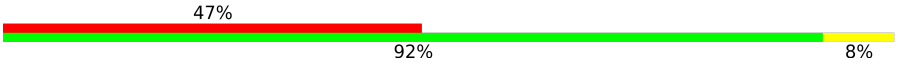


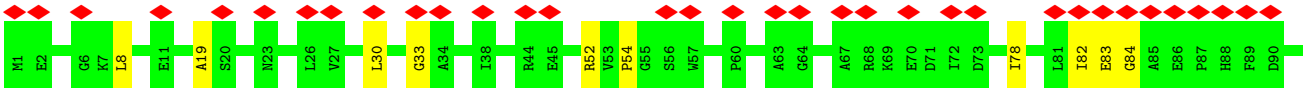


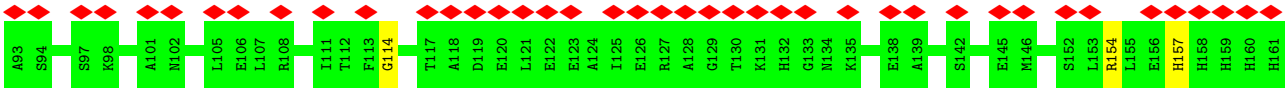


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CO:

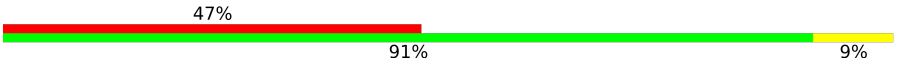


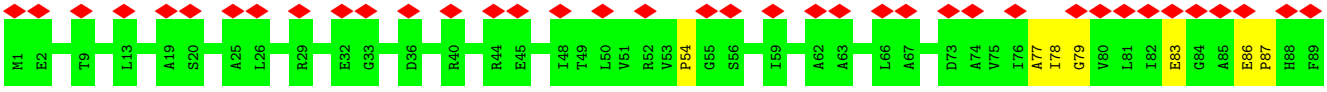


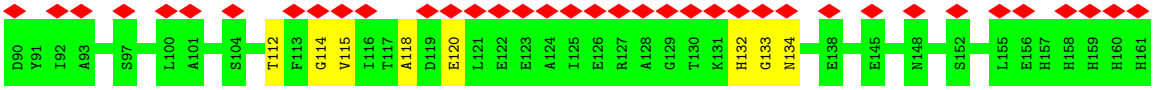


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DA:

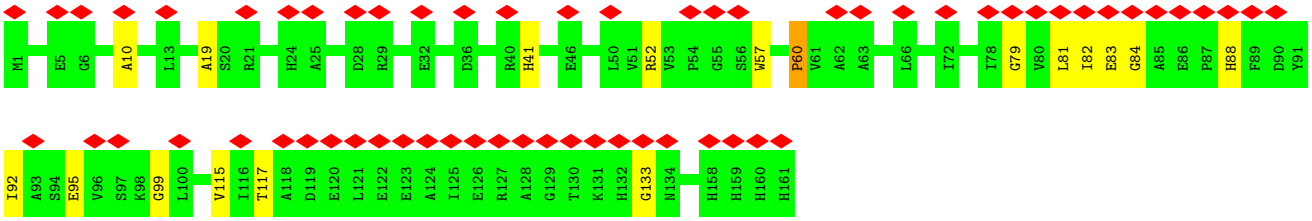






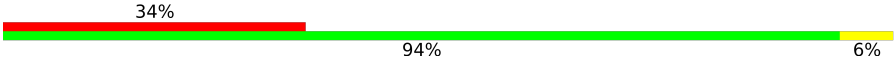
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

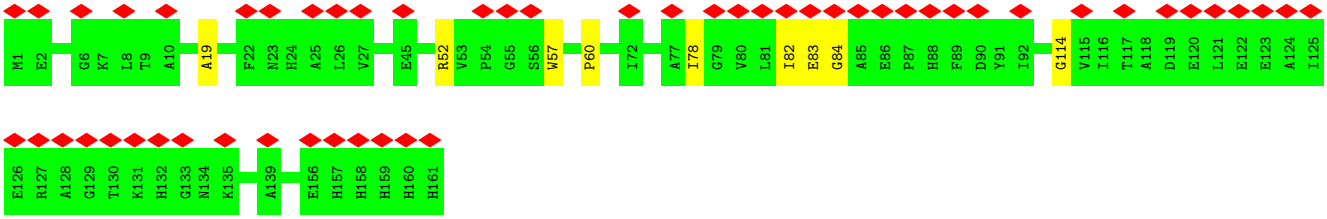
Chain DB:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

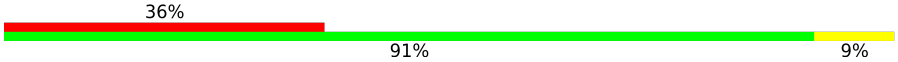
Chain DC:

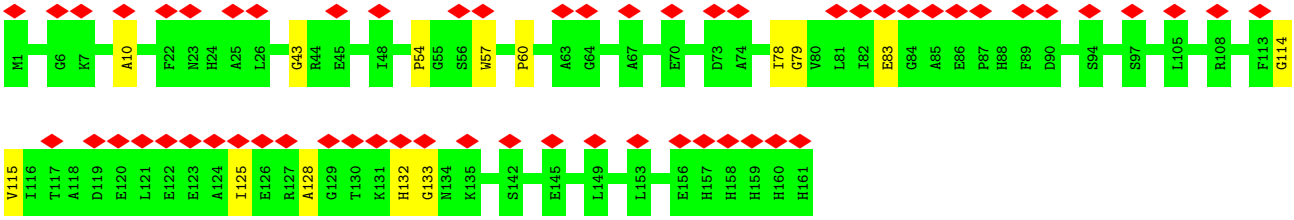




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

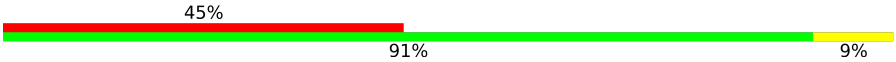
Chain DD:

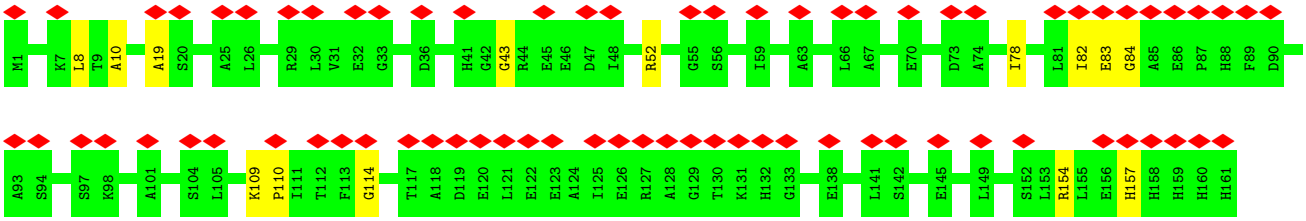




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

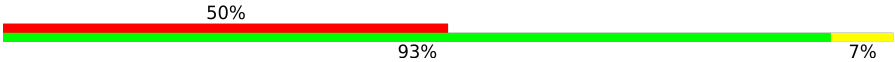
Chain DE:

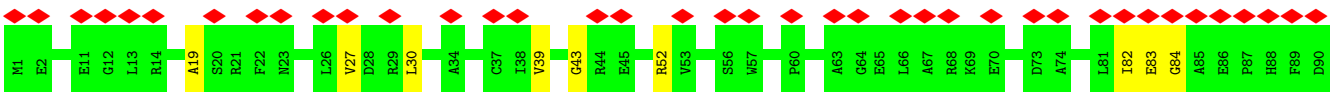


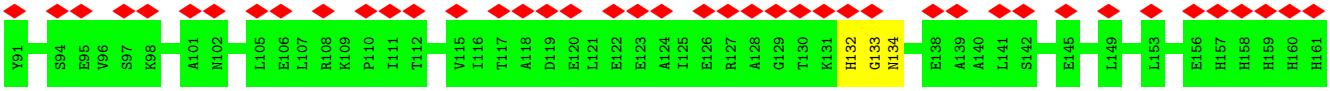


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DF:

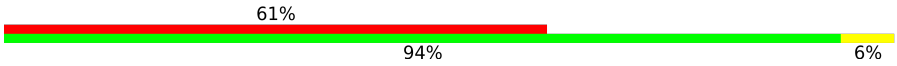


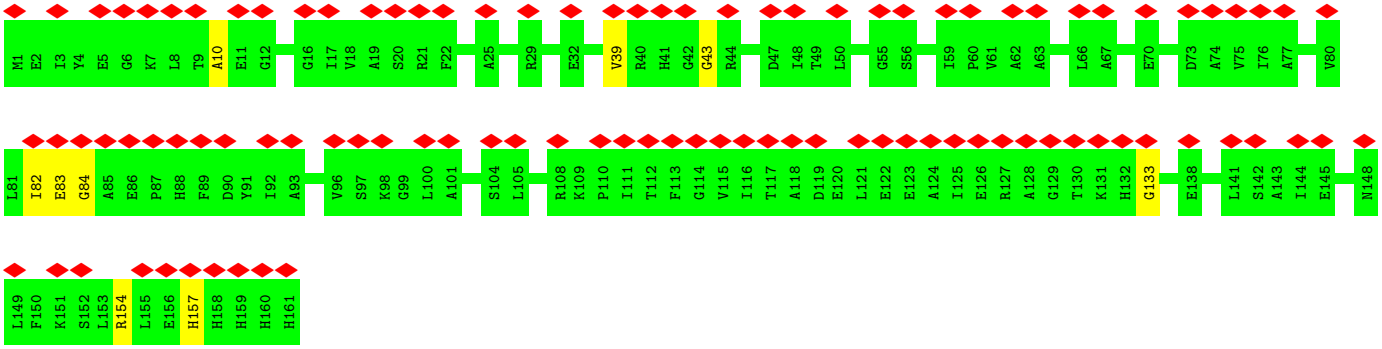




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

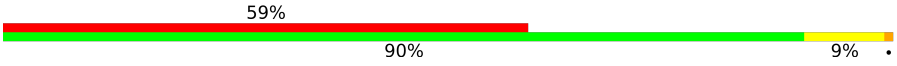
Chain DG:

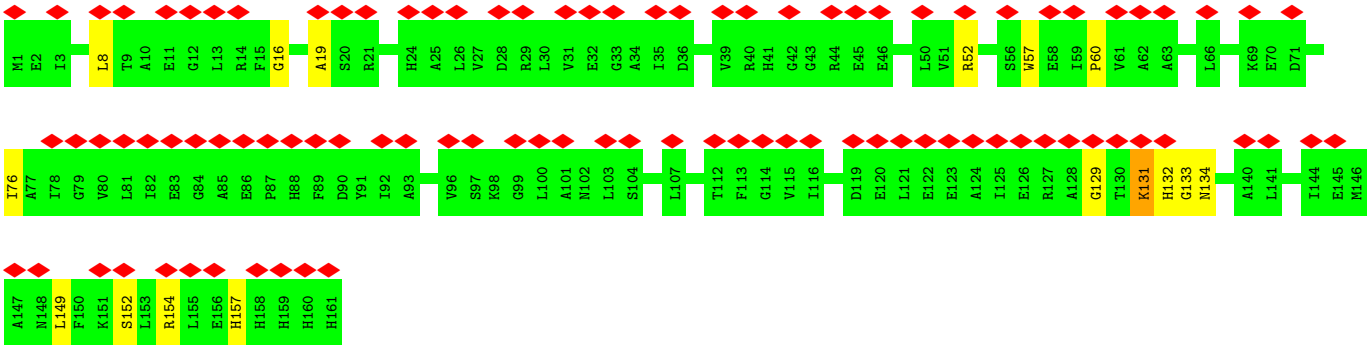




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

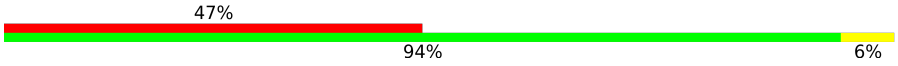
Chain DH:

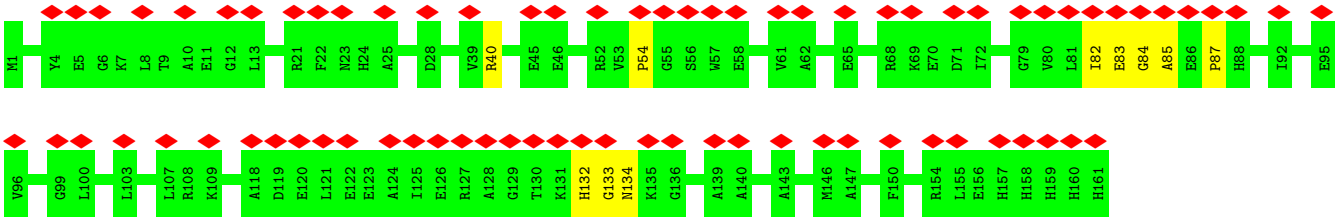




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

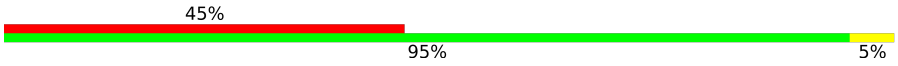
Chain DI:

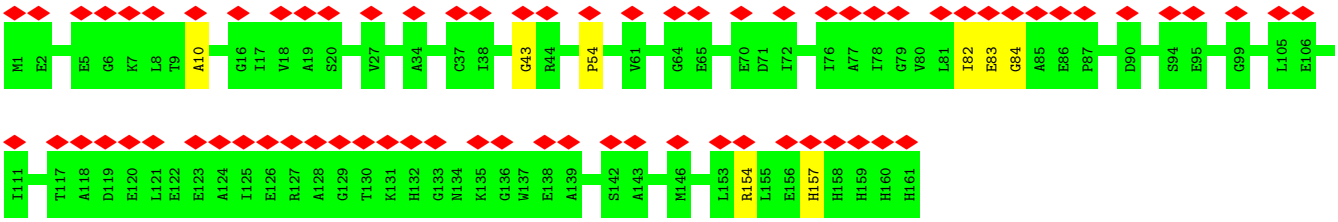




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

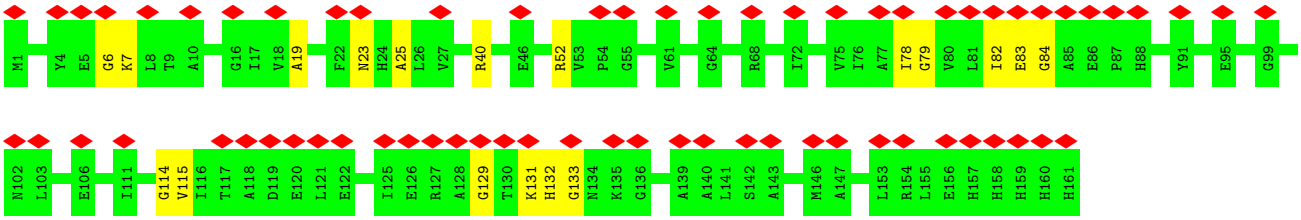
Chain DJ:





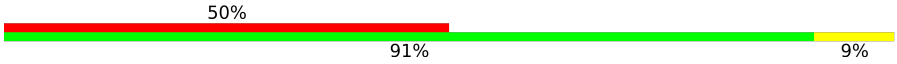
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

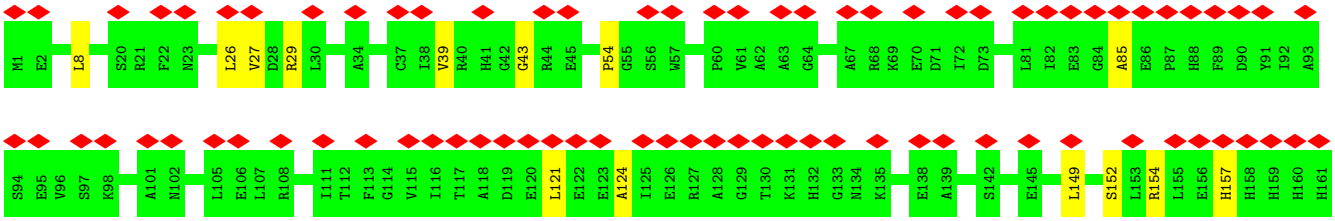
Chain DK:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

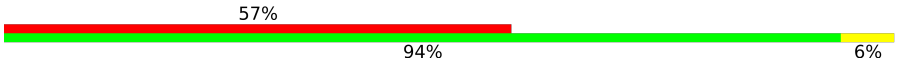
Chain DL:

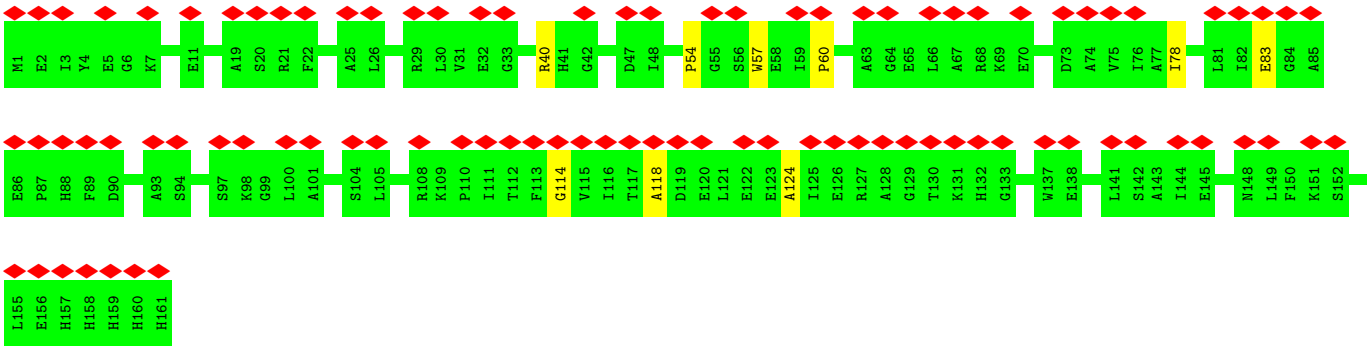




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

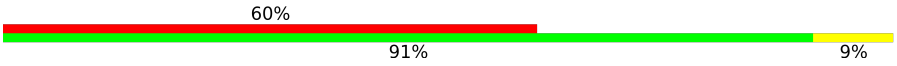
Chain DM:

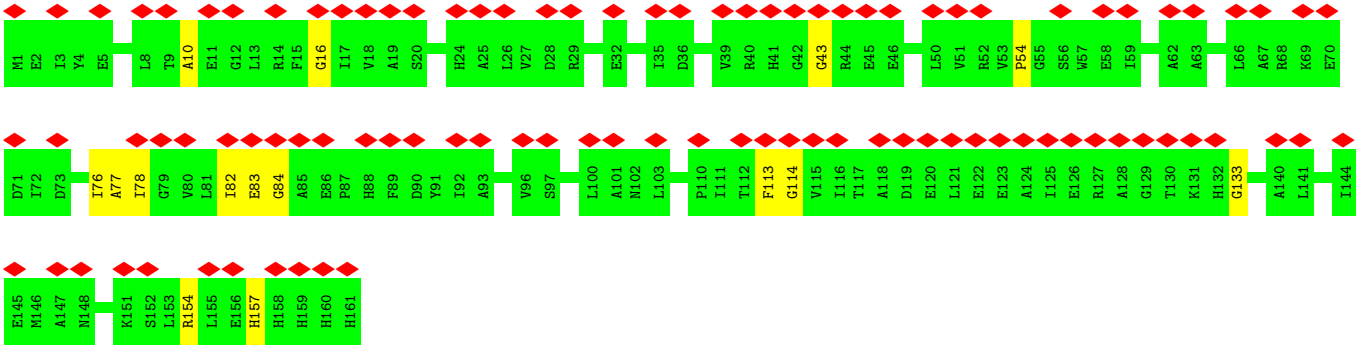




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

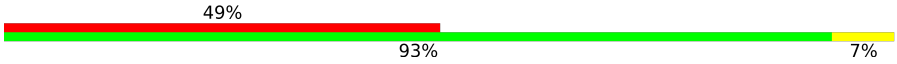
Chain DN:

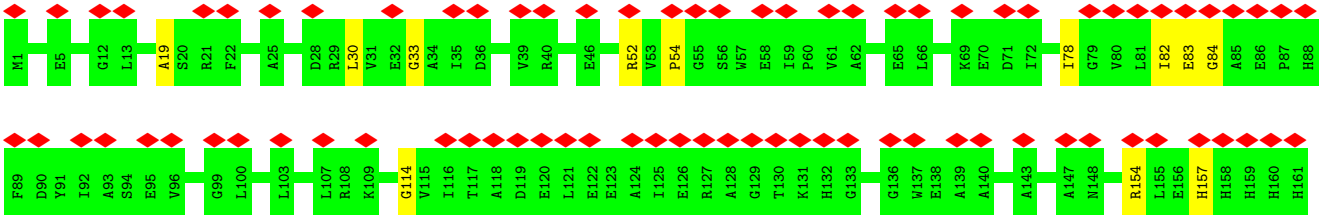




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

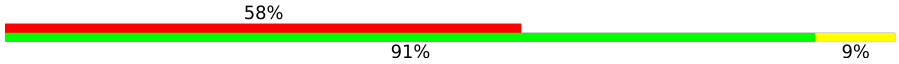
Chain DO:

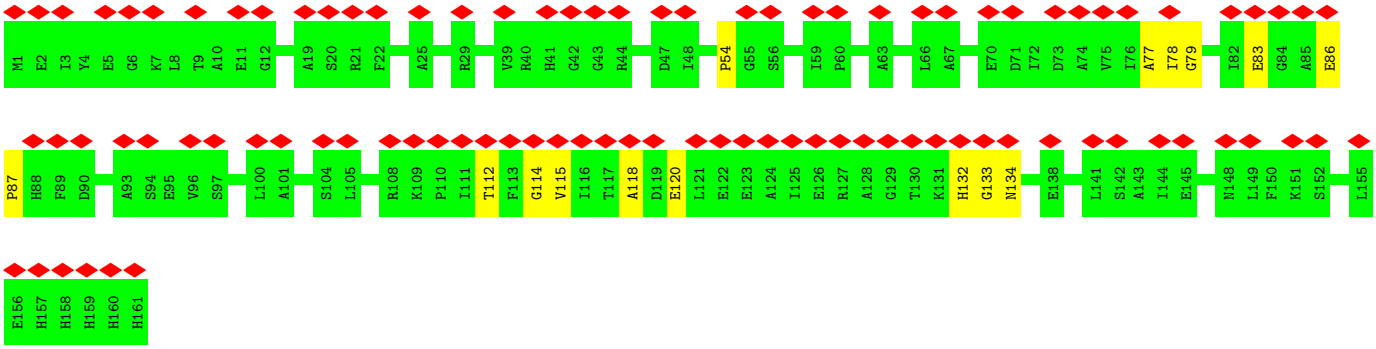




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

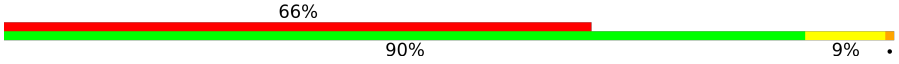
Chain EA:

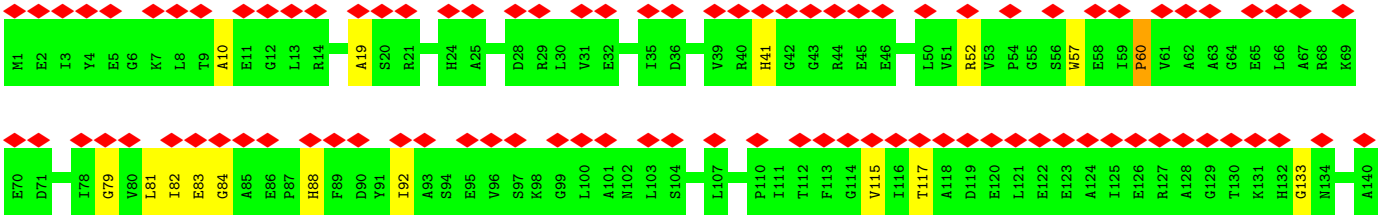


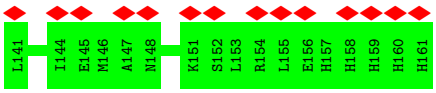


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EB:

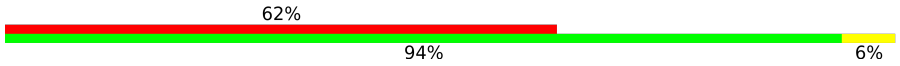


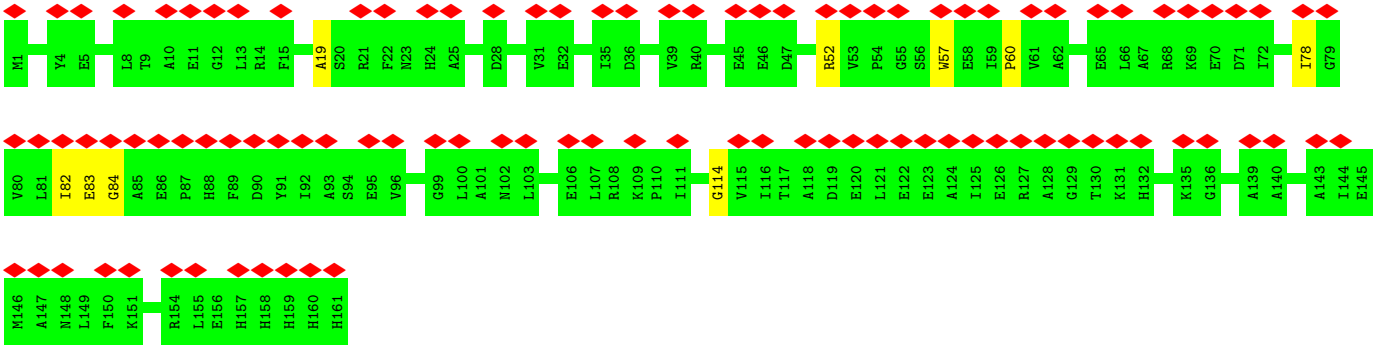




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

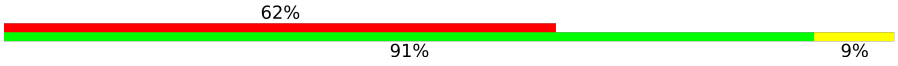
Chain EC:

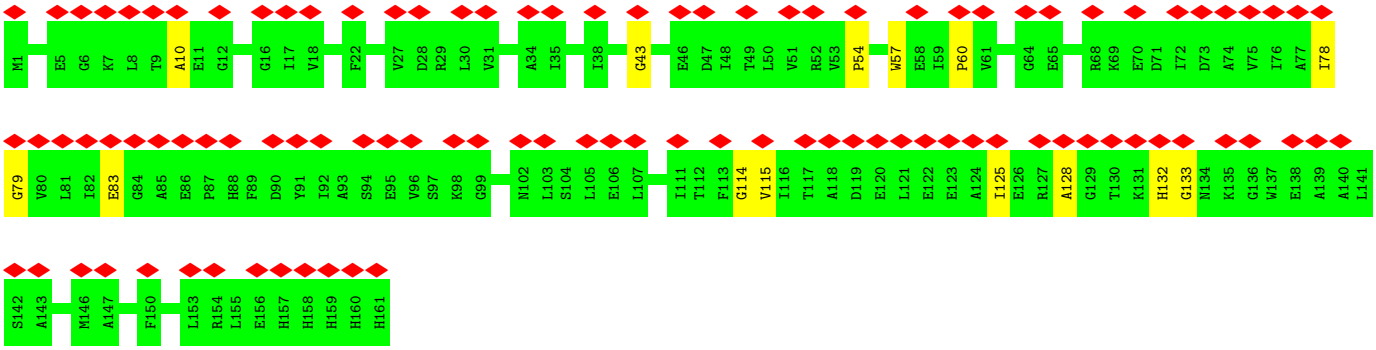




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

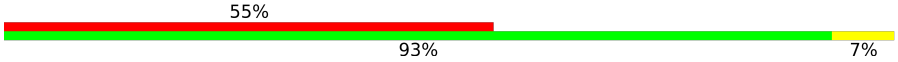
Chain ED:

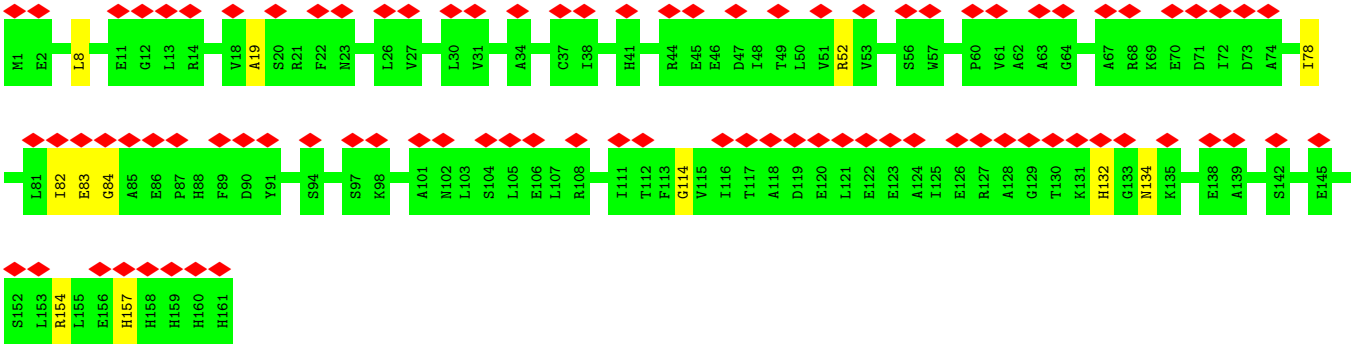




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

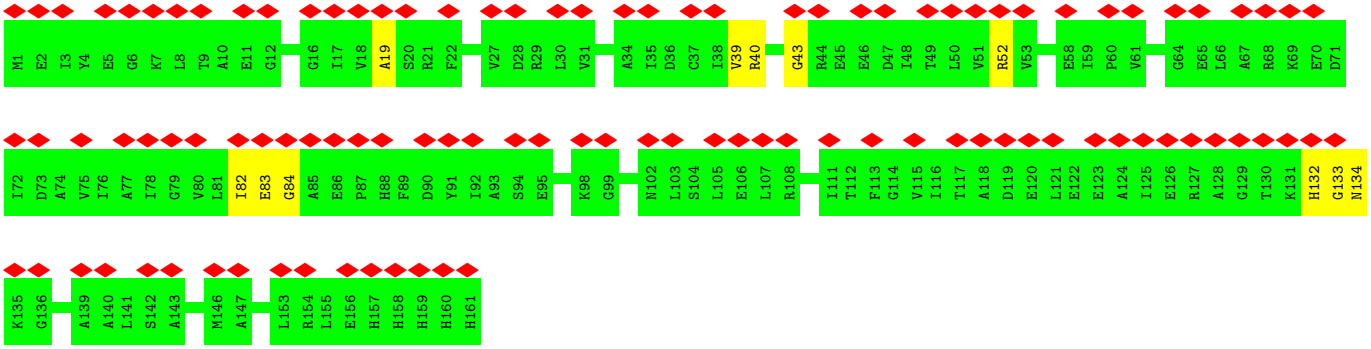
Chain EE:





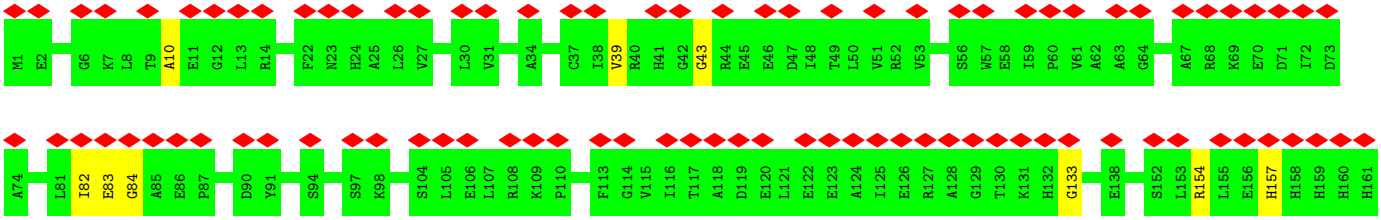
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EF: 65% 93% 7%



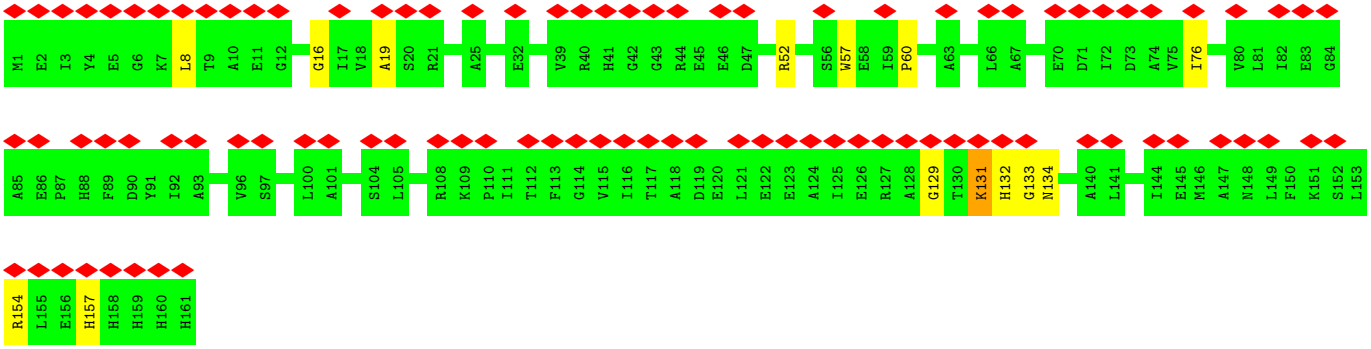
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EG: 55% 94% 6%



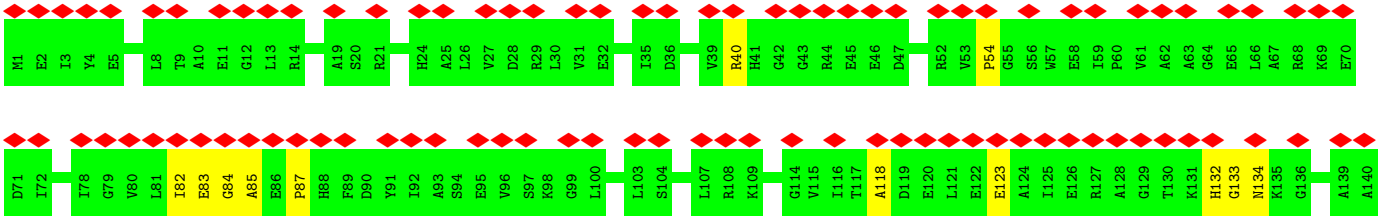
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

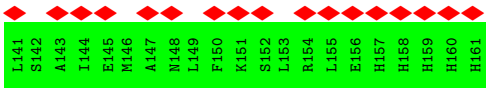
Chain EH: 59% 91% 8%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

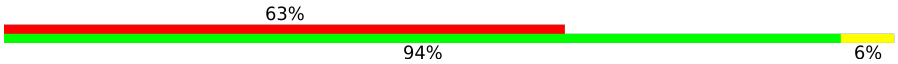
Chain EI: 68% 93% 7%

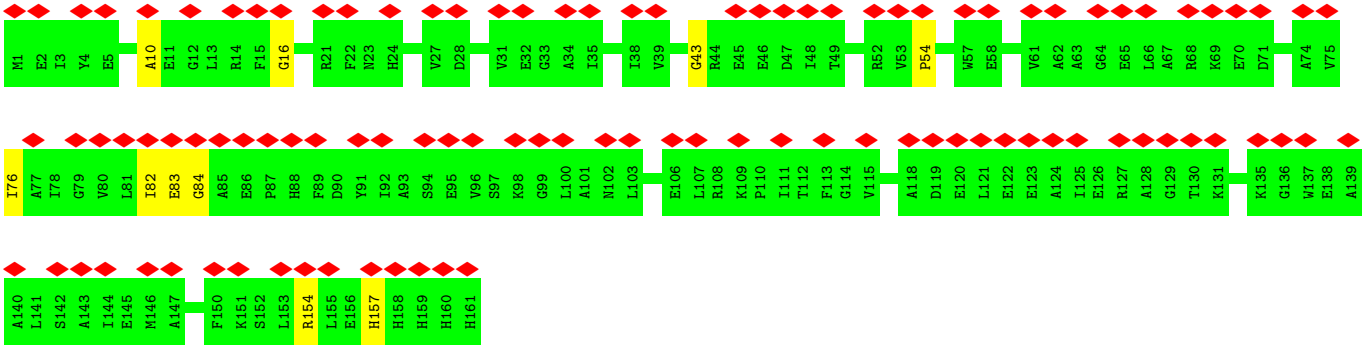




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

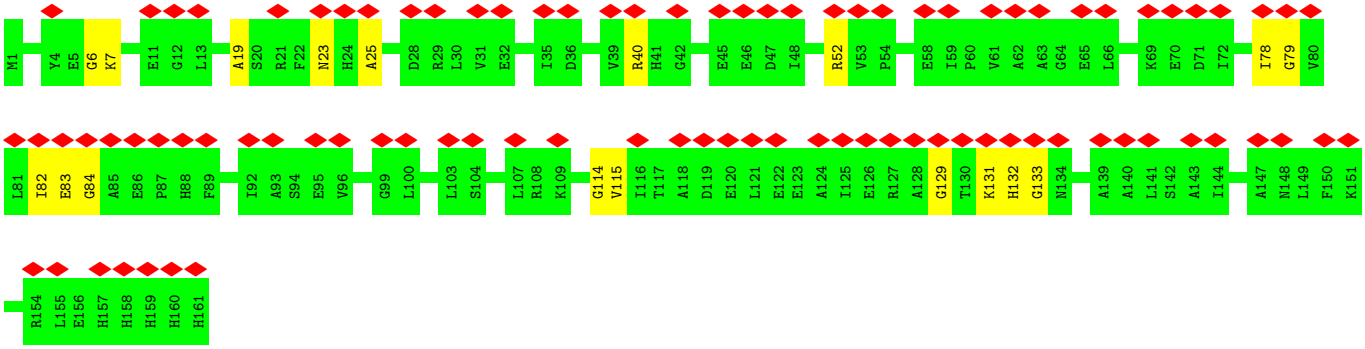
Chain EJ:





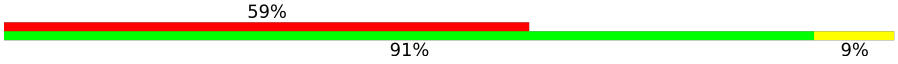
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

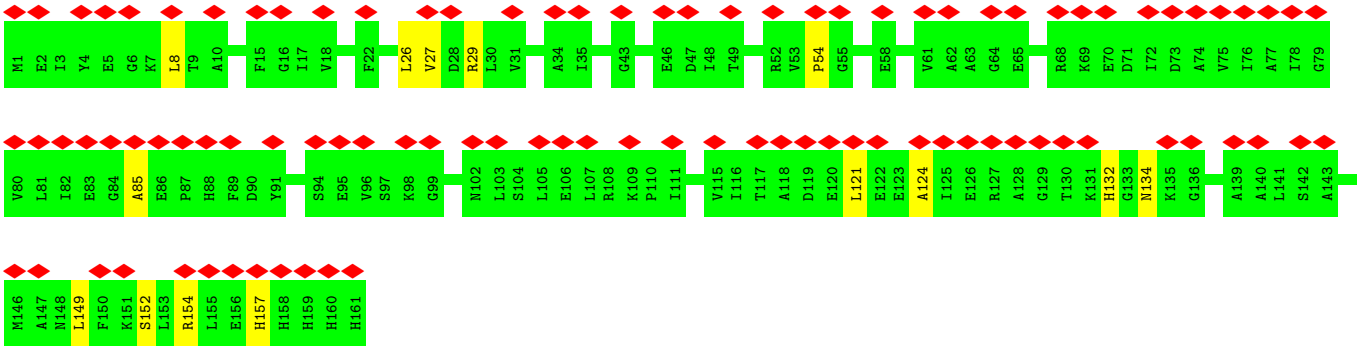
Chain EK:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

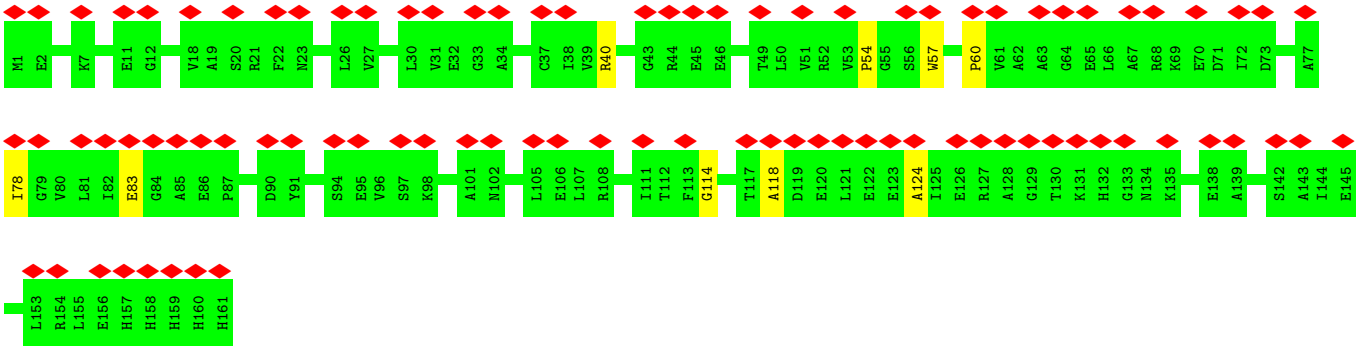
Chain EL:





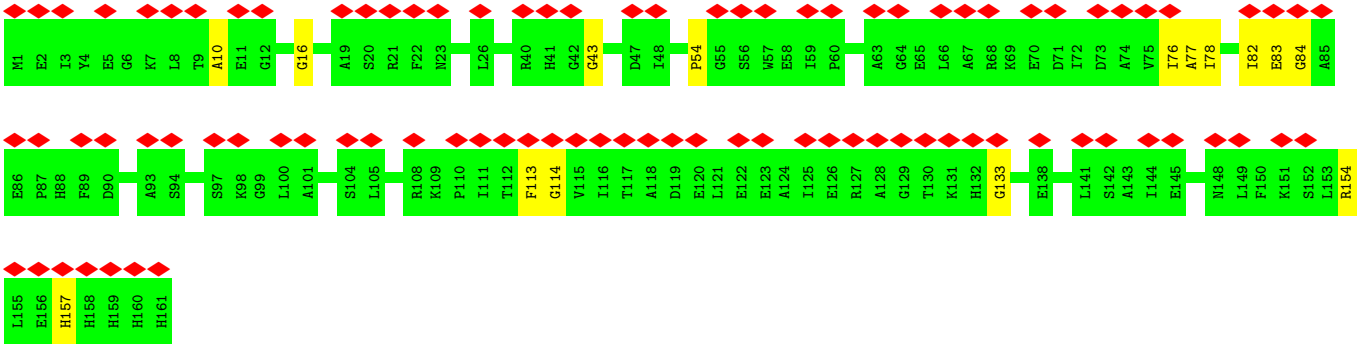
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EM: 55% 94% 6%



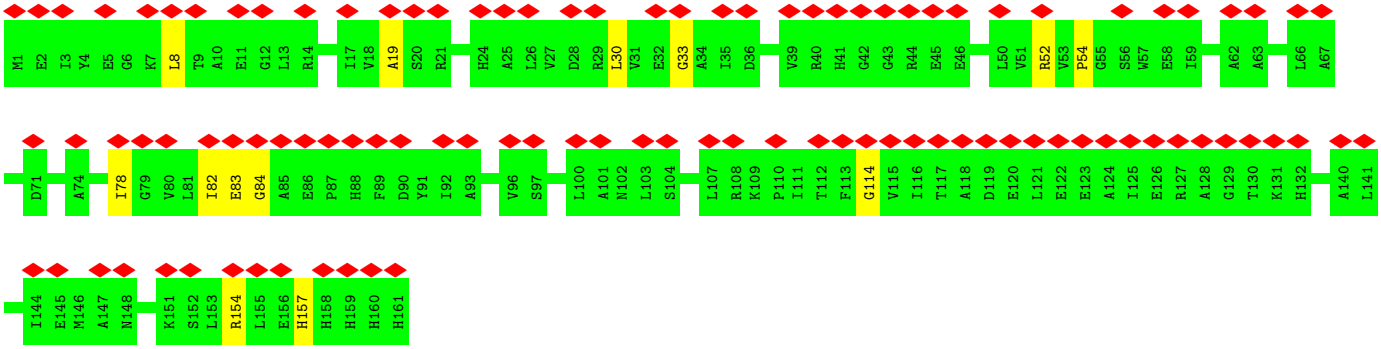
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EN: 57% 91% 9%



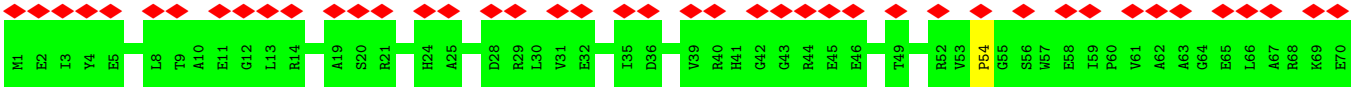
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

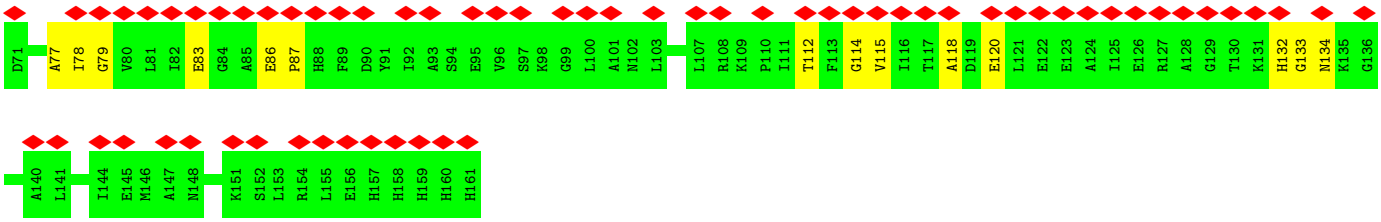
Chain EO: 63% 92% 8%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

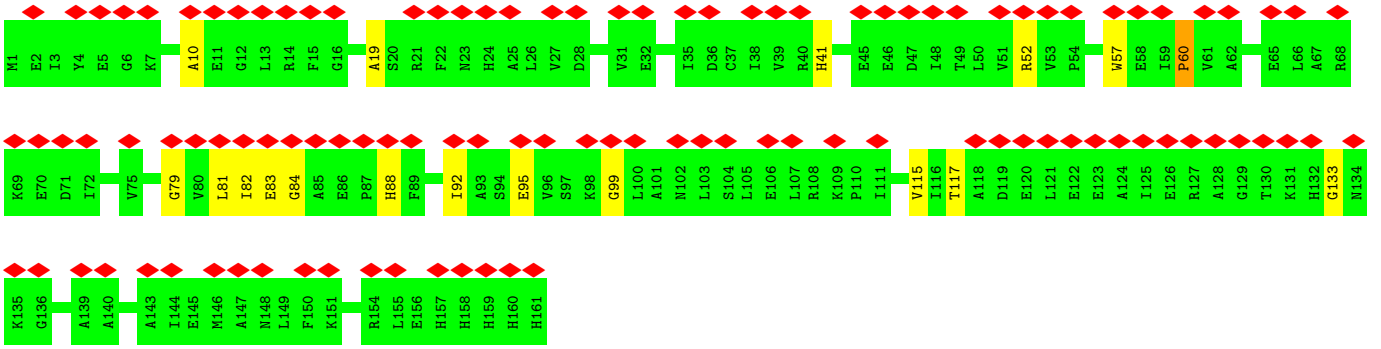
Chain FA: 66% 91% 9%





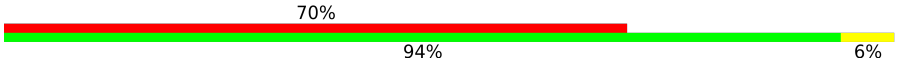
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

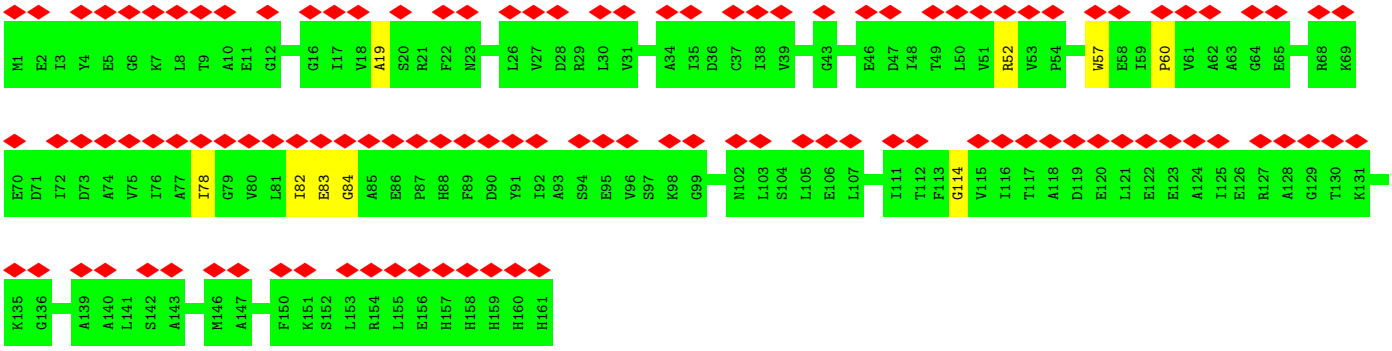
Chain FB:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

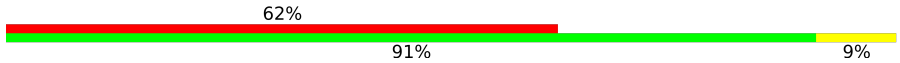
Chain FC:

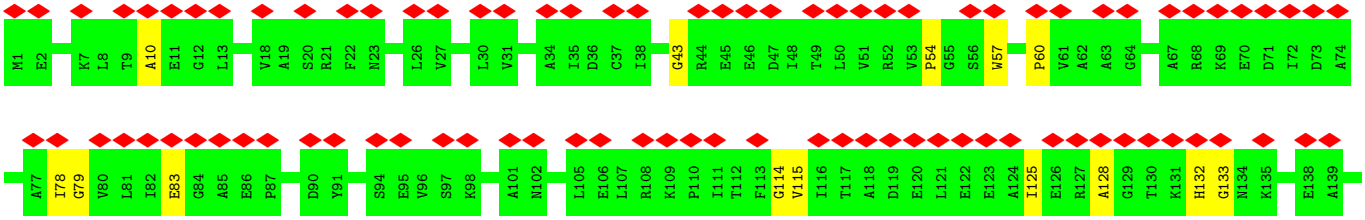


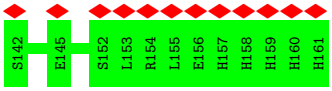


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FD:

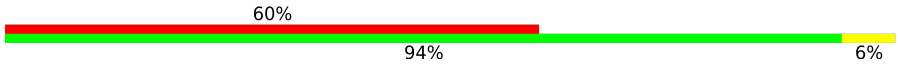


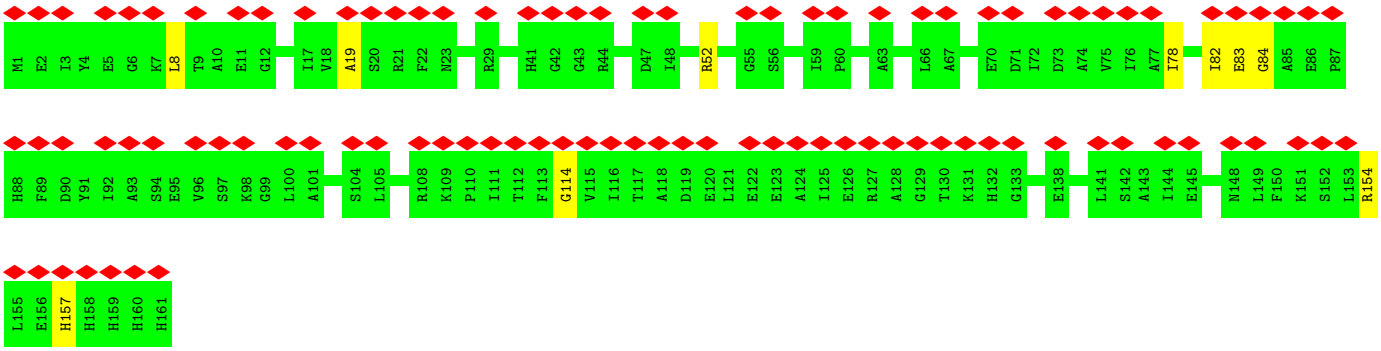




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

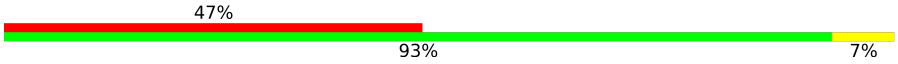
Chain FE:

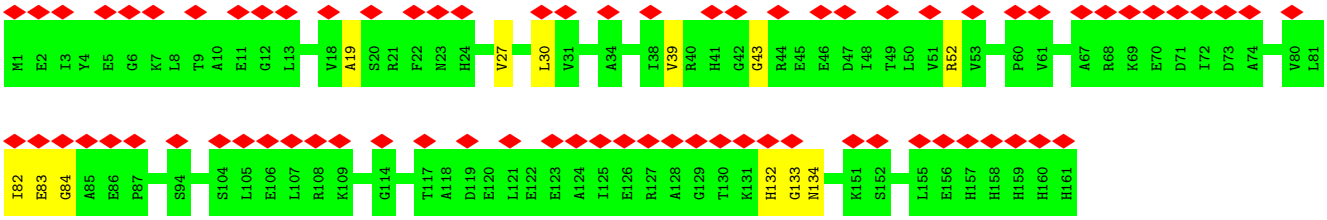




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

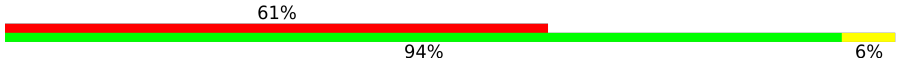
Chain FF:

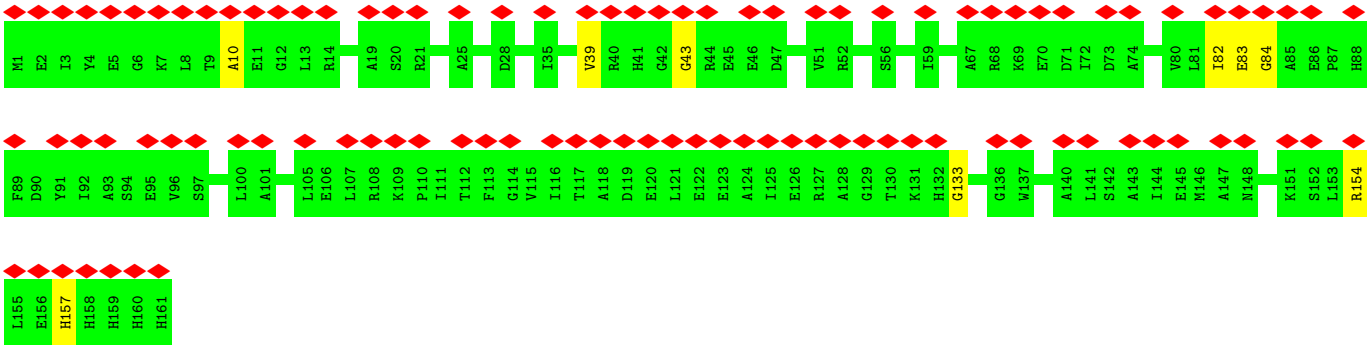




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

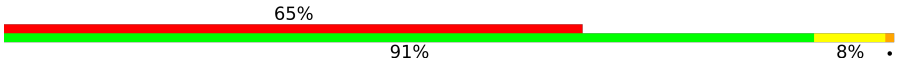
Chain FG:

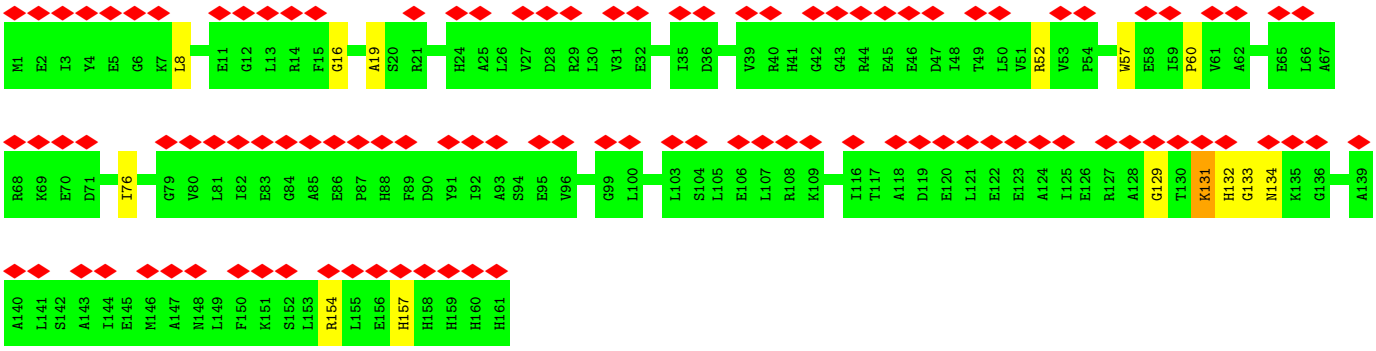




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

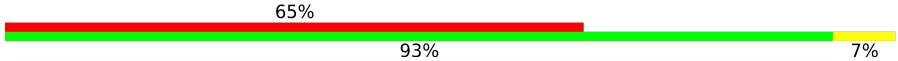
Chain FH:

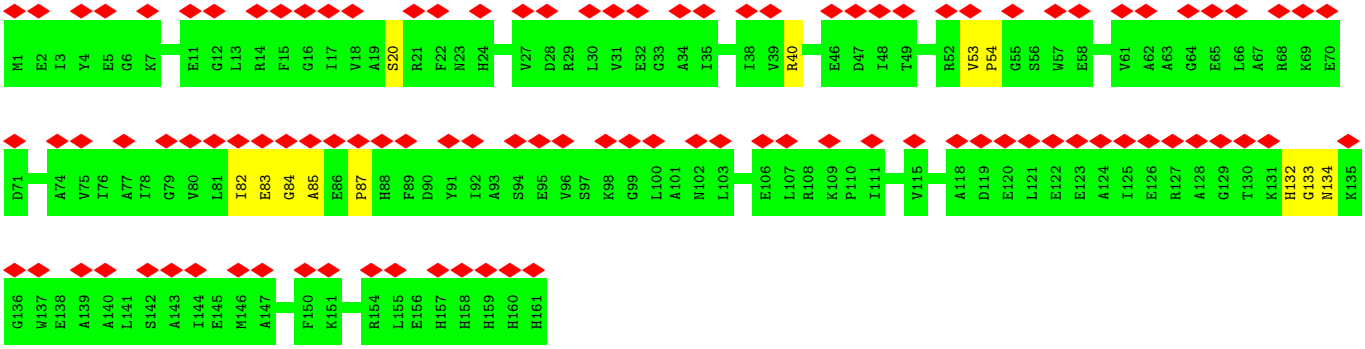




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

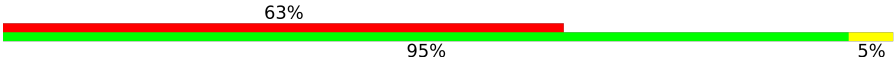
Chain FI:

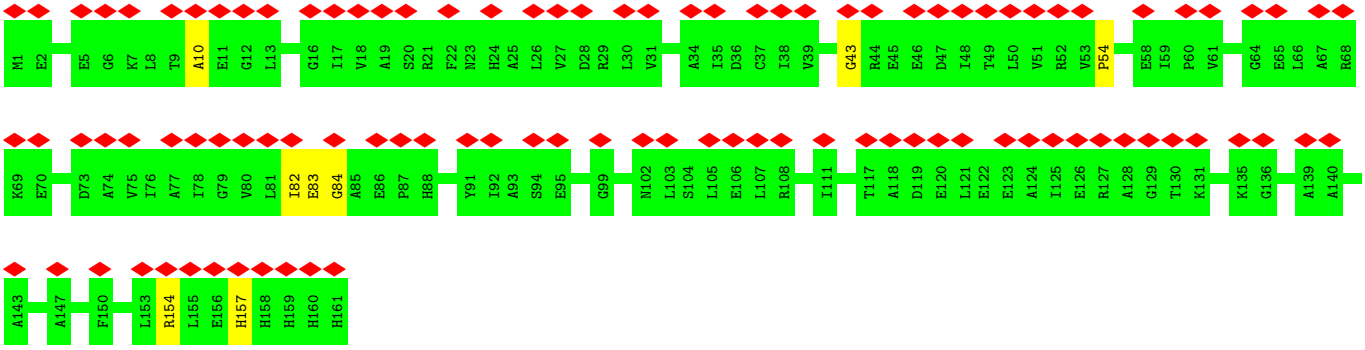




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

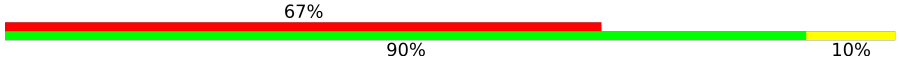
Chain FJ:

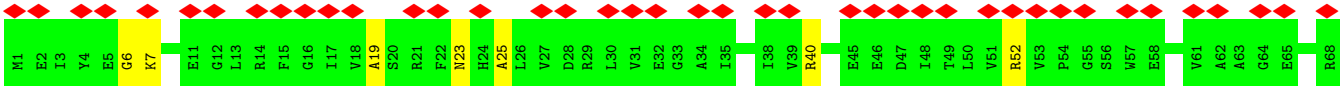


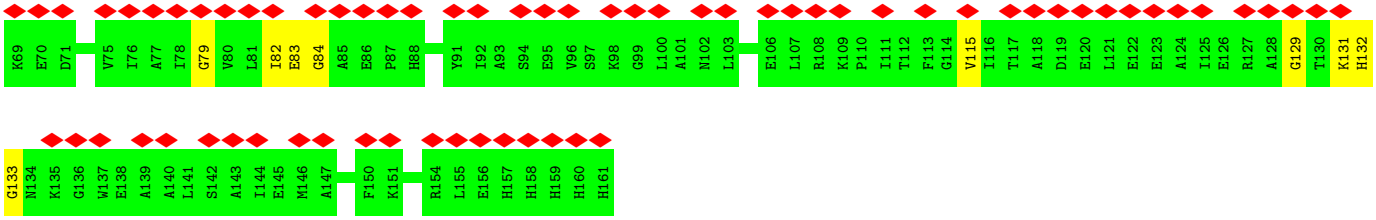


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FK:

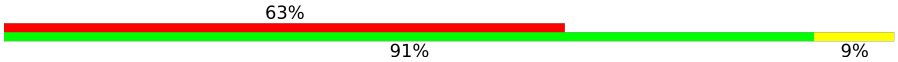


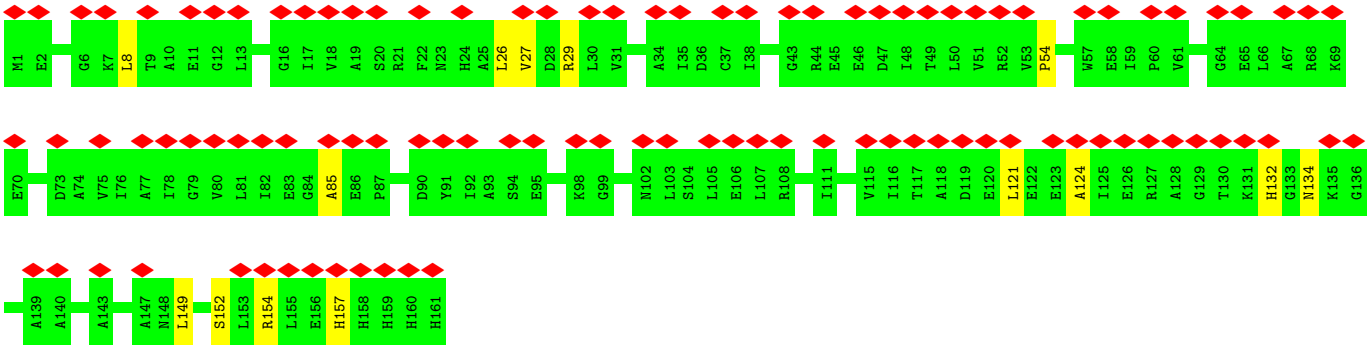




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

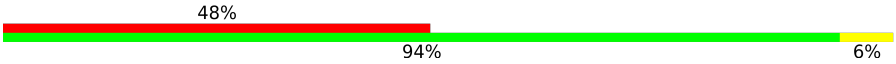
Chain FL:

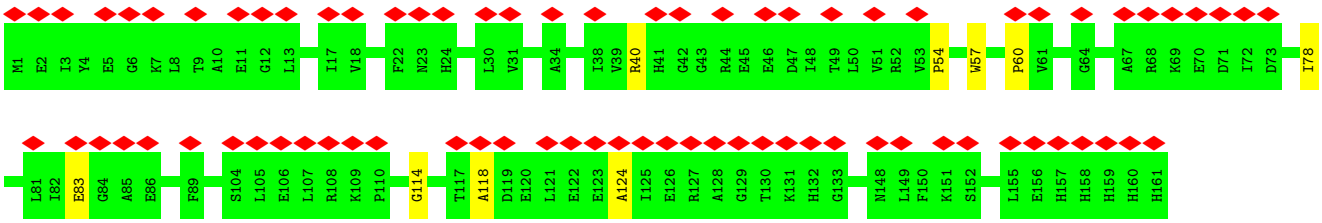




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

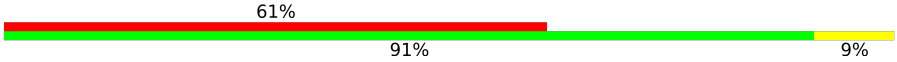
Chain FM:

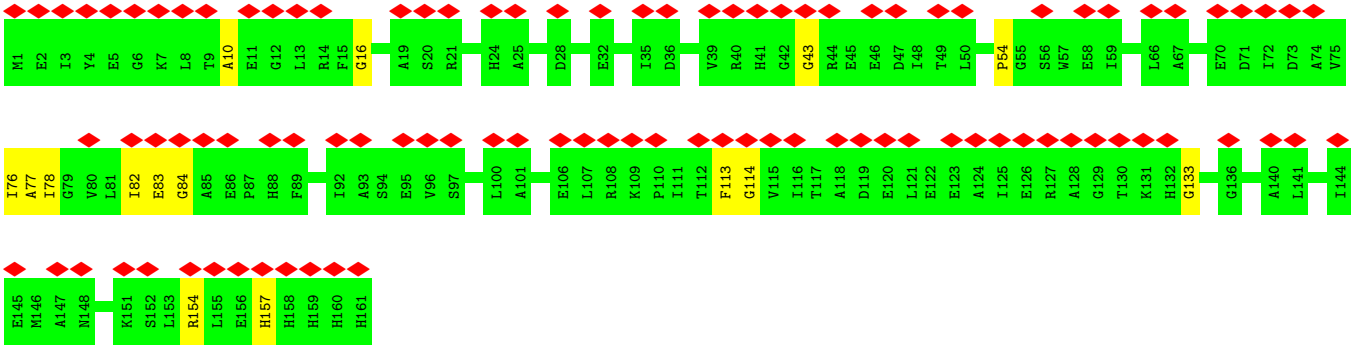




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

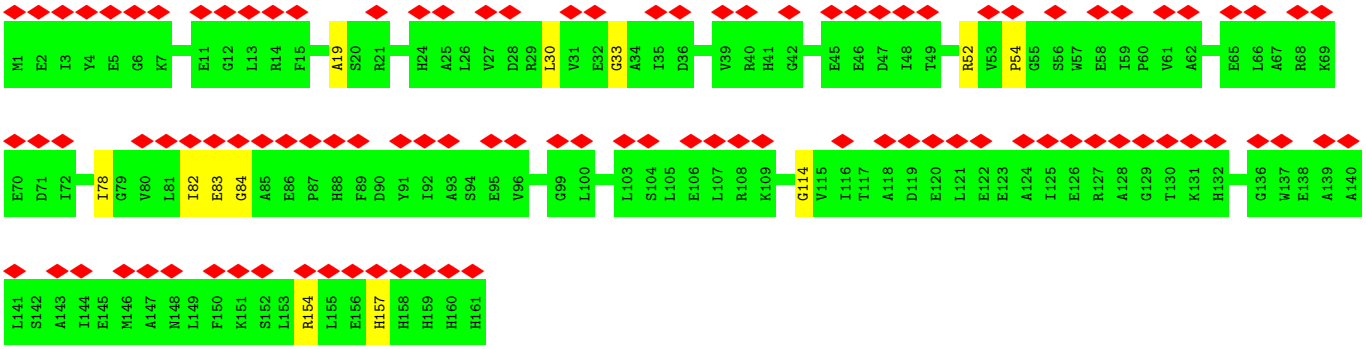
Chain FN:





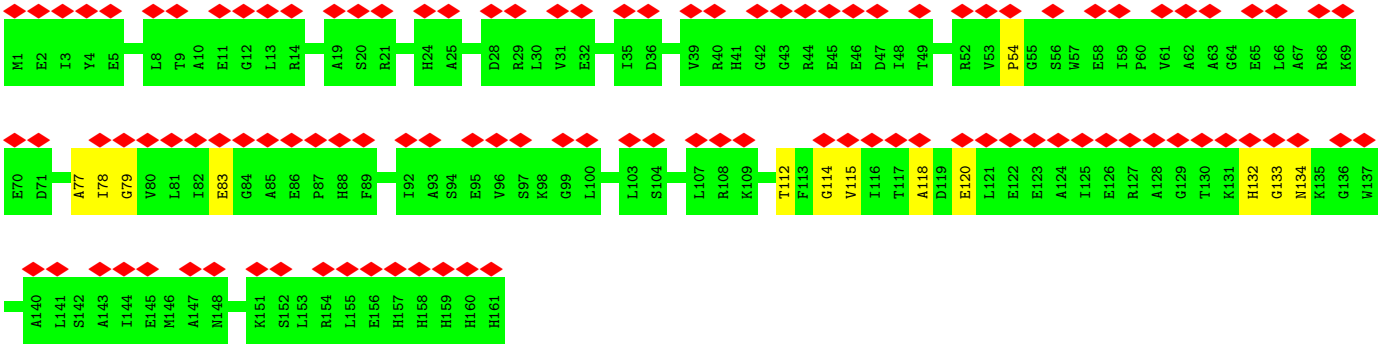
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FO: 63% 93% 7%



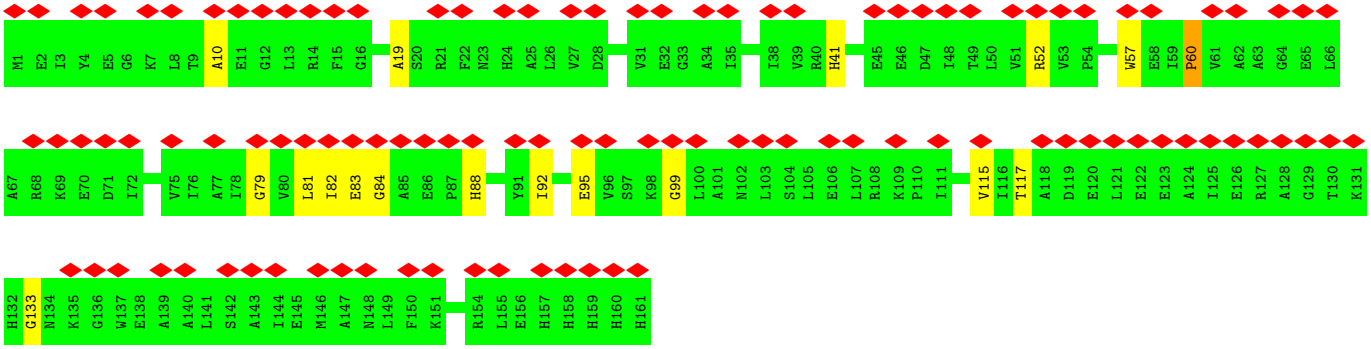
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GA: 68% 92% 8%



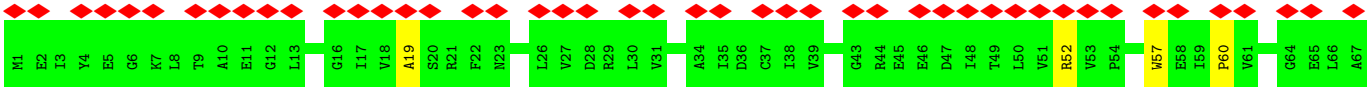
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

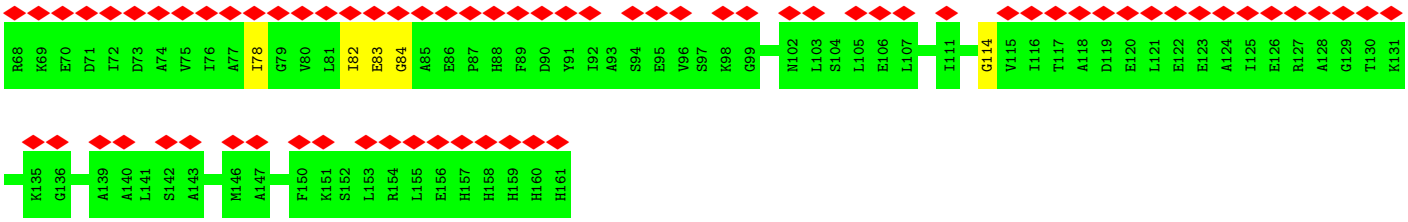
Chain GB: 66% 89% 11%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

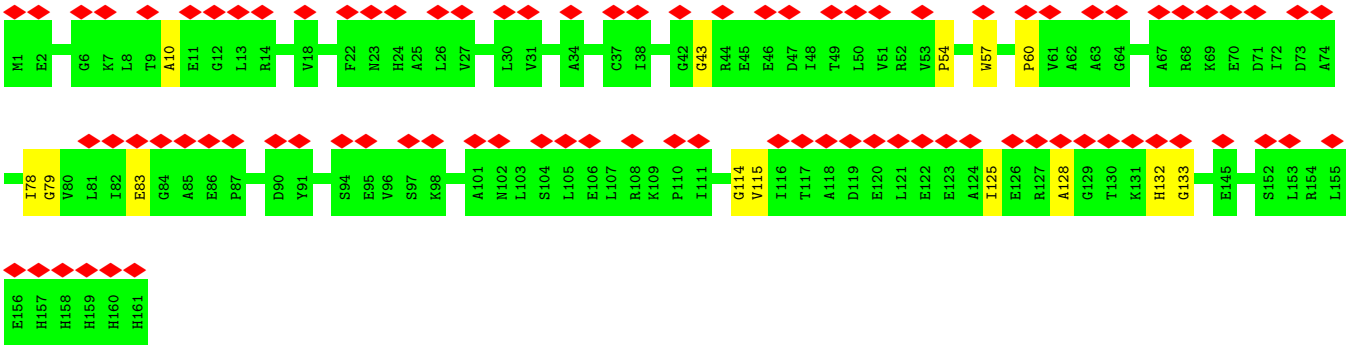
Chain GC: 73% 94% 6%





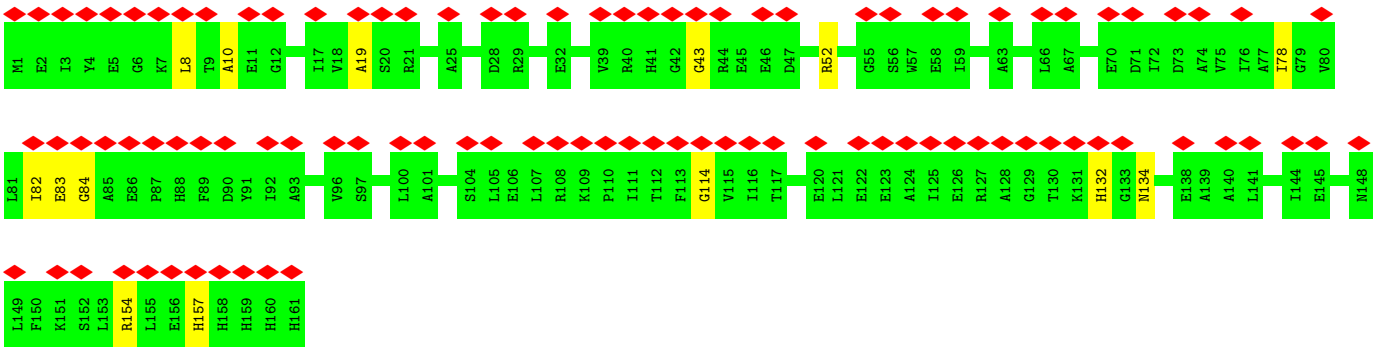
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GD: 55% 91% 9%



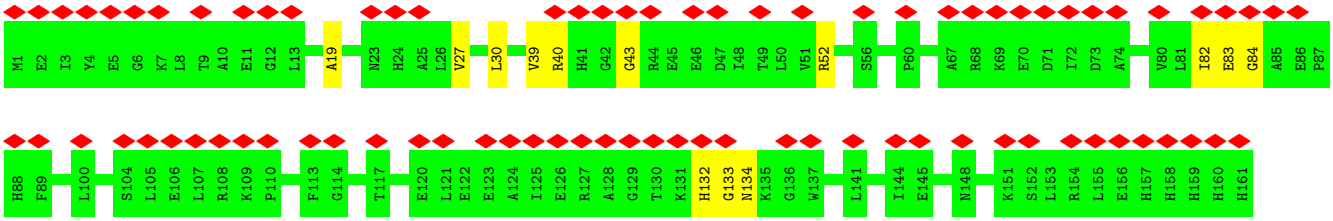
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GE: 61% 91% 9%



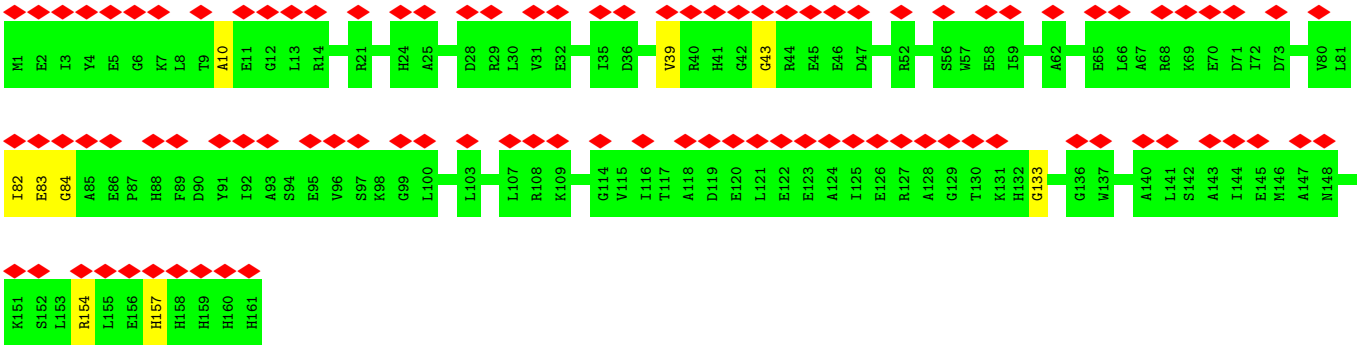
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GF: 50% 92% 8%



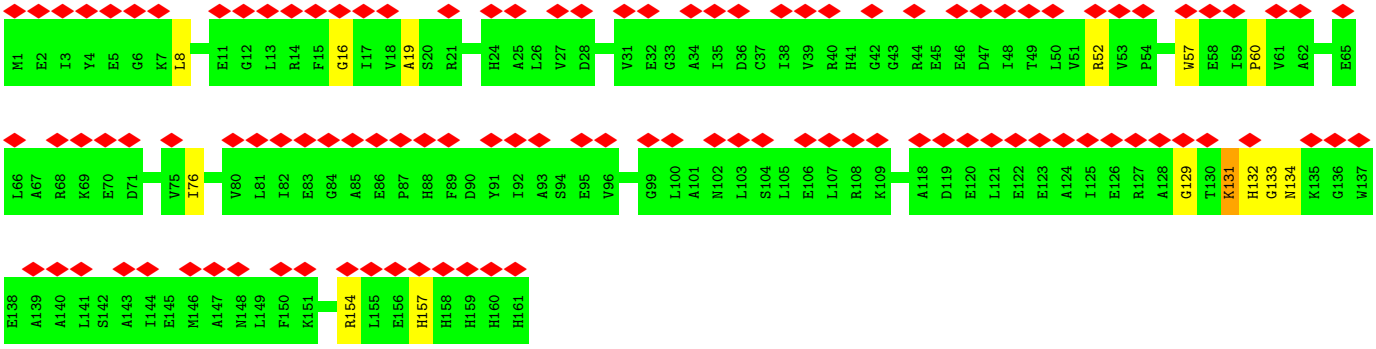
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GG: 60% 94% 6%



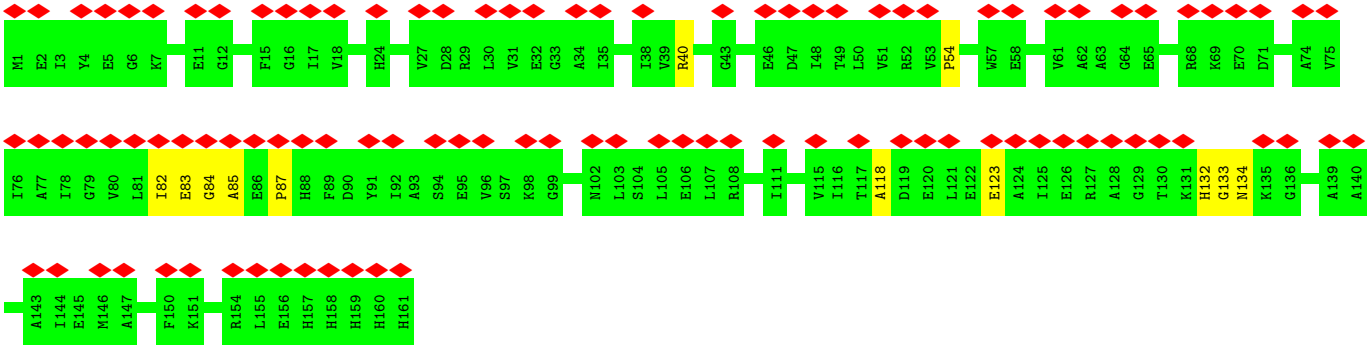
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GH: 68% 91% 8%



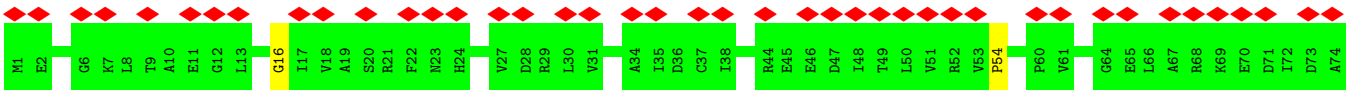
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

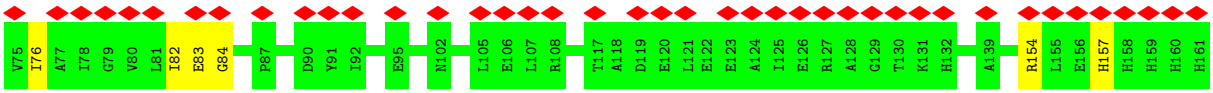
Chain GI: 63% 93% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

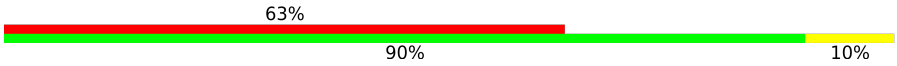
Chain GJ: 52% 95% 5%

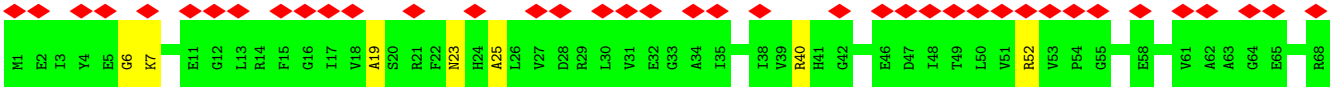


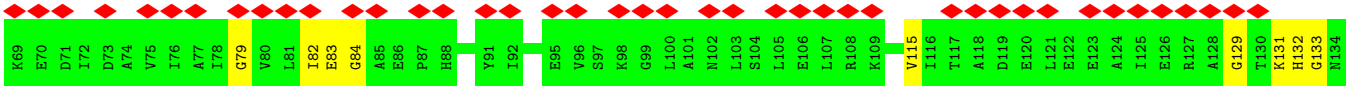


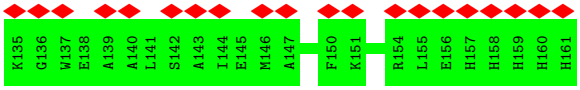
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GK:



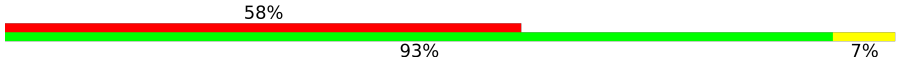


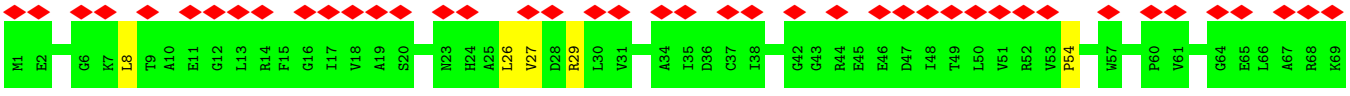


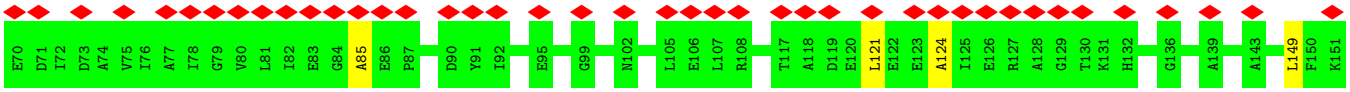


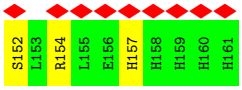
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GL:



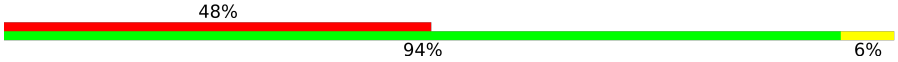


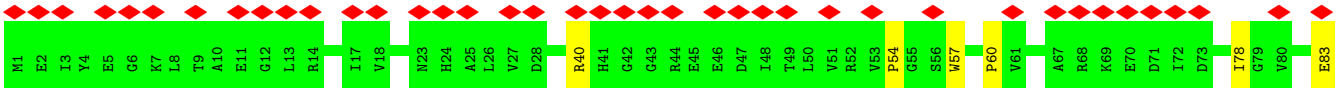


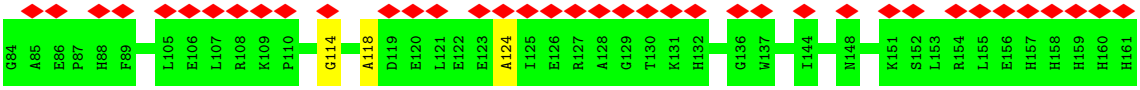


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GM:

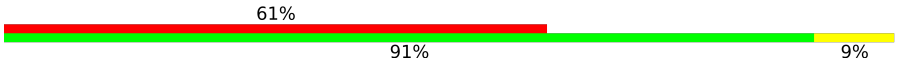


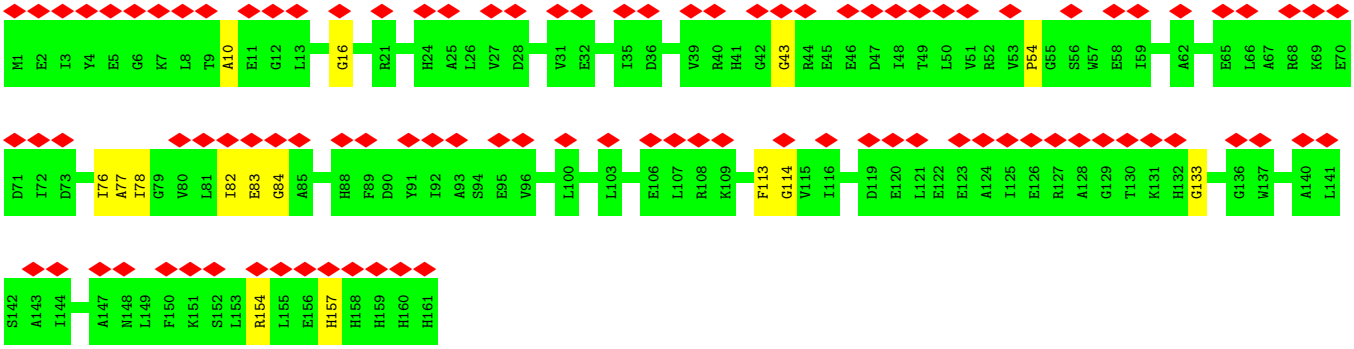




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

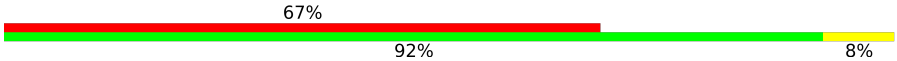
Chain GN:

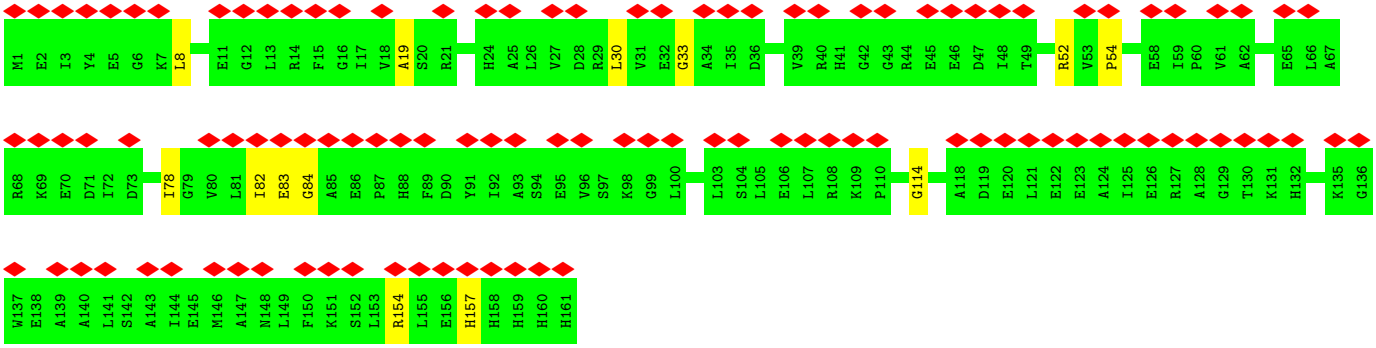




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

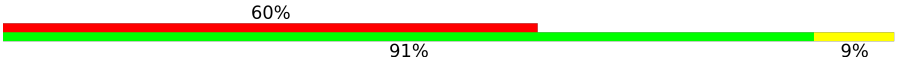
Chain GO:

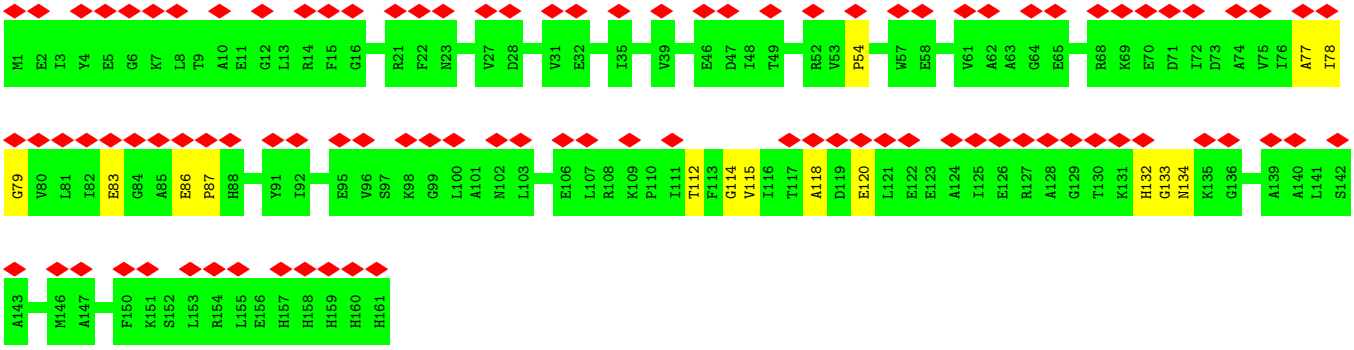




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

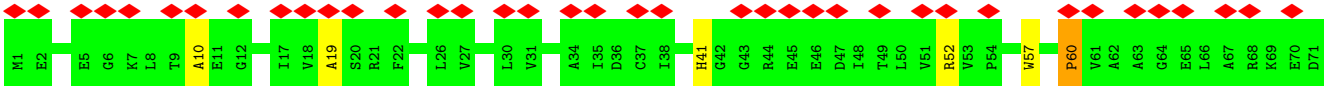
Chain HA:

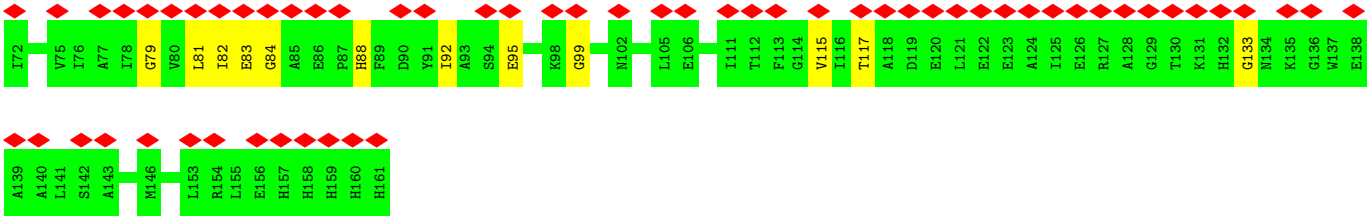




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

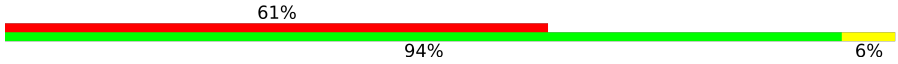
Chain HB:

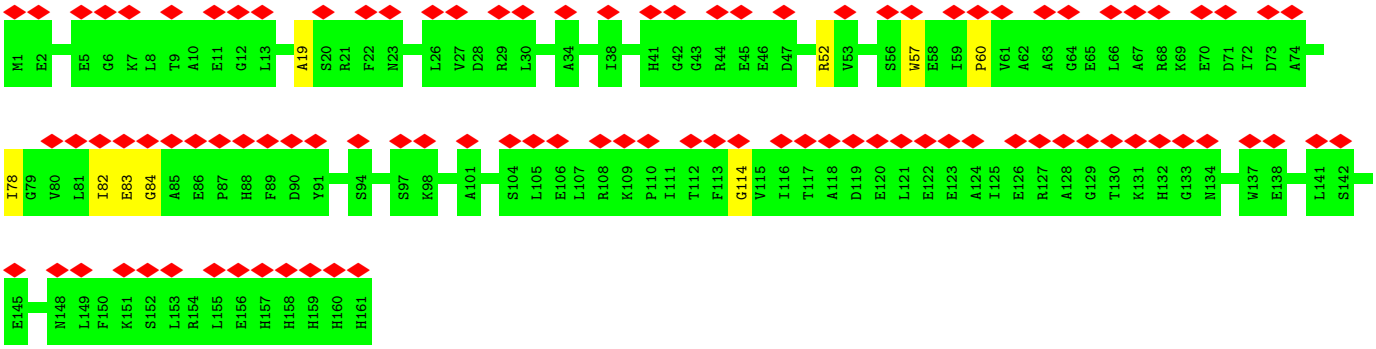




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

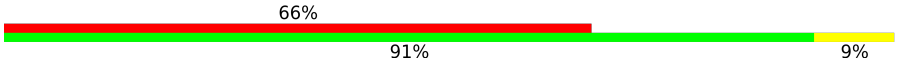
Chain HC:

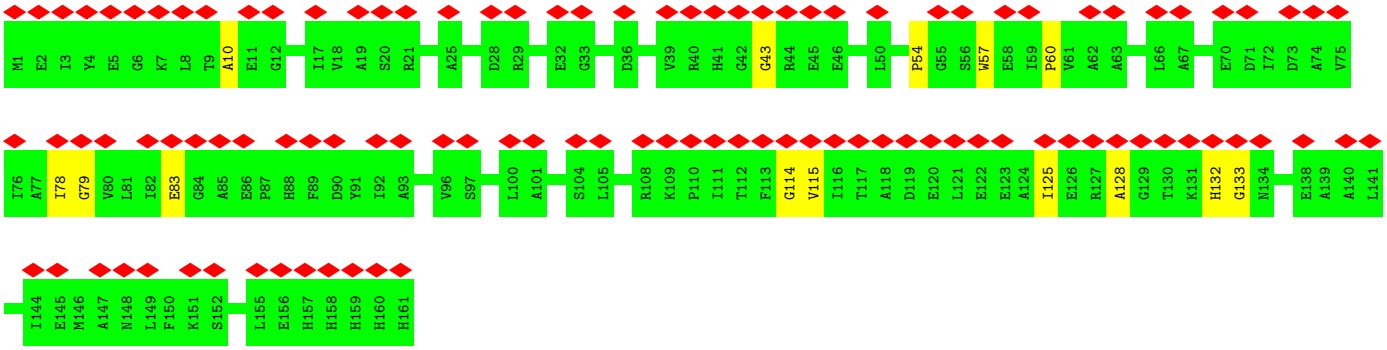




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

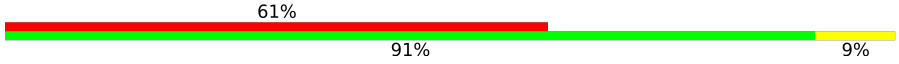
Chain HD:

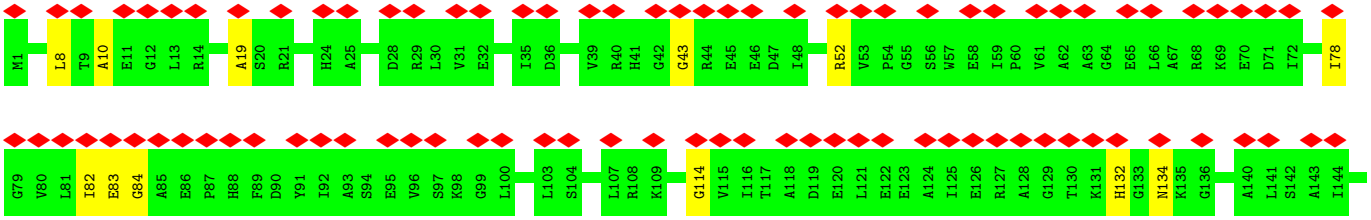


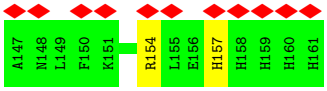


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HE:

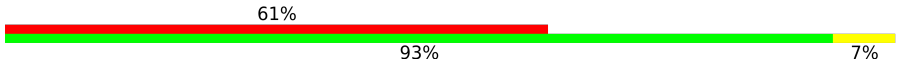


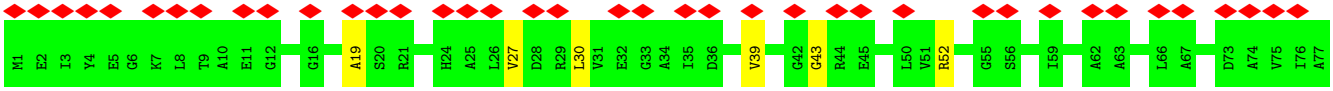


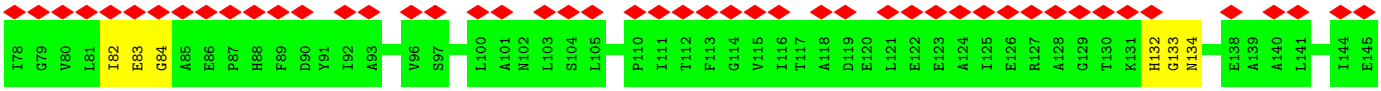


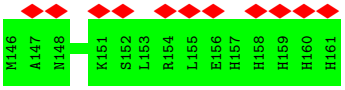
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HF:



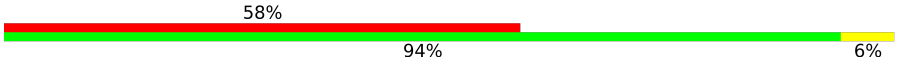


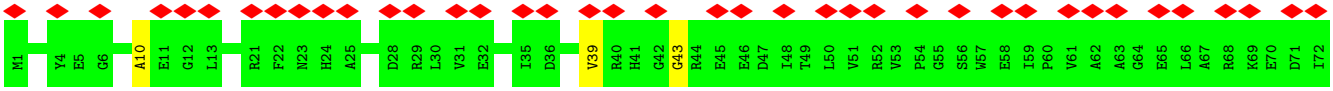


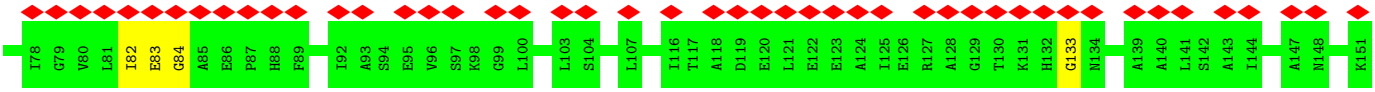


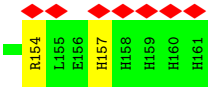
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HG:



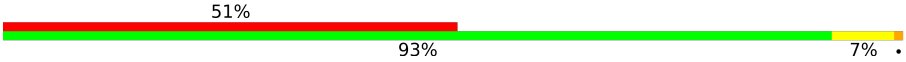


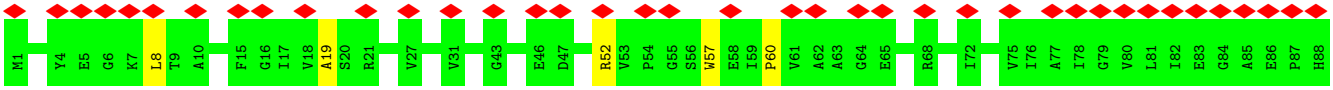


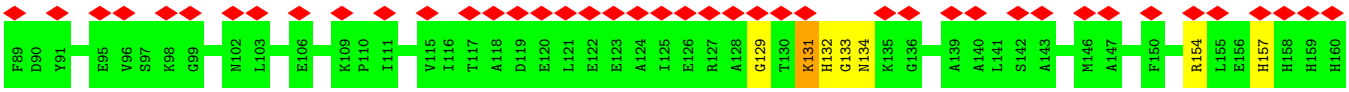


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HH:

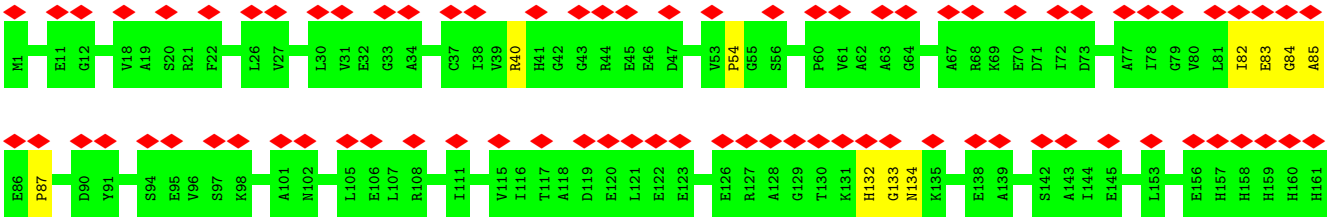






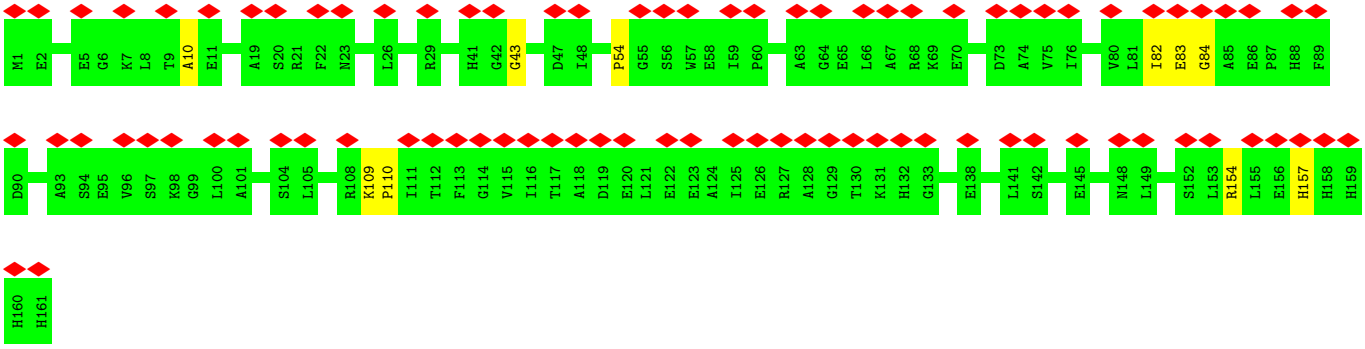
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HI: 50% 94% 6%



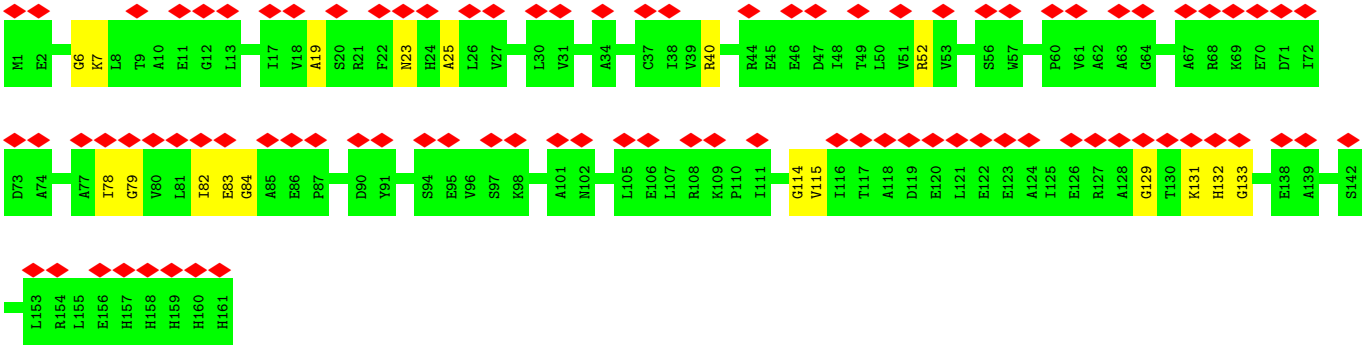
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HJ: 53% 94% 6%



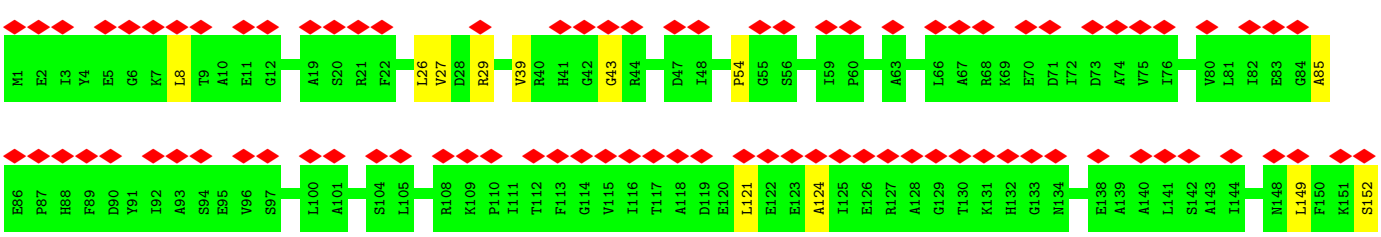
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

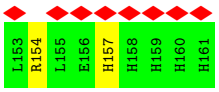
Chain HK: 56% 89% 11%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

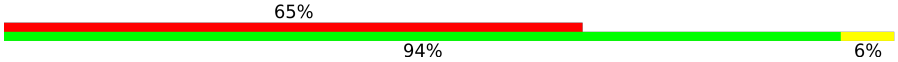
Chain HL: 59% 91% 9%

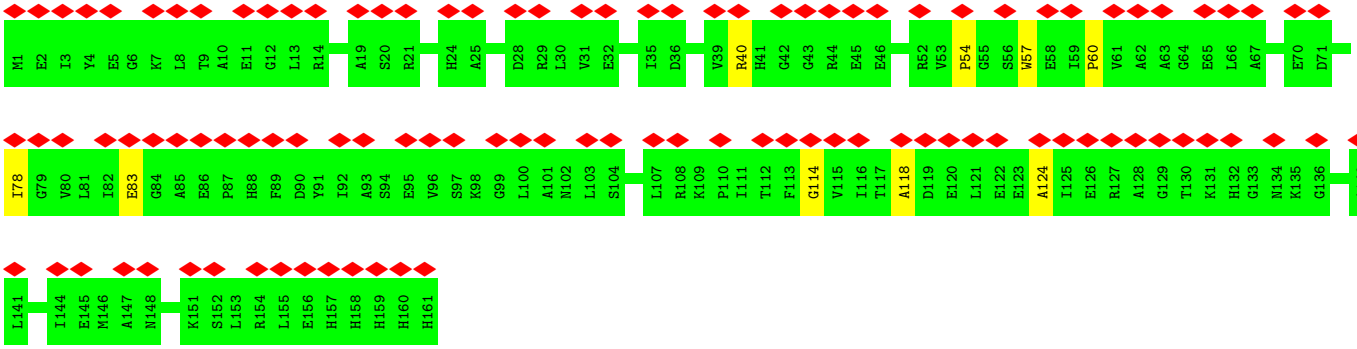




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

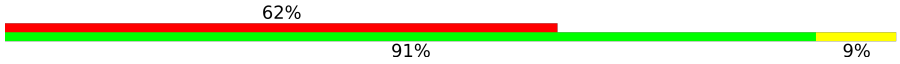
Chain HM:

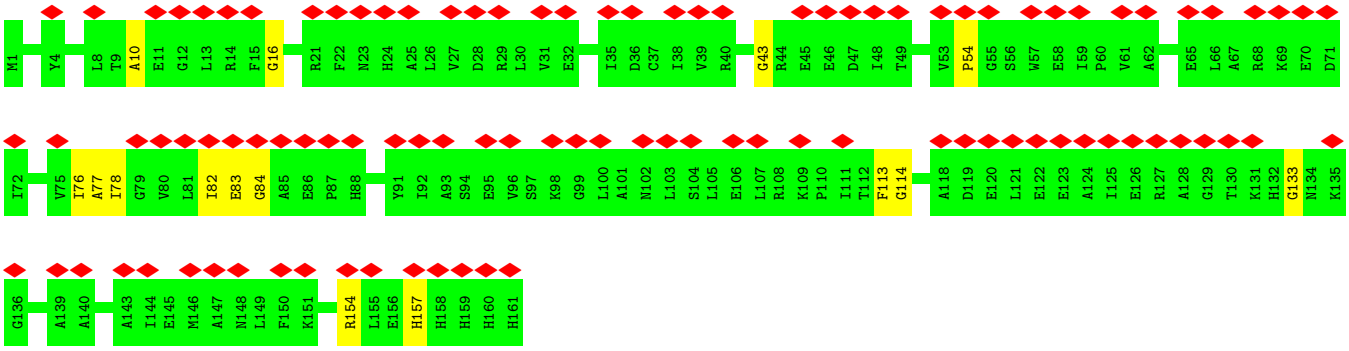




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

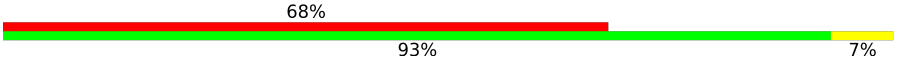
Chain HN:

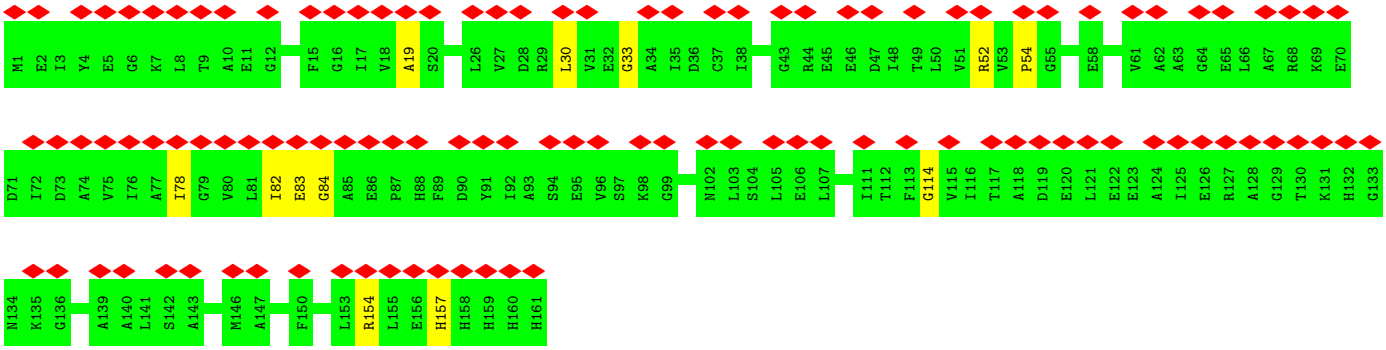




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

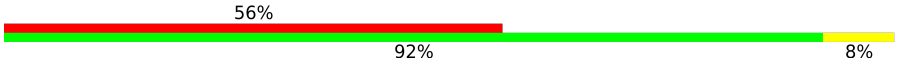
Chain HO:

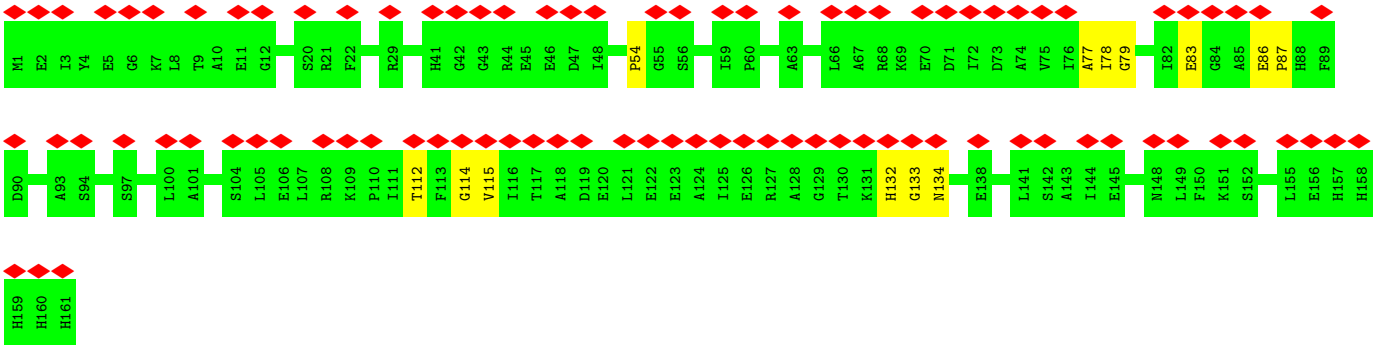




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

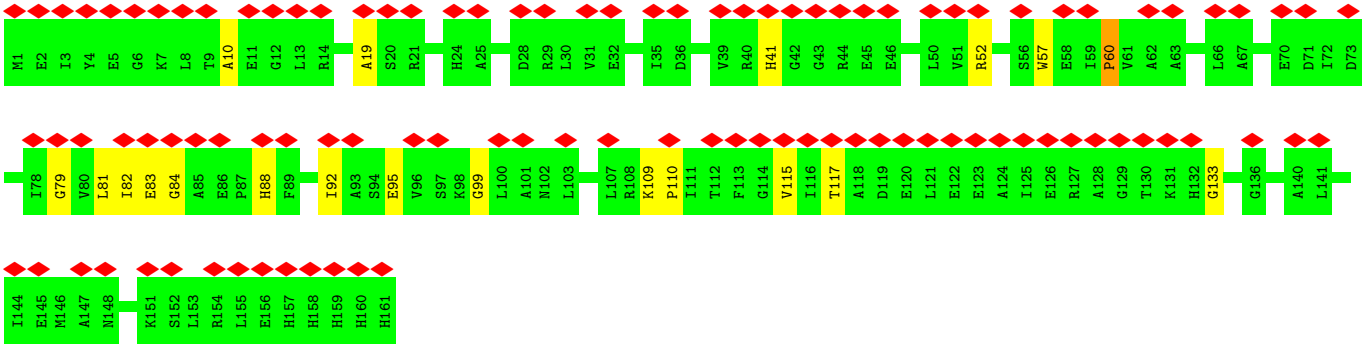
Chain IA:





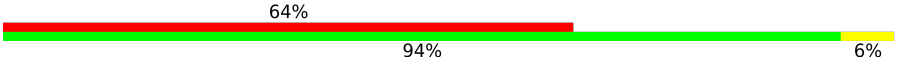
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

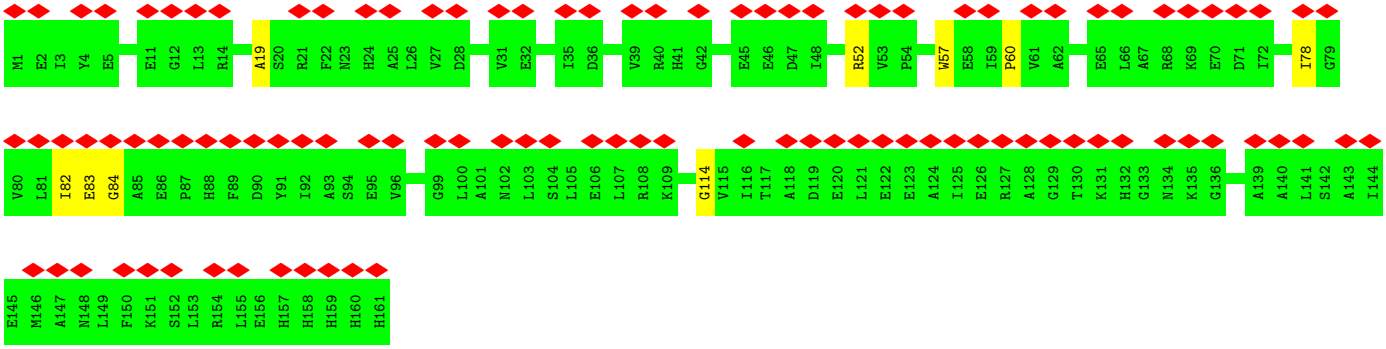
Chain IB:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

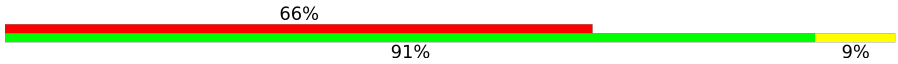
Chain IC:

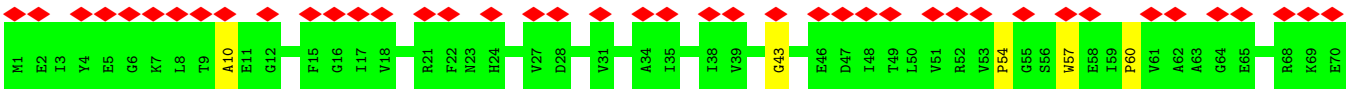


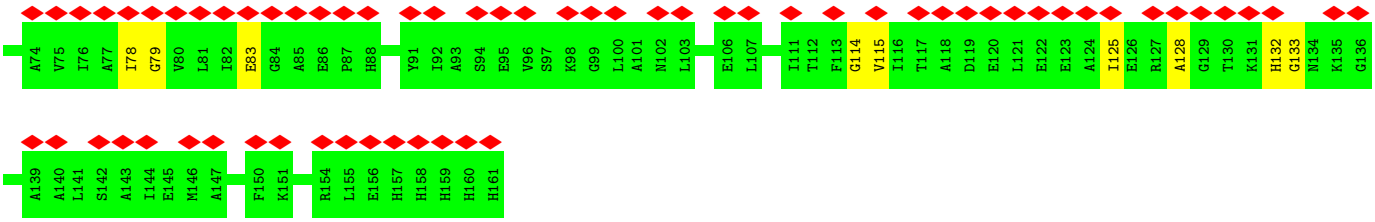


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ID:

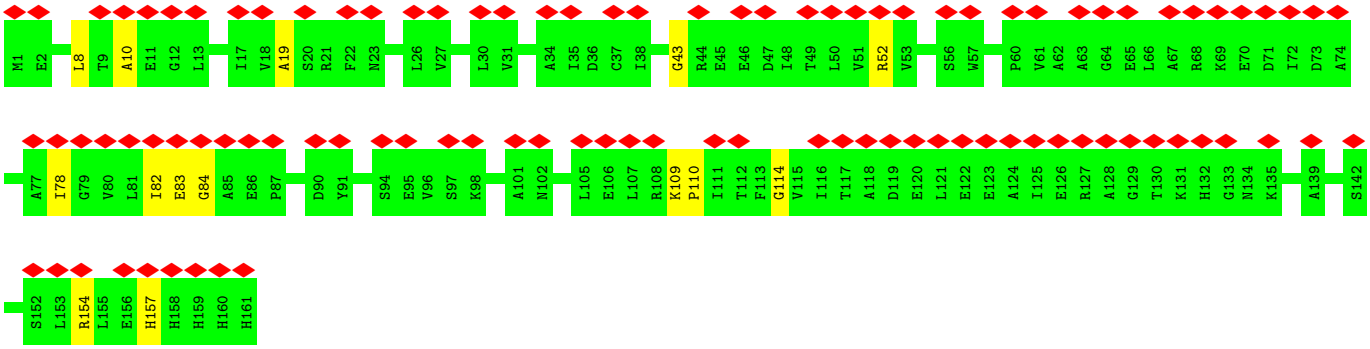






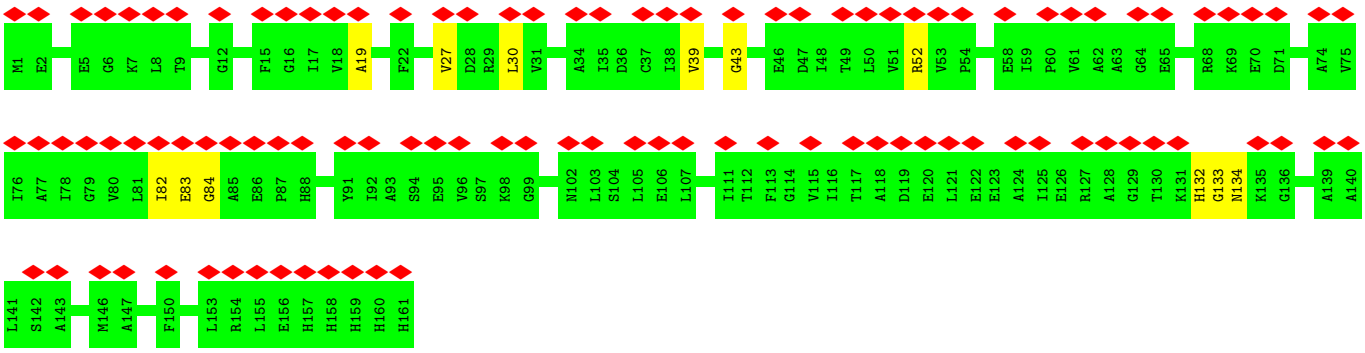
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IE: 61% 91% 9%



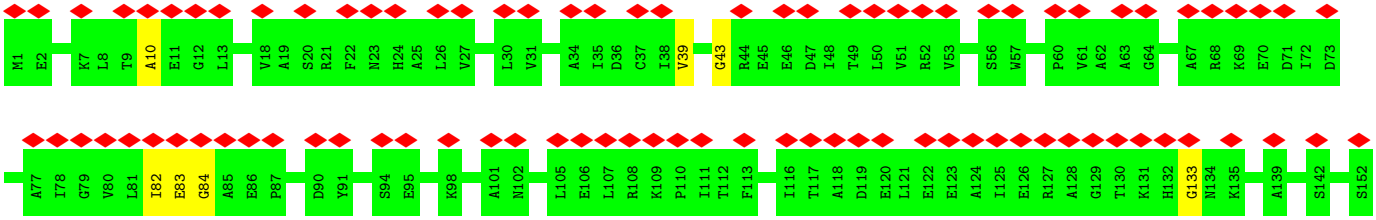
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

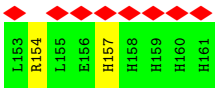
Chain IF: 64% 93% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

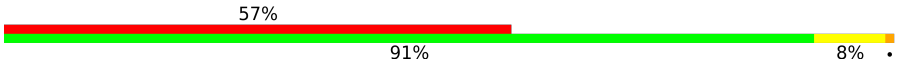
Chain IG: 60% 94% 6%

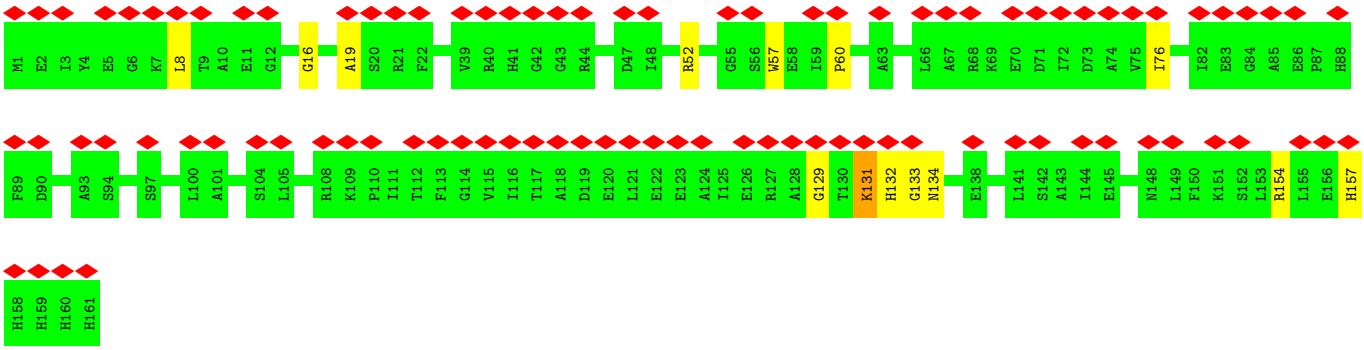




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

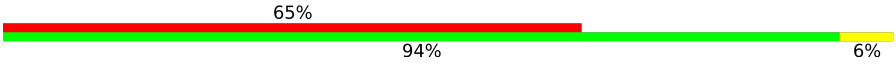
Chain IH:

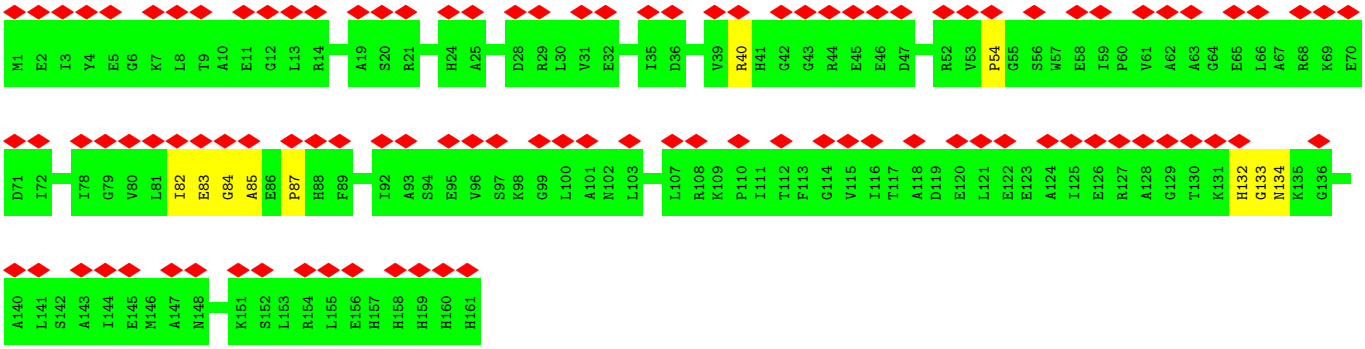




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

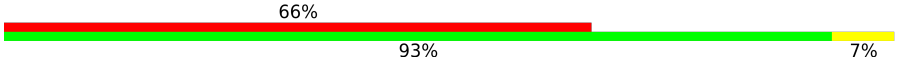
Chain II:

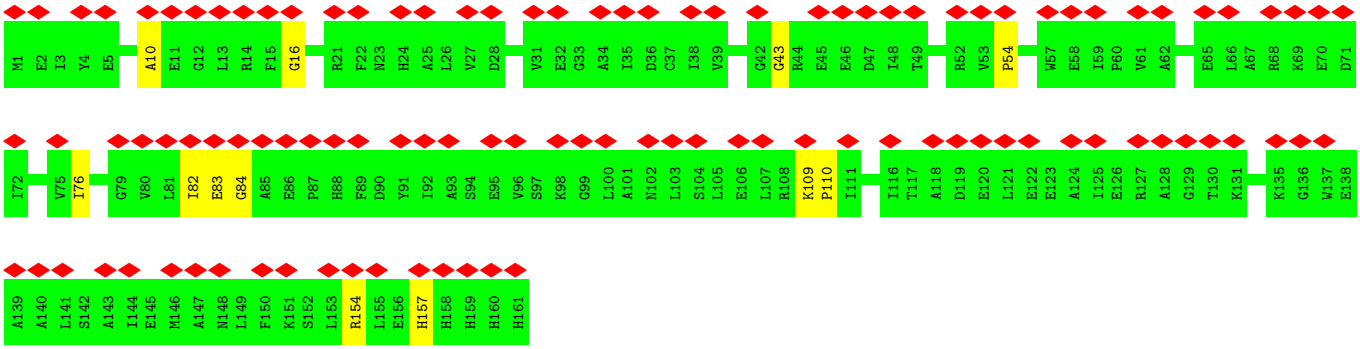




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

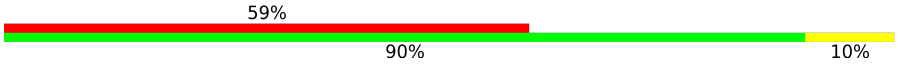
Chain IJ:

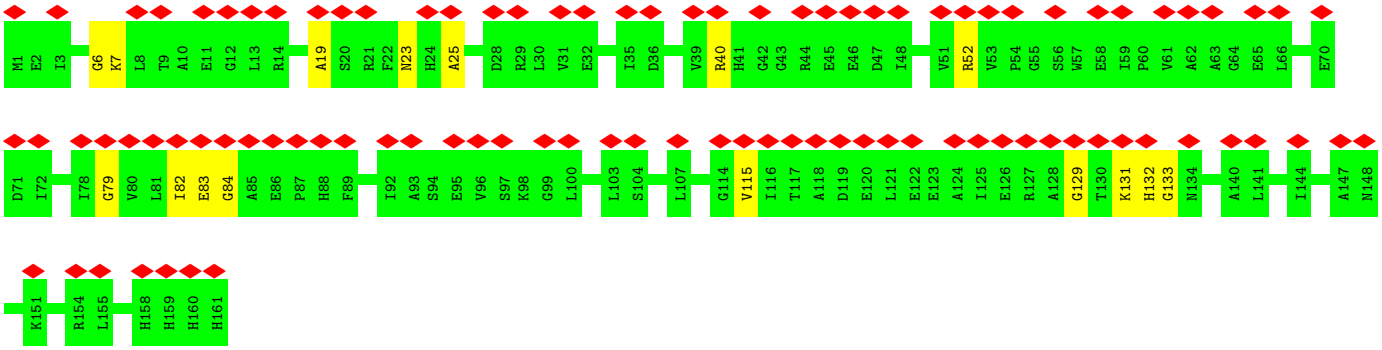




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

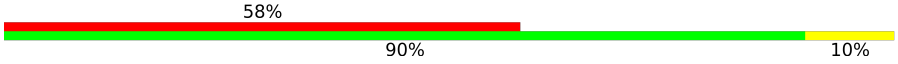
Chain IK:

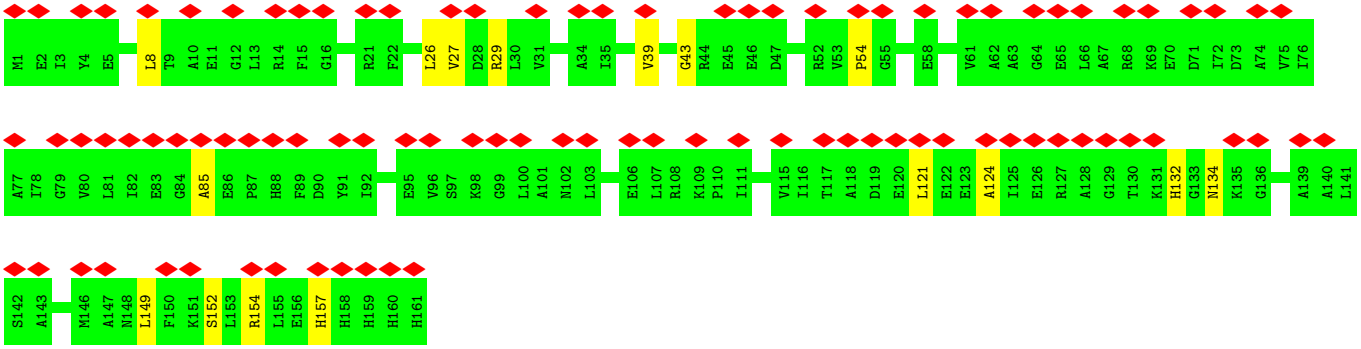




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

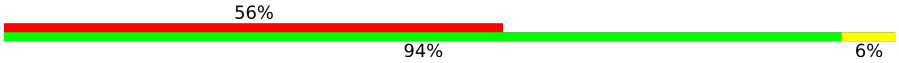
Chain IL:

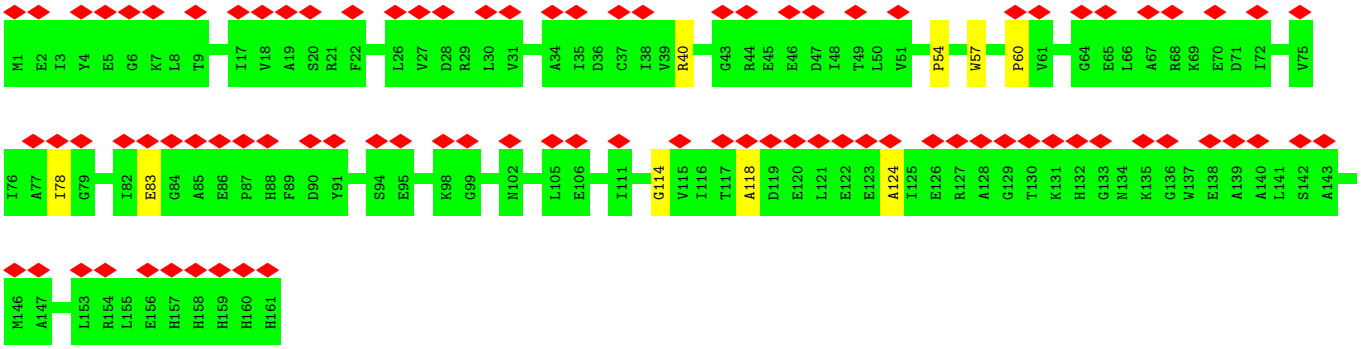




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

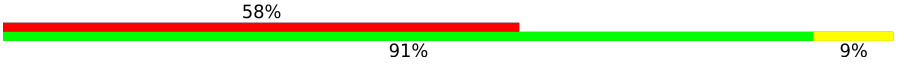
Chain IM:

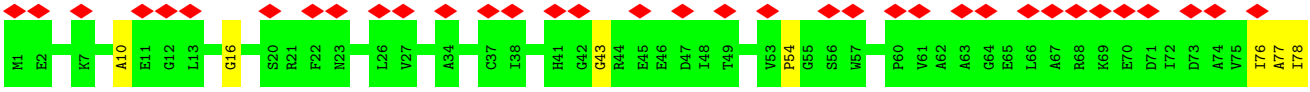


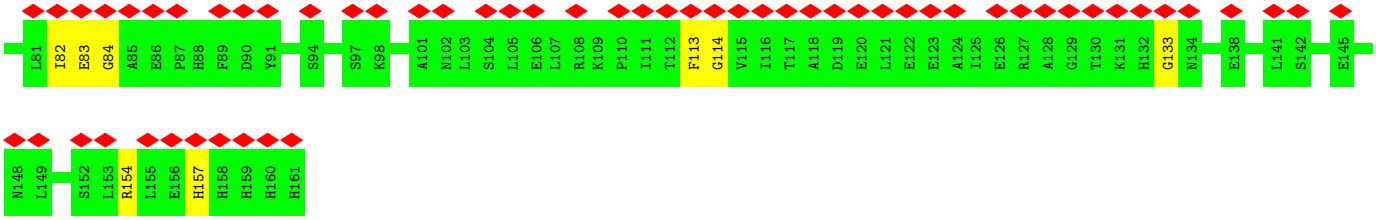


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IN:

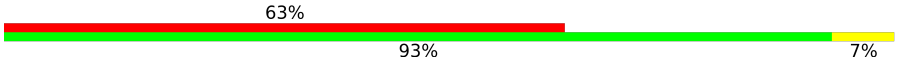


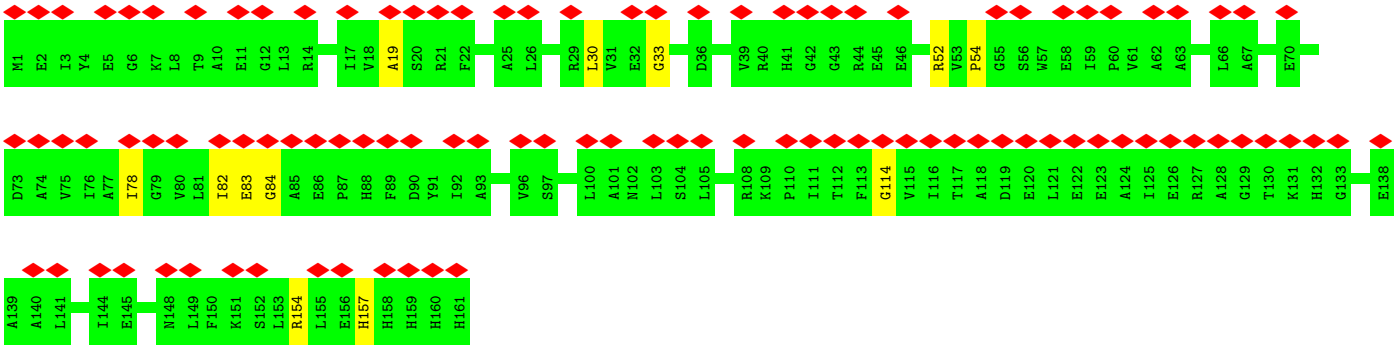




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

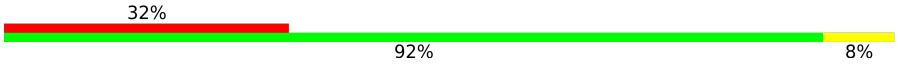
Chain IO:

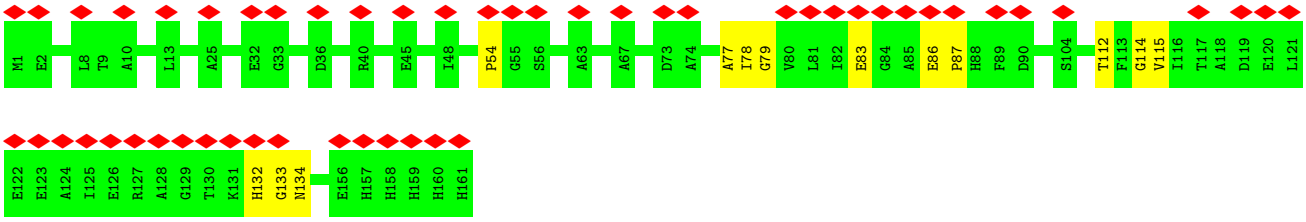




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

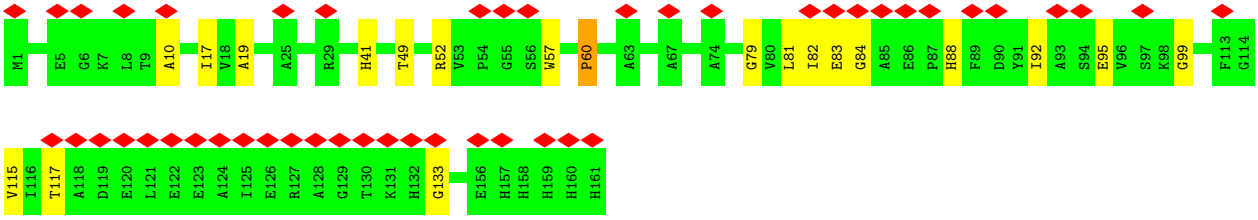
Chain JA:





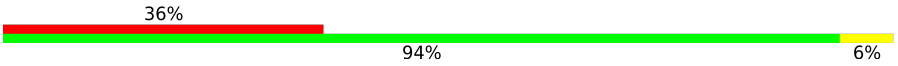
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

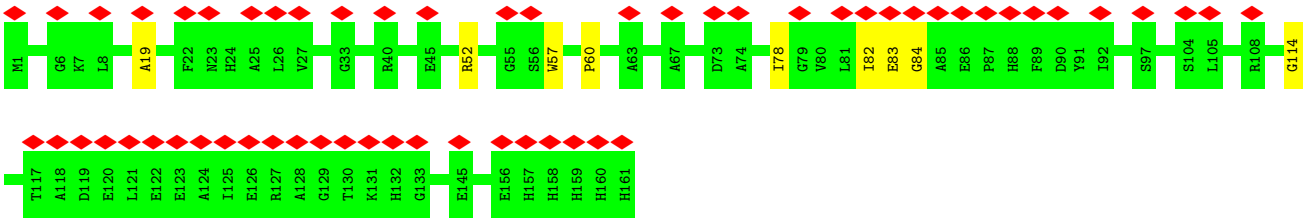
Chain JB:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

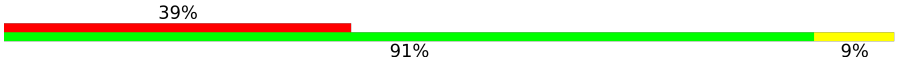
Chain JC:

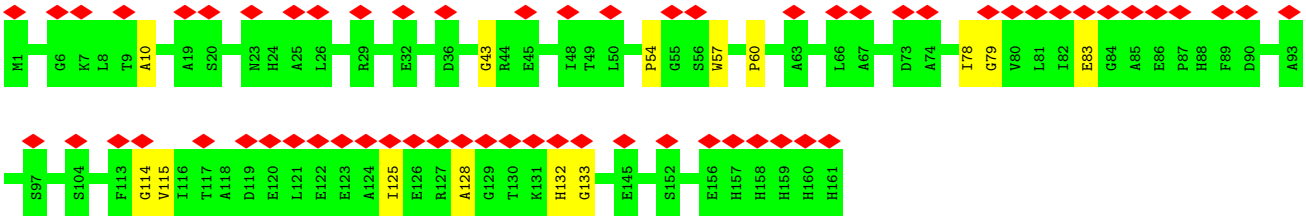




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

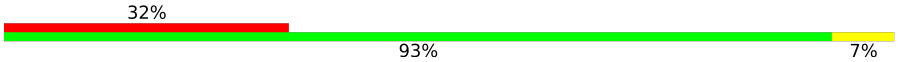
Chain JD:

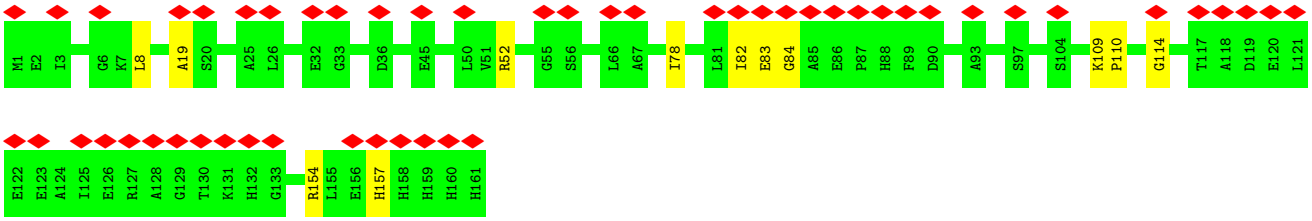




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

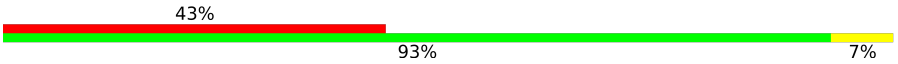
Chain JE:

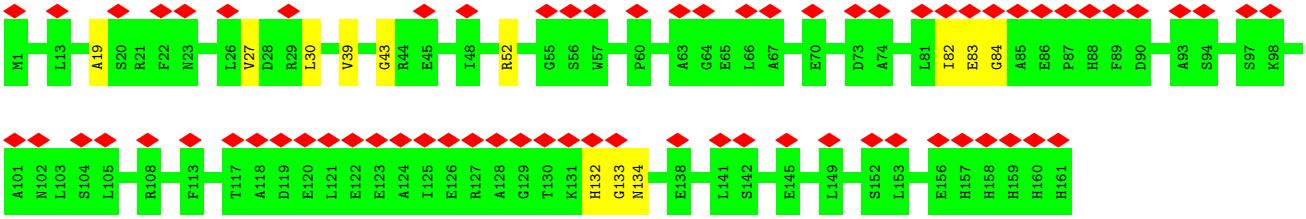




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

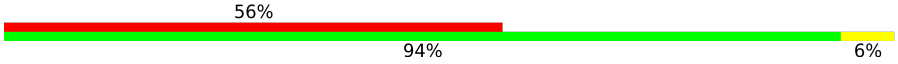
Chain JF:

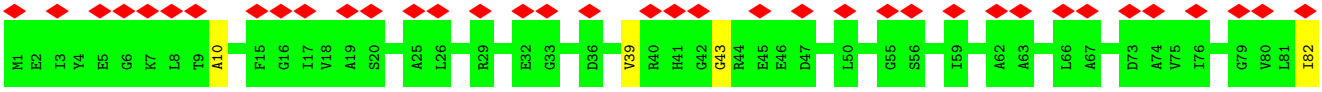


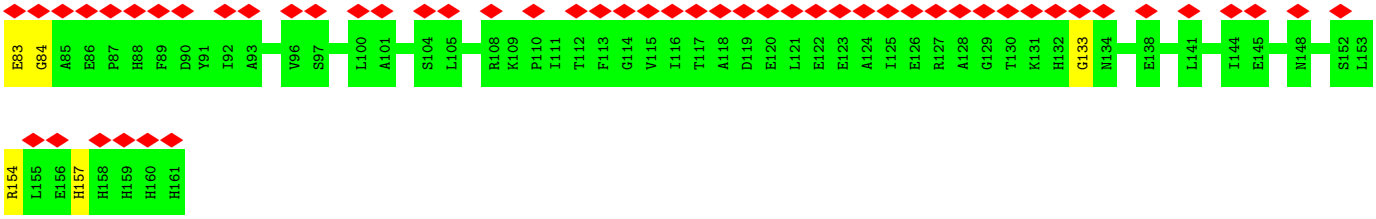


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JG:

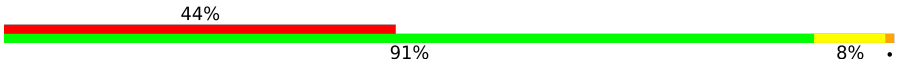


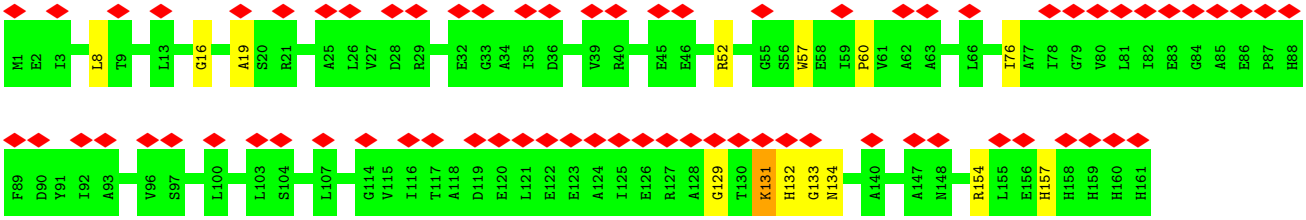




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

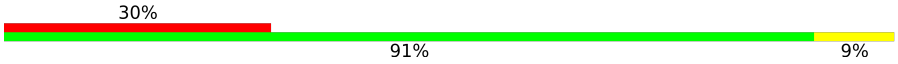
Chain JH:

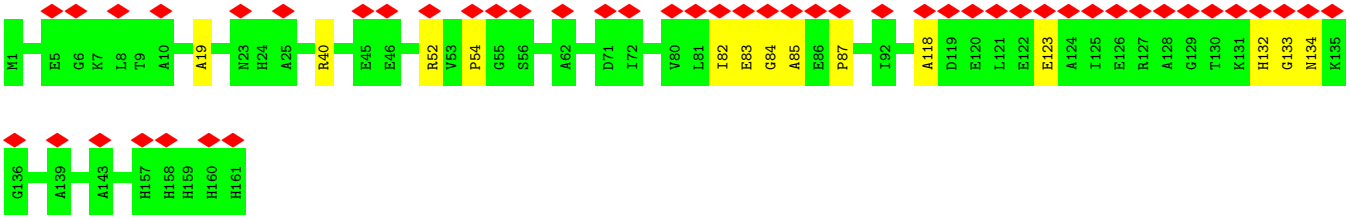




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

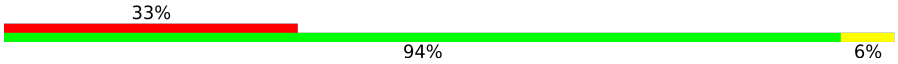
Chain JI:

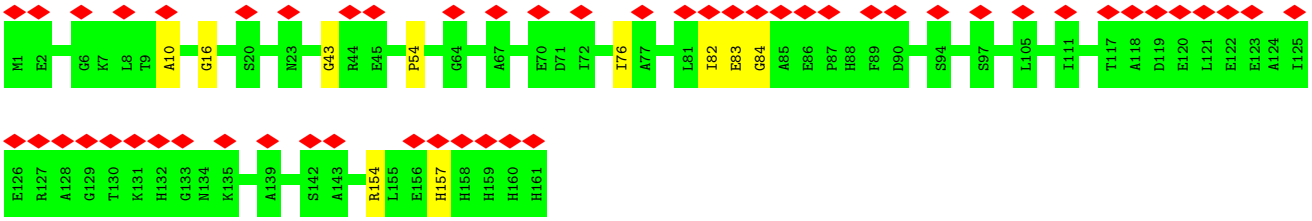




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

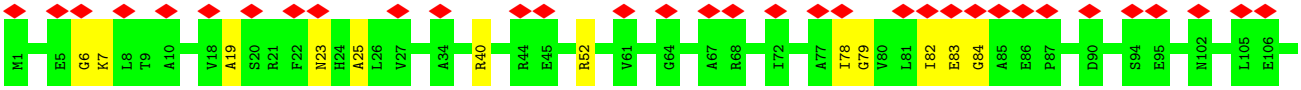
Chain JJ:

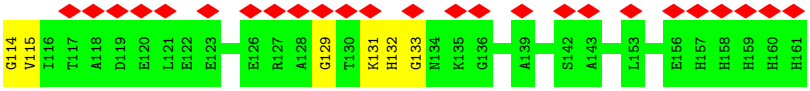




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

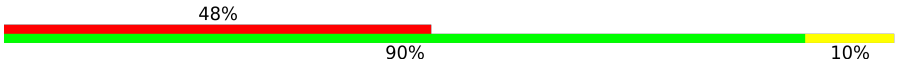
Chain JK:

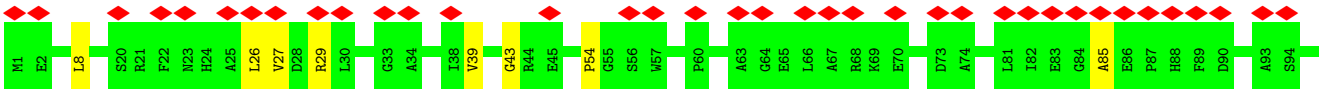


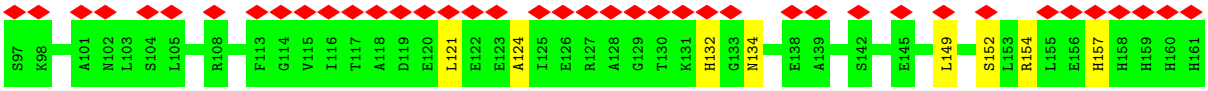


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JL:

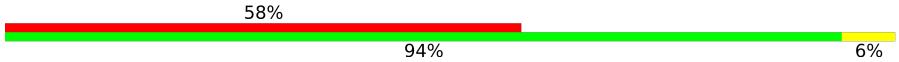


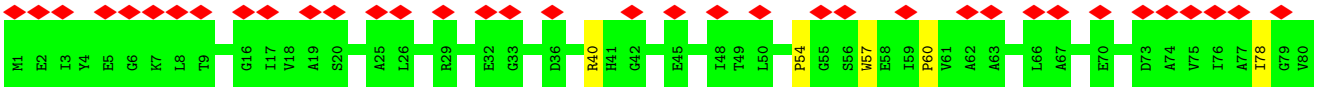


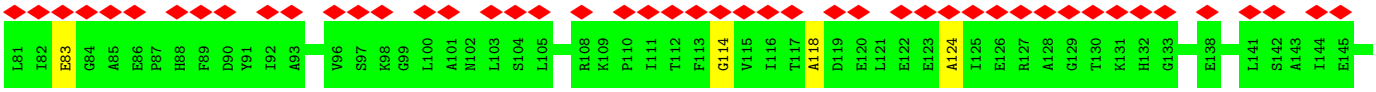


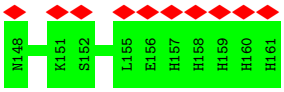
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JM:



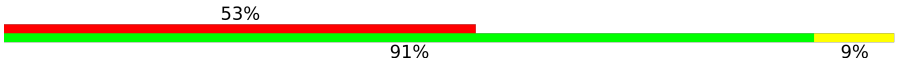


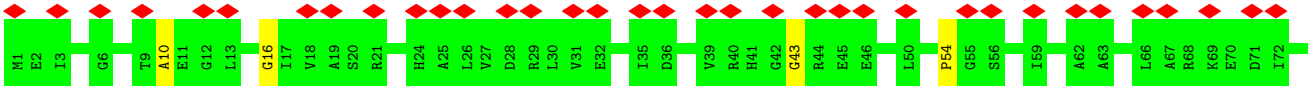


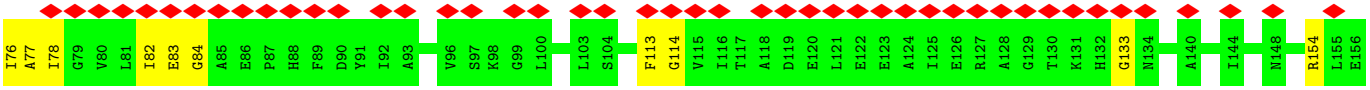


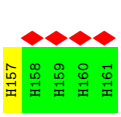
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JN:



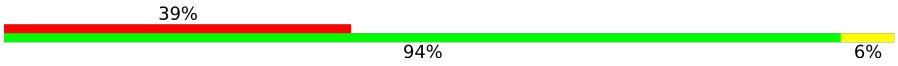


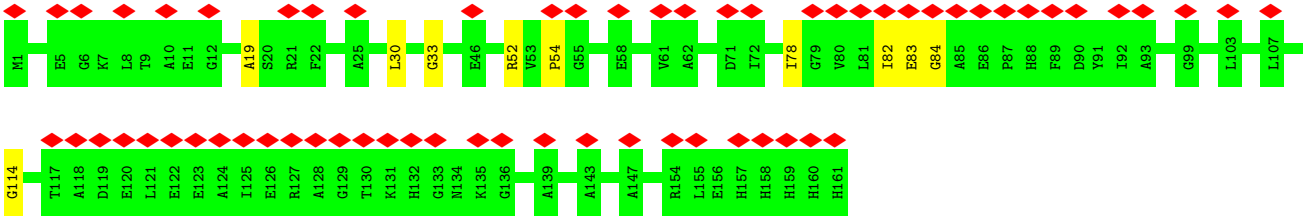




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

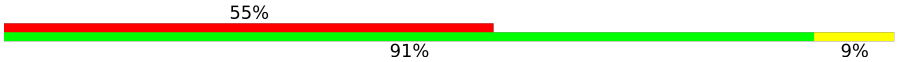
Chain JO:

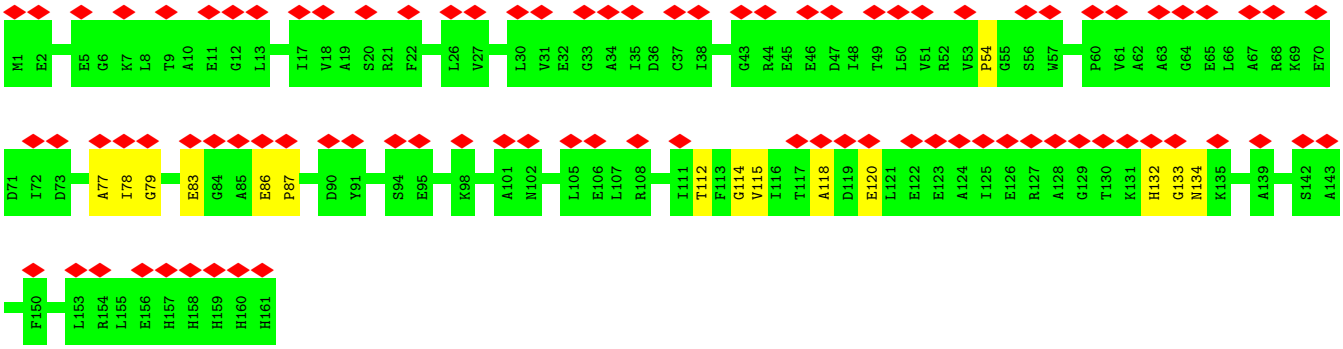




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

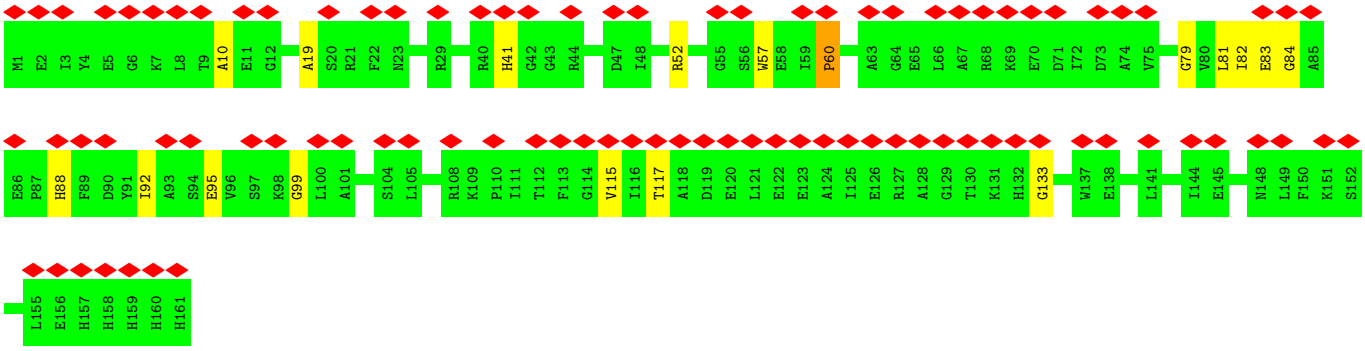
Chain KA:





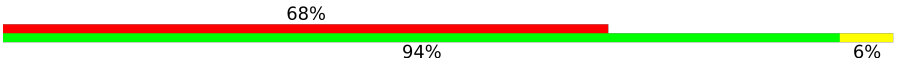
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

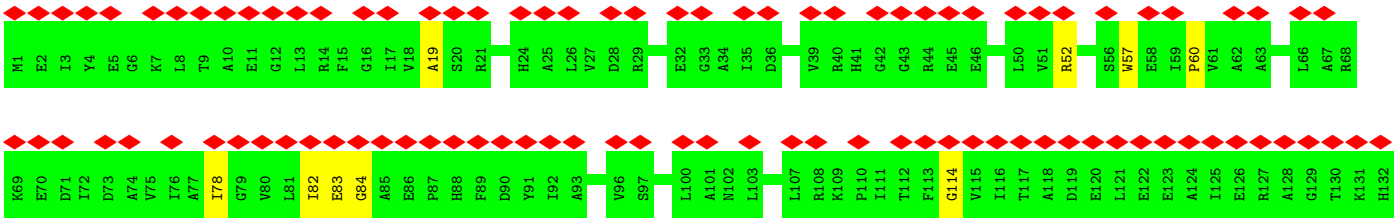
Chain KB:

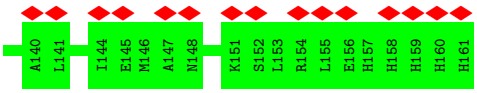


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KC:

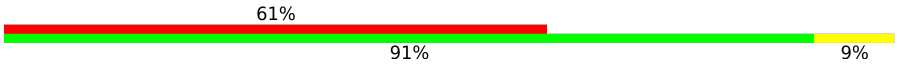


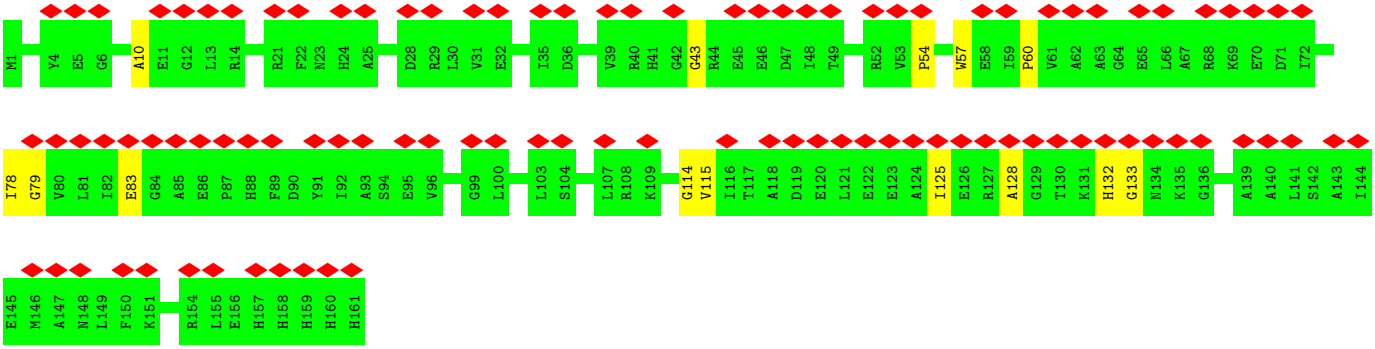




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

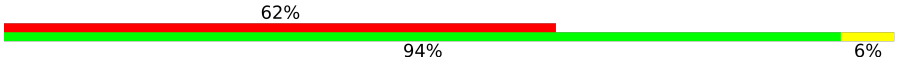
Chain KD:

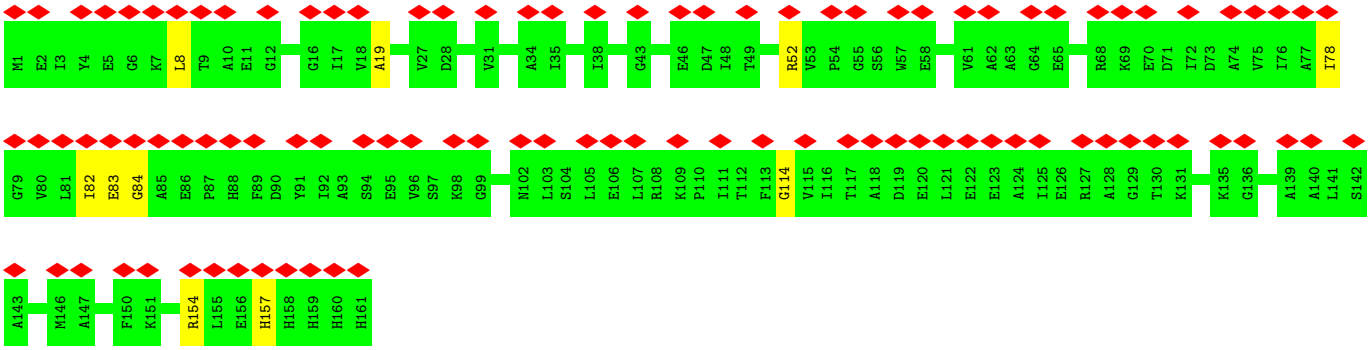




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

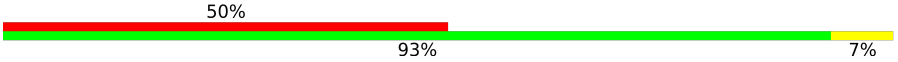
Chain KE:

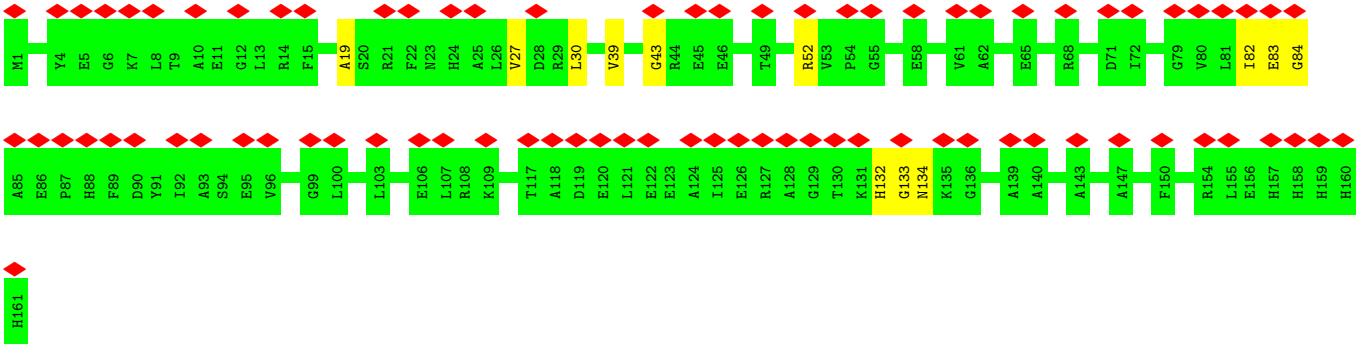




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

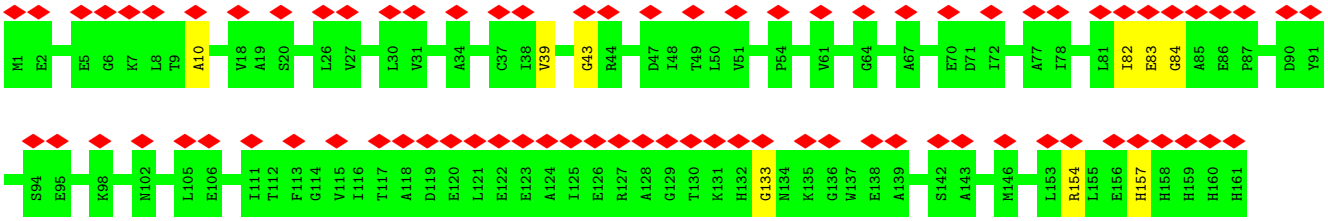
Chain KF:





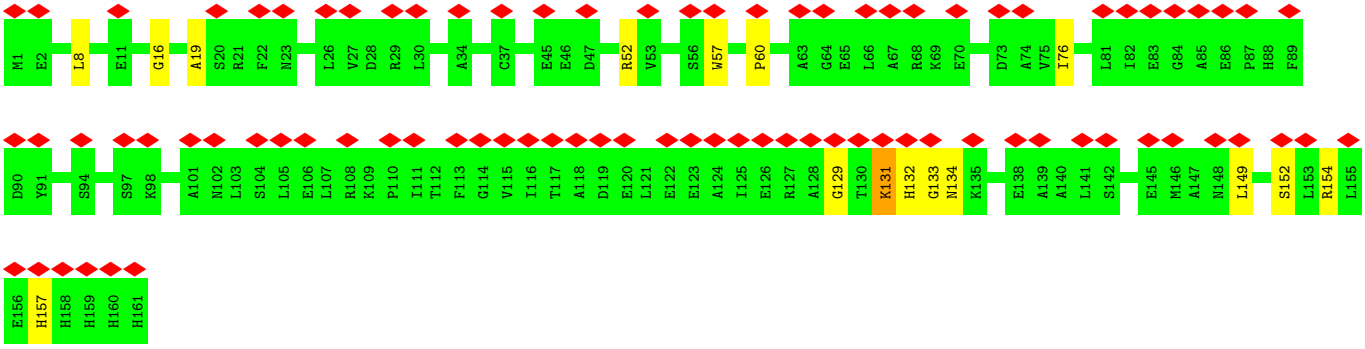
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KG: 49% 94% 6%



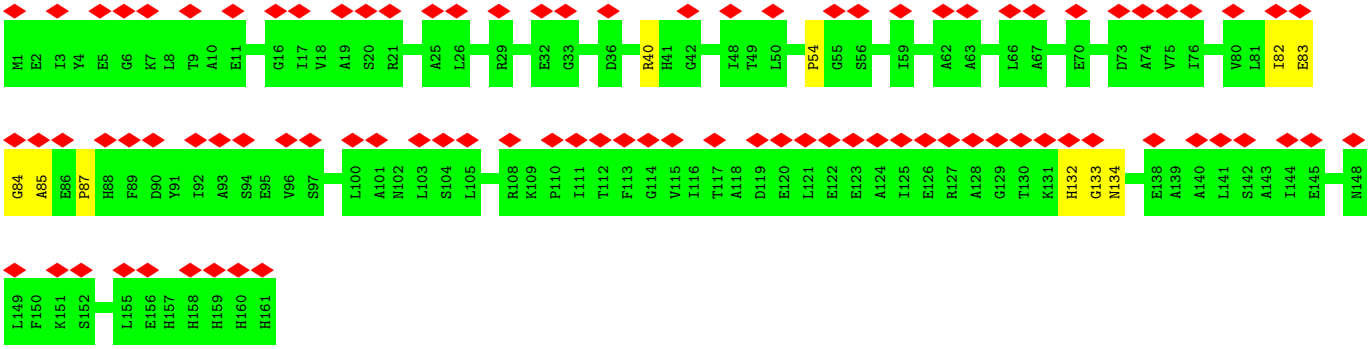
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KH: 53% 90% 9%



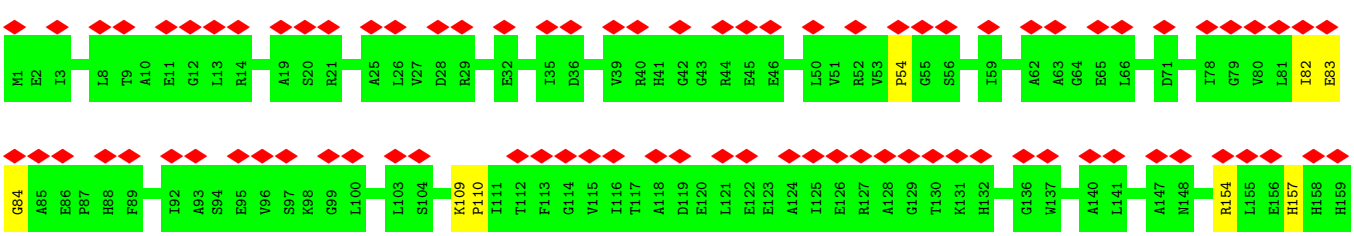
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KI: 57% 94% 6%



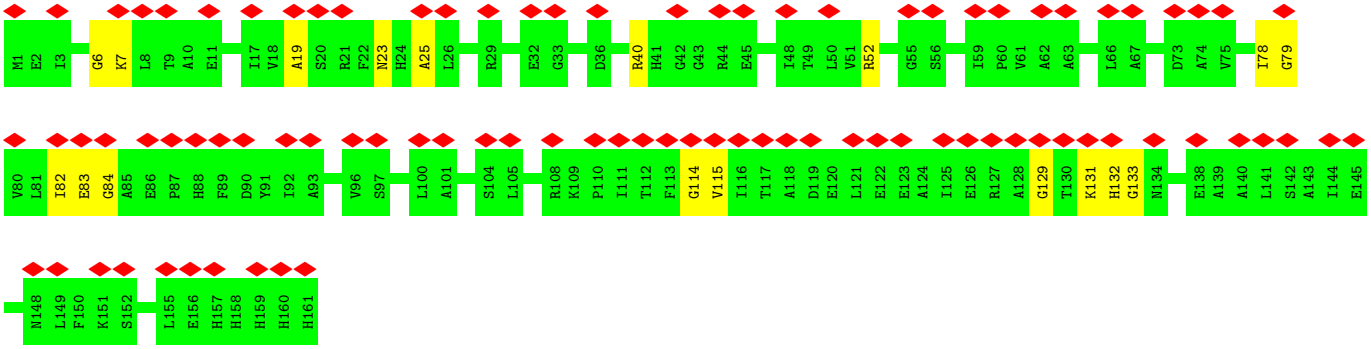
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KJ: 53% 95% 5%



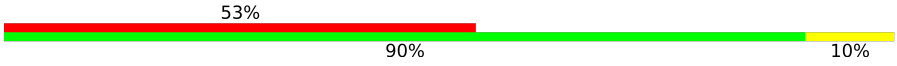
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

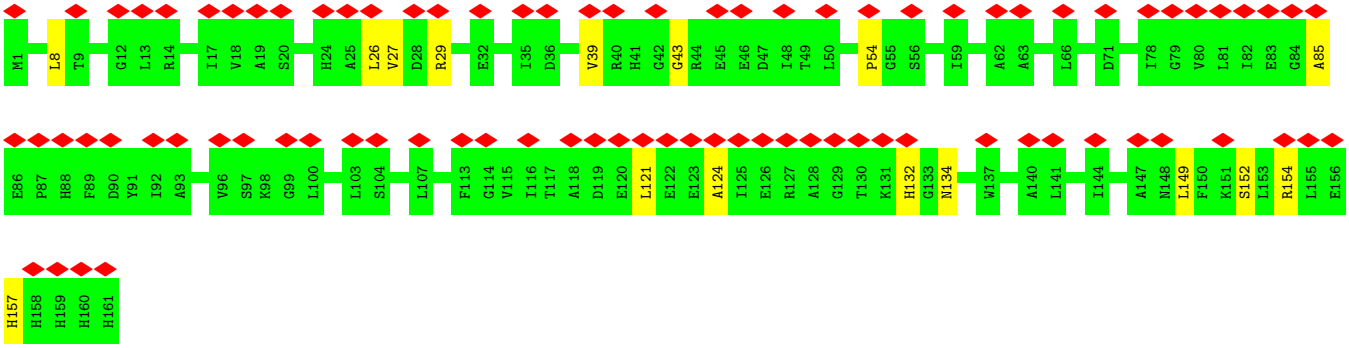
Chain KK:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

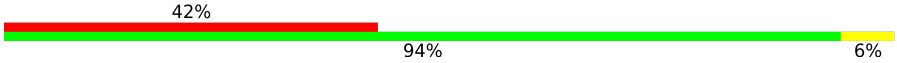
Chain KL:

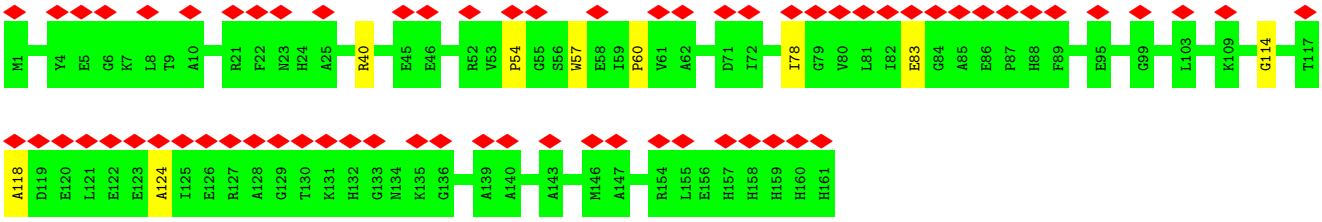




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

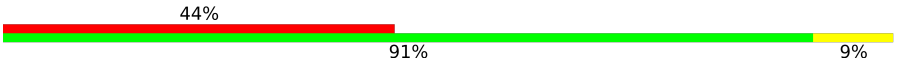
Chain KM:

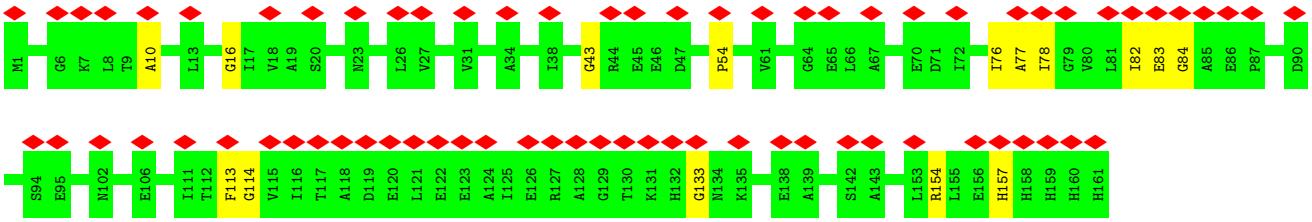




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

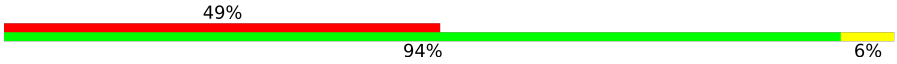
Chain KN:

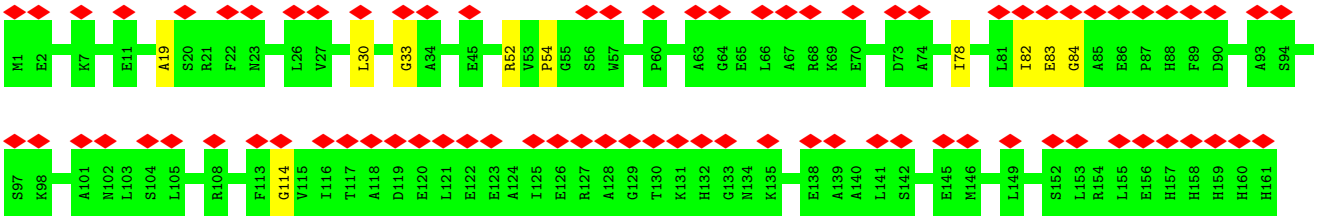




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

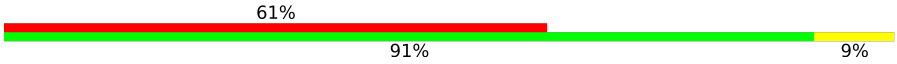
Chain KO:

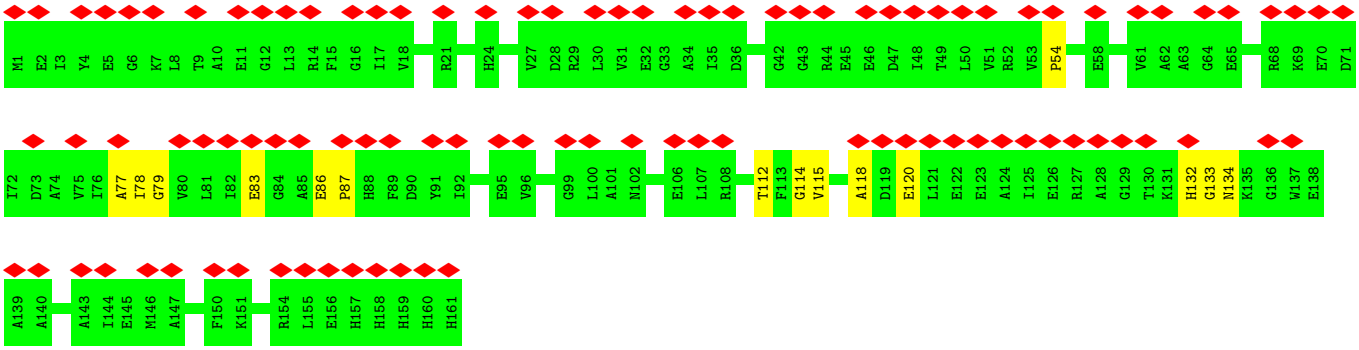




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

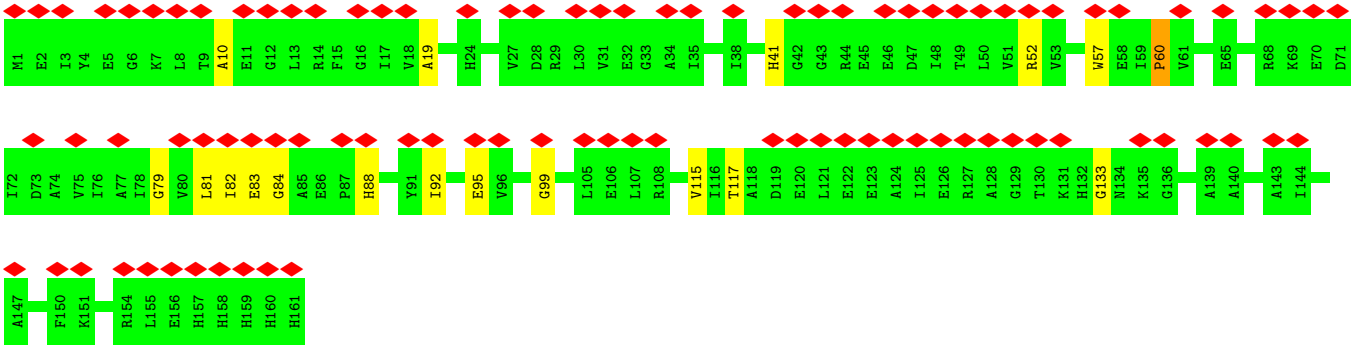
Chain LA:





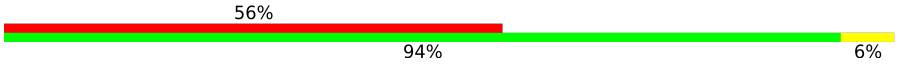
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

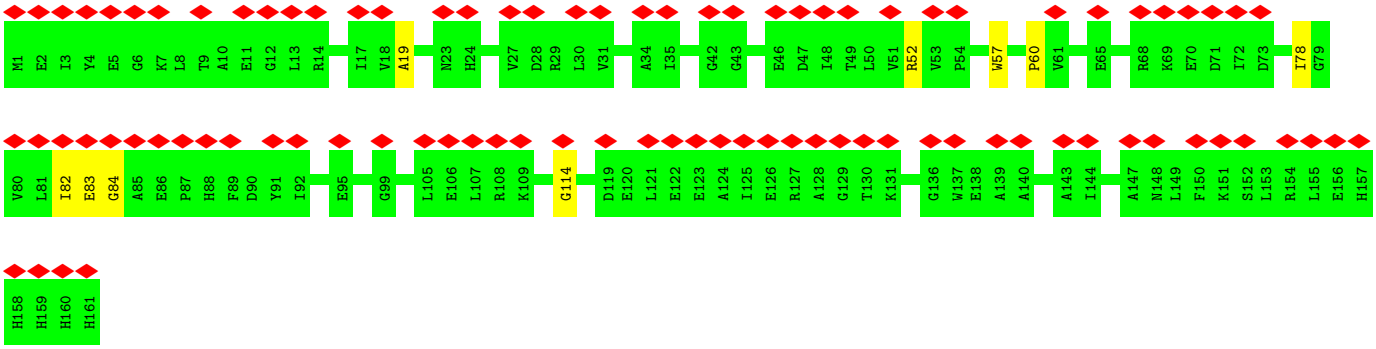
Chain LB:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

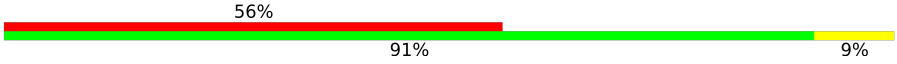
Chain LC:

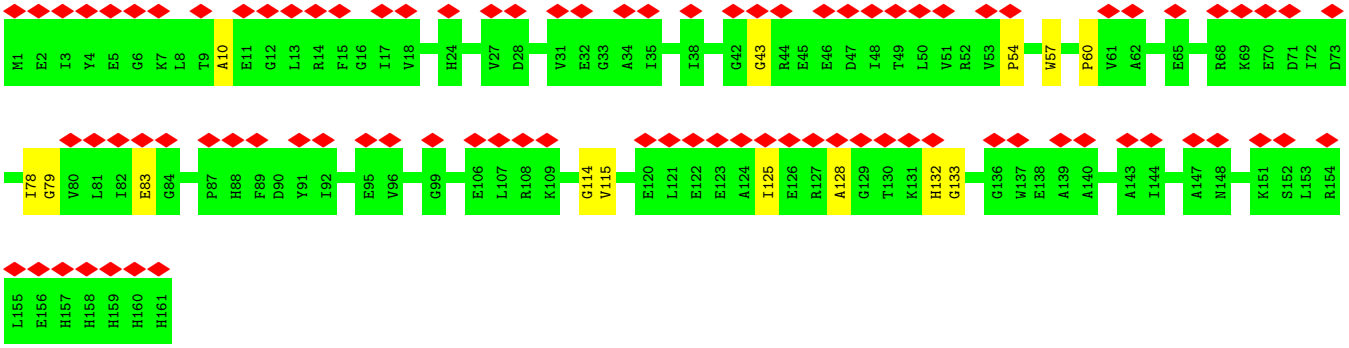




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

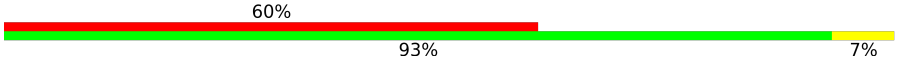
Chain LD:

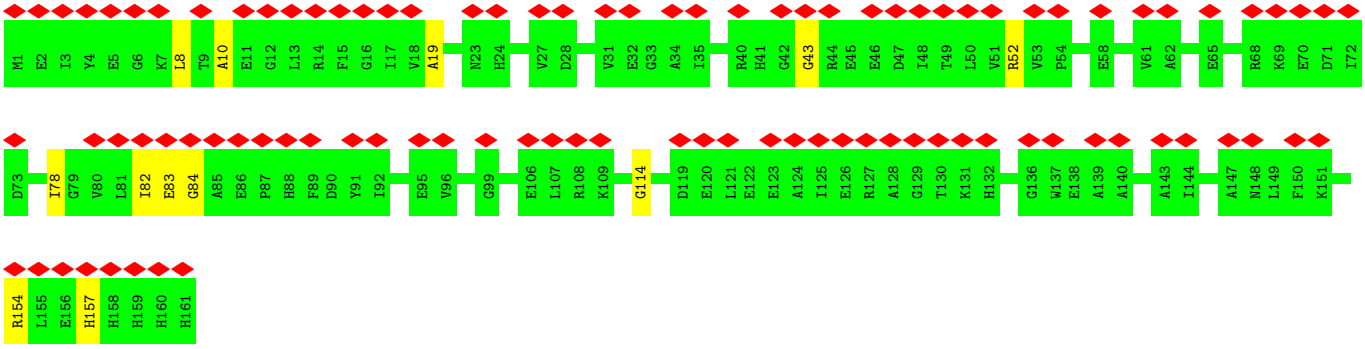




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

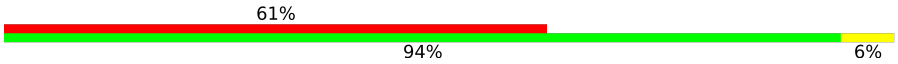
Chain LE:

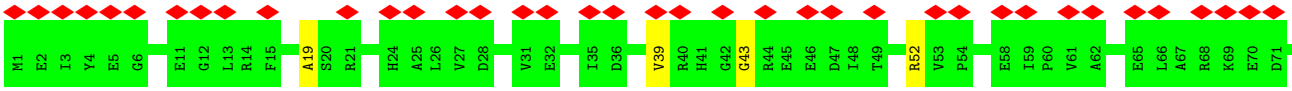


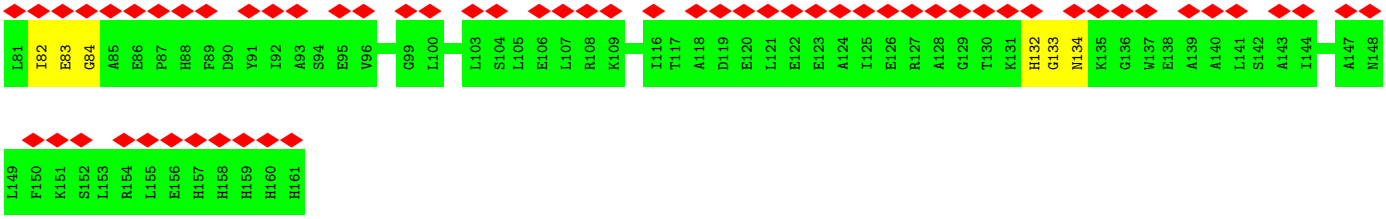


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LF:

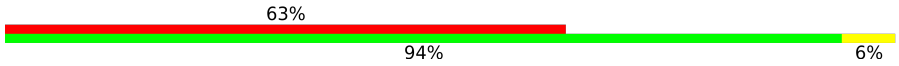


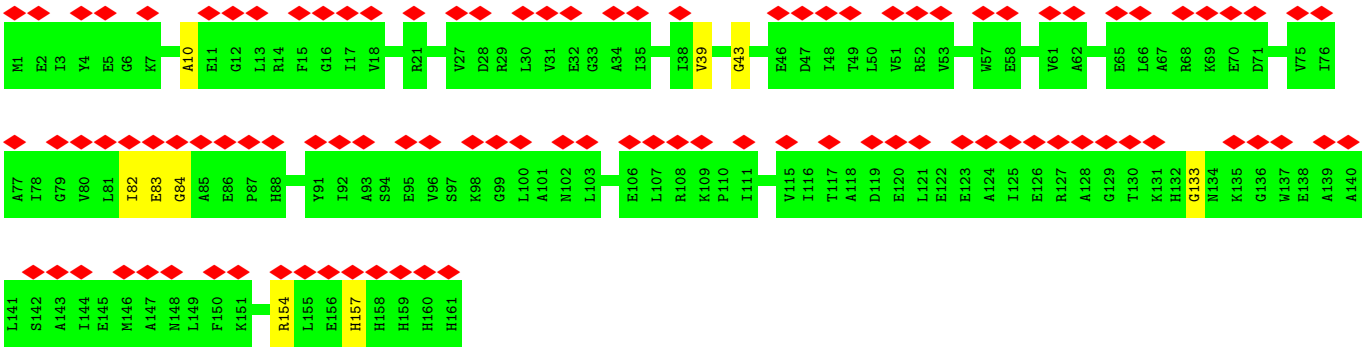




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

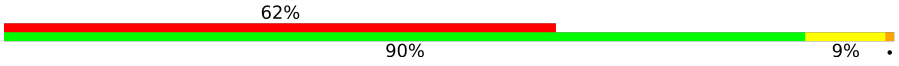
Chain LG:

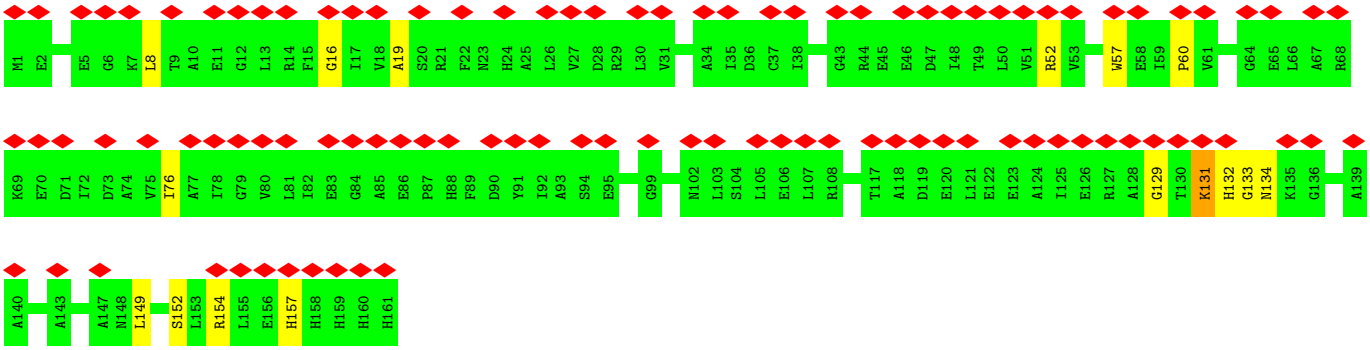




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

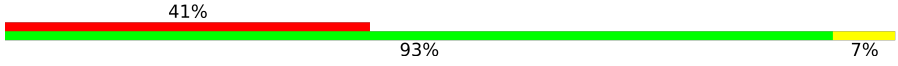
Chain LH:

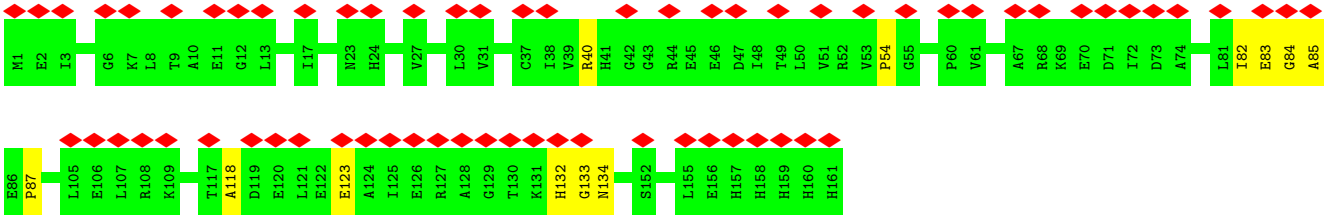




• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

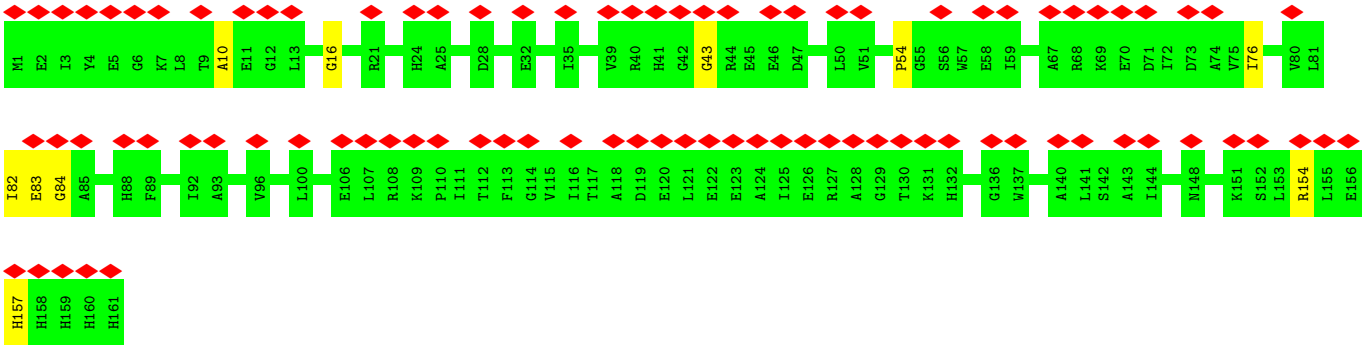
Chain LI:





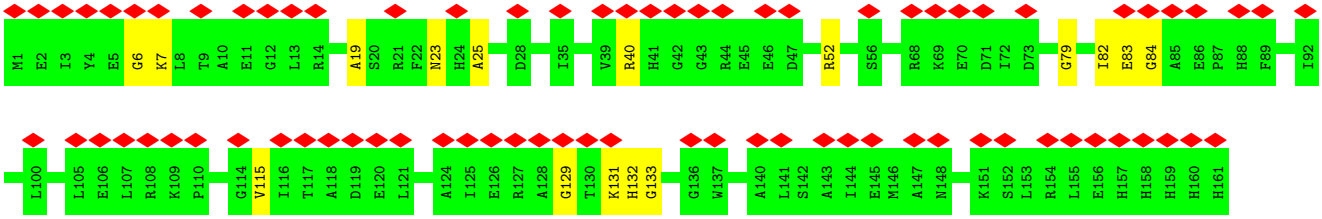
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LJ: 55% 94% 6%



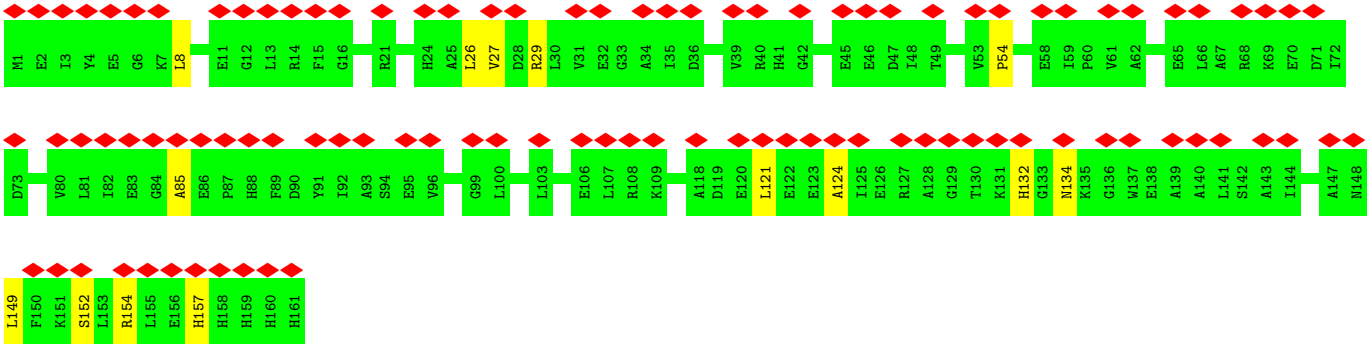
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LK: 48% 90% 10%



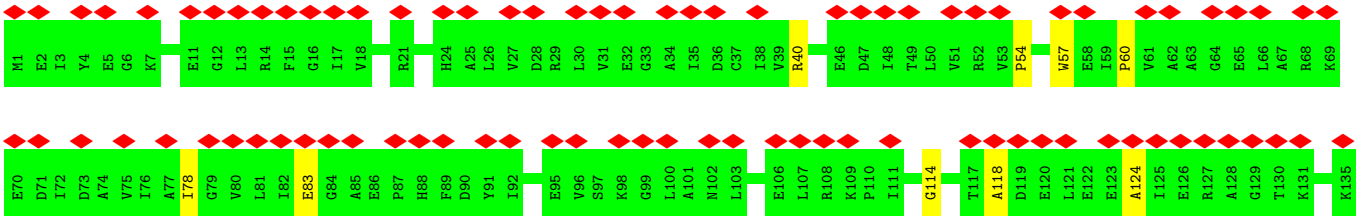
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

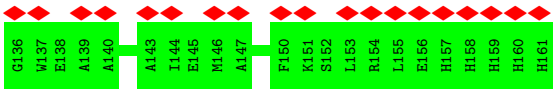
Chain LL: 61% 91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

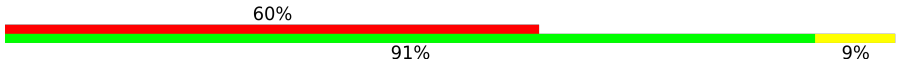
Chain LM: 65% 94% 6%

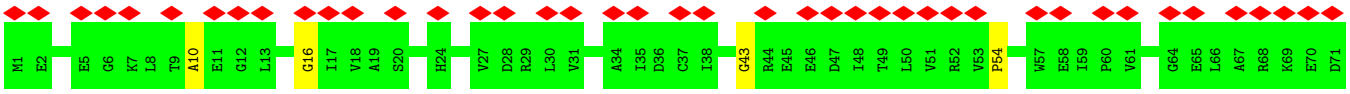


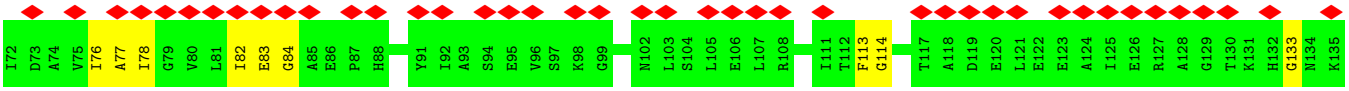


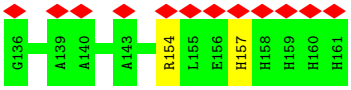
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LN:



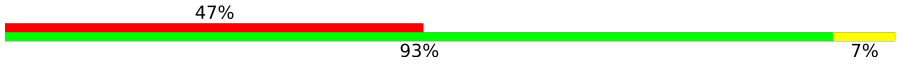


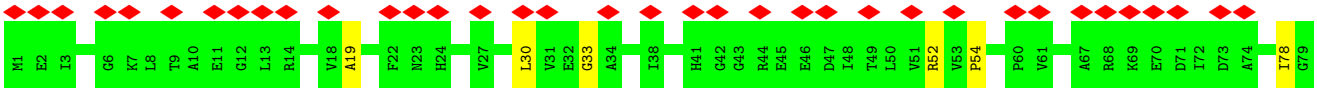


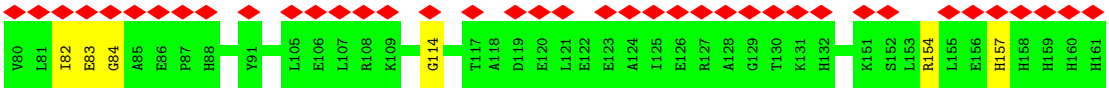


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LO:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	26769	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 ($e^-/Å^2$)	4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	417.0, 417.0, 417.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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	AA	0.33	0/801	0.57	0/1114
1	AB	0.35	0/801	0.59	0/1114
1	AC	0.34	0/801	0.55	0/1114
1	AD	0.33	0/801	0.57	0/1114
1	AE	0.33	0/801	0.55	0/1114
1	AF	0.35	0/801	0.56	0/1114
1	AG	0.31	0/801	0.57	0/1114
1	AH	0.37	0/801	0.61	1/1114 (0.1%)
1	AI	0.35	0/801	0.57	0/1114
1	AJ	0.35	0/801	0.57	0/1114
1	AK	0.34	0/801	0.53	0/1114
1	AL	0.36	0/801	0.55	0/1114
1	AM	0.35	0/801	0.55	0/1114
1	AN	0.33	0/801	0.57	0/1114
1	AO	0.34	0/801	0.56	0/1114
1	BA	0.33	0/801	0.57	0/1114
1	BB	0.35	0/801	0.59	0/1114
1	BC	0.35	0/801	0.55	0/1114
1	BD	0.33	0/801	0.57	0/1114
1	BE	0.34	0/801	0.55	0/1114
1	BF	0.35	0/801	0.56	0/1114
1	BG	0.31	0/801	0.57	0/1114
1	BH	0.37	0/801	0.61	1/1114 (0.1%)
1	BI	0.35	0/801	0.57	0/1114
1	BJ	0.35	0/801	0.57	0/1114
1	BK	0.34	0/801	0.53	0/1114
1	BL	0.36	0/801	0.55	0/1114
1	BM	0.35	0/801	0.55	0/1114
1	BN	0.33	0/801	0.57	0/1114
1	BO	0.34	0/801	0.56	0/1114
1	CA	0.33	0/801	0.57	0/1114
1	CB	0.35	0/801	0.59	0/1114
1	CC	0.34	0/801	0.55	0/1114
1	CD	0.33	0/801	0.57	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	CE	0.33	0/801	0.55	0/1114
1	CF	0.35	0/801	0.56	0/1114
1	CG	0.31	0/801	0.57	0/1114
1	CH	0.37	0/801	0.61	1/1114 (0.1%)
1	CI	0.35	0/801	0.57	0/1114
1	CJ	0.35	0/801	0.57	0/1114
1	CK	0.34	0/801	0.53	0/1114
1	CL	0.36	0/801	0.55	0/1114
1	CM	0.35	0/801	0.55	0/1114
1	CN	0.33	0/801	0.57	0/1114
1	CO	0.34	0/801	0.56	0/1114
1	DA	0.33	0/801	0.57	0/1114
1	DB	0.35	0/801	0.59	0/1114
1	DC	0.34	0/801	0.55	0/1114
1	DD	0.33	0/801	0.57	0/1114
1	DE	0.33	0/801	0.55	0/1114
1	DF	0.35	0/801	0.56	0/1114
1	DG	0.31	0/801	0.57	0/1114
1	DH	0.37	0/801	0.61	1/1114 (0.1%)
1	DI	0.35	0/801	0.57	0/1114
1	DJ	0.34	0/801	0.57	0/1114
1	DK	0.34	0/801	0.53	0/1114
1	DL	0.36	0/801	0.55	0/1114
1	DM	0.35	0/801	0.55	0/1114
1	DN	0.33	0/801	0.57	0/1114
1	DO	0.34	0/801	0.56	0/1114
1	EA	0.33	0/801	0.57	0/1114
1	EB	0.35	0/801	0.59	0/1114
1	EC	0.34	0/801	0.55	0/1114
1	ED	0.33	0/801	0.57	0/1114
1	EE	0.34	0/801	0.55	0/1114
1	EF	0.35	0/801	0.56	0/1114
1	EG	0.31	0/801	0.57	0/1114
1	EH	0.37	0/801	0.61	1/1114 (0.1%)
1	EI	0.35	0/801	0.57	0/1114
1	EJ	0.34	0/801	0.57	0/1114
1	EK	0.34	0/801	0.53	0/1114
1	EL	0.36	0/801	0.55	0/1114
1	EM	0.35	0/801	0.55	0/1114
1	EN	0.33	0/801	0.57	0/1114
1	EO	0.34	0/801	0.56	0/1114
1	FA	0.33	0/801	0.57	0/1114
1	FB	0.35	0/801	0.59	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	FC	0.35	0/801	0.55	0/1114
1	FD	0.33	0/801	0.57	0/1114
1	FE	0.34	0/801	0.55	0/1114
1	FF	0.35	0/801	0.56	0/1114
1	FG	0.31	0/801	0.57	0/1114
1	FH	0.37	0/801	0.61	1/1114 (0.1%)
1	FI	0.35	0/801	0.57	0/1114
1	FJ	0.35	0/801	0.57	0/1114
1	FK	0.34	0/801	0.53	0/1114
1	FL	0.36	0/801	0.55	0/1114
1	FM	0.35	0/801	0.55	0/1114
1	FN	0.33	0/801	0.57	0/1114
1	FO	0.34	0/801	0.56	0/1114
1	GA	0.33	0/801	0.57	0/1114
1	GB	0.35	0/801	0.59	0/1114
1	GC	0.34	0/801	0.55	0/1114
1	GD	0.33	0/801	0.57	0/1114
1	GE	0.33	0/801	0.55	0/1114
1	GF	0.35	0/801	0.56	0/1114
1	GG	0.31	0/801	0.57	0/1114
1	GH	0.37	0/801	0.61	1/1114 (0.1%)
1	GI	0.35	0/801	0.57	0/1114
1	GJ	0.35	0/801	0.57	0/1114
1	GK	0.34	0/801	0.53	0/1114
1	GL	0.36	0/801	0.55	0/1114
1	GM	0.35	0/801	0.55	0/1114
1	GN	0.33	0/801	0.57	0/1114
1	GO	0.34	0/801	0.56	0/1114
1	HA	0.33	0/801	0.57	0/1114
1	HB	0.35	0/801	0.59	0/1114
1	HC	0.34	0/801	0.55	0/1114
1	HD	0.33	0/801	0.57	0/1114
1	HE	0.34	0/801	0.55	0/1114
1	HF	0.35	0/801	0.56	0/1114
1	HG	0.31	0/801	0.57	0/1114
1	HH	0.37	0/801	0.61	1/1114 (0.1%)
1	HI	0.35	0/801	0.57	0/1114
1	HJ	0.35	0/801	0.57	0/1114
1	HK	0.34	0/801	0.53	0/1114
1	HL	0.36	0/801	0.55	0/1114
1	HM	0.35	0/801	0.55	0/1114
1	HN	0.33	0/801	0.57	0/1114
1	HO	0.34	0/801	0.56	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	IA	0.33	0/801	0.57	0/1114
1	IB	0.35	0/801	0.59	0/1114
1	IC	0.34	0/801	0.55	0/1114
1	ID	0.33	0/801	0.57	0/1114
1	IE	0.34	0/801	0.55	0/1114
1	IF	0.35	0/801	0.56	0/1114
1	IG	0.31	0/801	0.57	0/1114
1	IH	0.37	0/801	0.61	1/1114 (0.1%)
1	II	0.35	0/801	0.57	0/1114
1	IJ	0.35	0/801	0.57	0/1114
1	IK	0.33	0/801	0.53	0/1114
1	IL	0.36	0/801	0.55	0/1114
1	IM	0.35	0/801	0.55	0/1114
1	IN	0.33	0/801	0.57	0/1114
1	IO	0.34	0/801	0.56	0/1114
1	JA	0.33	0/801	0.57	0/1114
1	JB	0.35	0/801	0.59	0/1114
1	JC	0.34	0/801	0.55	0/1114
1	JD	0.33	0/801	0.57	0/1114
1	JE	0.33	0/801	0.55	0/1114
1	JF	0.35	0/801	0.56	0/1114
1	JG	0.31	0/801	0.57	0/1114
1	JH	0.37	0/801	0.61	1/1114 (0.1%)
1	JI	0.35	0/801	0.57	0/1114
1	JJ	0.35	0/801	0.57	0/1114
1	JK	0.34	0/801	0.53	0/1114
1	JL	0.36	0/801	0.55	0/1114
1	JM	0.35	0/801	0.55	0/1114
1	JN	0.33	0/801	0.57	0/1114
1	JO	0.34	0/801	0.56	0/1114
1	KA	0.33	0/801	0.57	0/1114
1	KB	0.35	0/801	0.59	0/1114
1	KC	0.34	0/801	0.55	0/1114
1	KD	0.33	0/801	0.57	0/1114
1	KE	0.34	0/801	0.55	0/1114
1	KF	0.35	0/801	0.56	0/1114
1	KG	0.31	0/801	0.57	0/1114
1	KH	0.37	0/801	0.61	1/1114 (0.1%)
1	KI	0.35	0/801	0.57	0/1114
1	KJ	0.34	0/801	0.57	0/1114
1	KK	0.34	0/801	0.53	0/1114
1	KL	0.36	0/801	0.55	0/1114
1	KM	0.35	0/801	0.55	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	KN	0.33	0/801	0.57	0/1114
1	KO	0.34	0/801	0.56	0/1114
1	LA	0.33	0/801	0.57	0/1114
1	LB	0.35	0/801	0.59	0/1114
1	LC	0.34	0/801	0.55	0/1114
1	LD	0.33	0/801	0.57	0/1114
1	LE	0.33	0/801	0.55	0/1114
1	LF	0.35	0/801	0.56	0/1114
1	LG	0.31	0/801	0.57	0/1114
1	LH	0.37	0/801	0.61	1/1114 (0.1%)
1	LI	0.35	0/801	0.57	0/1114
1	LJ	0.35	0/801	0.57	0/1114
1	LK	0.34	0/801	0.53	0/1114
1	LL	0.36	0/801	0.55	0/1114
1	LM	0.35	0/801	0.55	0/1114
1	LN	0.33	0/801	0.57	0/1114
1	LO	0.34	0/801	0.56	0/1114
All	All	0.34	0/144180	0.57	12/200520 (0.0%)

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	AK	0	1
1	BK	0	1
1	CK	0	1
1	DK	0	1
1	EK	0	1
1	FK	0	1
1	GK	0	1
1	HK	0	1
1	IK	0	1
1	JK	0	1
1	KK	0	1
1	LK	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	IH	133	GLY	N-CA-C	-5.74	98.75	113.10
1	CH	133	GLY	N-CA-C	-5.73	98.77	113.10
1	FH	133	GLY	N-CA-C	-5.73	98.77	113.10
1	LH	133	GLY	N-CA-C	-5.73	98.78	113.10
1	EH	133	GLY	N-CA-C	-5.72	98.79	113.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AK	6	GLY	Peptide
1	BK	6	GLY	Peptide
1	CK	6	GLY	Peptide
1	DK	6	GLY	Peptide
1	EK	6	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	798	0	416	5	0
1	AB	798	0	416	8	0
1	AC	798	0	416	4	0
1	AD	798	0	416	6	0
1	AE	798	0	416	5	0
1	AF	798	0	416	5	0
1	AG	798	0	416	5	0
1	AH	798	0	416	7	0
1	AI	798	0	416	4	0
1	AJ	798	0	416	3	0
1	AK	798	0	416	8	0
1	AL	798	0	416	7	0
1	AM	798	0	416	4	0
1	AN	798	0	416	7	0
1	AO	798	0	416	6	0
1	BA	798	0	416	5	0
1	BB	798	0	416	9	0
1	BC	798	0	416	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BD	798	0	416	6	0
1	BE	798	0	416	8	0
1	BF	798	0	416	5	0
1	BG	798	0	416	5	0
1	BH	798	0	416	7	0
1	BI	798	0	416	5	0
1	BJ	798	0	416	2	0
1	BK	798	0	416	7	0
1	BL	798	0	416	6	0
1	BM	798	0	416	4	0
1	BN	798	0	416	6	0
1	BO	798	0	416	5	0
1	CA	798	0	416	6	0
1	CB	798	0	416	8	0
1	CC	798	0	416	4	0
1	CD	798	0	416	6	0
1	CE	798	0	416	8	0
1	CF	798	0	416	6	0
1	CG	798	0	416	5	0
1	CH	798	0	416	7	0
1	CI	798	0	416	5	0
1	CJ	798	0	416	3	0
1	CK	798	0	416	8	0
1	CL	798	0	416	7	0
1	CM	798	0	416	4	0
1	CN	798	0	416	7	0
1	CO	798	0	416	6	0
1	DA	798	0	416	6	0
1	DB	798	0	416	8	0
1	DC	798	0	416	4	0
1	DD	798	0	416	6	0
1	DE	798	0	416	7	0
1	DF	798	0	416	5	0
1	DG	798	0	416	5	0
1	DH	798	0	416	7	0
1	DI	798	0	416	4	0
1	DJ	798	0	416	3	0
1	DK	798	0	416	8	0
1	DL	798	0	416	6	0
1	DM	798	0	416	4	0
1	DN	798	0	416	7	0
1	DO	798	0	416	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EA	798	0	416	6	0
1	EB	798	0	416	7	0
1	EC	798	0	416	4	0
1	ED	798	0	416	6	0
1	EE	798	0	416	6	0
1	EF	798	0	416	5	0
1	EG	798	0	416	5	0
1	EH	798	0	416	6	0
1	EI	798	0	416	5	0
1	EJ	798	0	416	4	0
1	EK	798	0	416	8	0
1	EL	798	0	416	6	0
1	EM	798	0	416	4	0
1	EN	798	0	416	7	0
1	EO	798	0	416	6	0
1	FA	798	0	416	6	0
1	FB	798	0	416	8	0
1	FC	798	0	416	4	0
1	FD	798	0	416	6	0
1	FE	798	0	416	5	0
1	FF	798	0	416	5	0
1	FG	798	0	416	5	0
1	FH	798	0	416	6	0
1	FI	798	0	416	5	0
1	FJ	798	0	416	3	0
1	FK	798	0	416	6	0
1	FL	798	0	416	6	0
1	FM	798	0	416	4	0
1	FN	798	0	416	8	0
1	FO	798	0	416	5	0
1	GA	798	0	416	5	0
1	GB	798	0	416	8	0
1	GC	798	0	416	4	0
1	GD	798	0	416	6	0
1	GE	798	0	416	7	0
1	GF	798	0	416	6	0
1	GG	798	0	416	5	0
1	GH	798	0	416	6	0
1	GI	798	0	416	5	0
1	GJ	798	0	416	3	0
1	GK	798	0	416	7	0
1	GL	798	0	416	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GM	798	0	416	4	0
1	GN	798	0	416	7	0
1	GO	798	0	416	6	0
1	HA	798	0	416	6	0
1	HB	798	0	416	8	0
1	HC	798	0	416	4	0
1	HD	798	0	416	6	0
1	HE	798	0	416	7	0
1	HF	798	0	416	5	0
1	HG	798	0	416	5	0
1	HH	798	0	416	5	0
1	HI	798	0	416	4	0
1	HJ	798	0	416	4	0
1	HK	798	0	416	8	0
1	HL	798	0	416	6	0
1	HM	798	0	416	4	0
1	HN	798	0	416	7	0
1	HO	798	0	416	5	0
1	IA	798	0	416	5	0
1	IB	798	0	416	9	0
1	IC	798	0	416	4	0
1	ID	798	0	416	6	0
1	IE	798	0	416	7	0
1	IF	798	0	416	5	0
1	IG	798	0	416	5	0
1	IH	798	0	416	6	0
1	II	798	0	416	4	0
1	IJ	798	0	416	5	0
1	IK	798	0	416	6	0
1	IL	798	0	416	7	0
1	IM	798	0	416	4	0
1	IN	798	0	416	8	0
1	IO	798	0	416	5	0
1	JA	798	0	416	5	0
1	JB	798	0	416	9	0
1	JC	798	0	416	4	0
1	JD	798	0	416	6	0
1	JE	798	0	416	6	0
1	JF	798	0	416	5	0
1	JG	798	0	416	5	0
1	JH	798	0	416	6	0
1	JI	798	0	416	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JJ	798	0	416	4	0
1	JK	798	0	416	7	0
1	JL	798	0	416	7	0
1	JM	798	0	416	4	0
1	JN	798	0	416	8	0
1	JO	798	0	416	4	0
1	KA	798	0	416	6	0
1	KB	798	0	416	8	0
1	KC	798	0	416	4	0
1	KD	798	0	416	6	0
1	KE	798	0	416	5	0
1	KF	798	0	416	5	0
1	KG	798	0	416	5	0
1	KH	798	0	416	7	0
1	KI	798	0	416	4	0
1	KJ	798	0	416	3	0
1	KK	798	0	416	7	0
1	KL	798	0	416	7	0
1	KM	798	0	416	4	0
1	KN	798	0	416	8	0
1	KO	798	0	416	4	0
1	LA	798	0	416	6	0
1	LB	798	0	416	8	0
1	LC	798	0	416	4	0
1	LD	798	0	416	6	0
1	LE	798	0	416	6	0
1	LF	798	0	416	4	0
1	LG	798	0	416	5	0
1	LH	798	0	416	7	0
1	LI	798	0	416	5	0
1	LJ	798	0	416	4	0
1	LK	798	0	416	7	0
1	LL	798	0	416	6	0
1	LM	798	0	416	4	0
1	LN	798	0	416	7	0
1	LO	798	0	416	5	0
All	All	143640	0	74880	977	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 977 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IL:26:LEU:O	1:IL:29:ARG:N	2.17	0.76
1:JL:26:LEU:O	1:JL:29:ARG:N	2.17	0.75
1:LL:26:LEU:O	1:LL:29:ARG:N	2.17	0.73
1:DL:26:LEU:O	1:DL:29:ARG:N	2.17	0.73
1:GL:26:LEU:O	1:GL:29:ARG:N	2.17	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8 39
1	AB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8 39
1	AC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25 65
1	AD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5 34
1	AE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25 65
1	AF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12 48
1	AG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12 48
1	AH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8 39
1	AI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8 39
1	AJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12 48
1	AK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5 34
1	AL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8 39
1	AM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12 48
1	AN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8 39
1	AO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12 48
1	BA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	BC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	BD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	BE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	BF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	BG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	BH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	BI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	BJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	BK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	BL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	BM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	BN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	BO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	CA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	CB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	CC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	CD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	CE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	CF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	CG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	CH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	CI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	CJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	CK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	CL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	CM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	CN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	CO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	DA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	DB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	DD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	DE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	DF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	DG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	DH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	DI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	DJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	DK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	DL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	DM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	DN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	DO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	EA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	EB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	EC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	ED	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	EE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	EF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	EG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	EH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	EI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	EJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	EK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	EL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	EM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	EN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	EO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	FA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	FB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	FC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	FE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	FF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	FG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	FH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	FI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	FJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	FK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	FL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	FM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	FN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	FO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	GA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	GB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	GC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	GD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	GE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	GF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	GG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	GH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	GI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	GJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	GK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	GL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	GM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	GN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	GO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	HA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	HB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	HC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	HD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	HF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	HG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	HH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	HI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	HJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	HK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	HL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	HM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	HN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	HO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	IA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	IB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	IC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	ID	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	IE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	IF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	IG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	IH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	II	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	IJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	IK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	IL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	IM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	IN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	IO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	JA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	JB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	JC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	JD	159/161 (99%)	149 (94%)	6 (4%)	4 (2%)	5	34
1	JE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	JG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	JH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	JI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	JJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	JK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	JL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	JM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	JN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	JO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	KA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	KB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	KC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	KD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	KE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	KF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	KG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	KH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	KI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	KJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	KK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	KL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	KM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	KN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	KO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
1	LA	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	39
1	LB	159/161 (99%)	145 (91%)	11 (7%)	3 (2%)	8	39
1	LC	159/161 (99%)	146 (92%)	12 (8%)	1 (1%)	25	65
1	LD	159/161 (99%)	148 (93%)	7 (4%)	4 (2%)	5	34
1	LE	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	65
1	LF	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LG	159/161 (99%)	150 (94%)	7 (4%)	2 (1%)	12	48
1	LH	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	8	39
1	LI	159/161 (99%)	149 (94%)	7 (4%)	3 (2%)	8	39
1	LJ	159/161 (99%)	144 (91%)	13 (8%)	2 (1%)	12	48
1	LK	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	5	34
1	LL	159/161 (99%)	146 (92%)	10 (6%)	3 (2%)	8	39
1	LM	159/161 (99%)	148 (93%)	9 (6%)	2 (1%)	12	48
1	LN	159/161 (99%)	148 (93%)	8 (5%)	3 (2%)	8	39
1	LO	159/161 (99%)	145 (91%)	12 (8%)	2 (1%)	12	48
All	All	28620/28980 (99%)	26305 (92%)	1859 (6%)	456 (2%)	13	44

5 of 456 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	133	GLY
1	AB	83	GLU
1	AF	83	GLU
1	AF	133	GLY
1	AG	83	GLU

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	AA	4/127 (3%)	4 (100%)	0	100	100
1	AB	4/127 (3%)	4 (100%)	0	100	100
1	AC	4/127 (3%)	4 (100%)	0	100	100
1	AD	4/127 (3%)	4 (100%)	0	100	100
1	AE	4/127 (3%)	4 (100%)	0	100	100
1	AF	4/127 (3%)	4 (100%)	0	100	100
1	AG	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	4/127 (3%)	4 (100%)	0	100	100
1	AI	4/127 (3%)	4 (100%)	0	100	100
1	AJ	4/127 (3%)	4 (100%)	0	100	100
1	AK	4/127 (3%)	4 (100%)	0	100	100
1	AL	4/127 (3%)	4 (100%)	0	100	100
1	AM	4/127 (3%)	4 (100%)	0	100	100
1	AN	4/127 (3%)	4 (100%)	0	100	100
1	AO	4/127 (3%)	4 (100%)	0	100	100
1	BA	4/127 (3%)	4 (100%)	0	100	100
1	BB	4/127 (3%)	4 (100%)	0	100	100
1	BC	4/127 (3%)	4 (100%)	0	100	100
1	BD	4/127 (3%)	4 (100%)	0	100	100
1	BE	4/127 (3%)	4 (100%)	0	100	100
1	BF	4/127 (3%)	4 (100%)	0	100	100
1	BG	4/127 (3%)	4 (100%)	0	100	100
1	BH	4/127 (3%)	4 (100%)	0	100	100
1	BI	4/127 (3%)	4 (100%)	0	100	100
1	BJ	4/127 (3%)	4 (100%)	0	100	100
1	BK	4/127 (3%)	4 (100%)	0	100	100
1	BL	4/127 (3%)	4 (100%)	0	100	100
1	BM	4/127 (3%)	4 (100%)	0	100	100
1	BN	4/127 (3%)	4 (100%)	0	100	100
1	BO	4/127 (3%)	4 (100%)	0	100	100
1	CA	4/127 (3%)	4 (100%)	0	100	100
1	CB	4/127 (3%)	4 (100%)	0	100	100
1	CC	4/127 (3%)	4 (100%)	0	100	100
1	CD	4/127 (3%)	4 (100%)	0	100	100
1	CE	4/127 (3%)	4 (100%)	0	100	100
1	CF	4/127 (3%)	4 (100%)	0	100	100
1	CG	4/127 (3%)	4 (100%)	0	100	100
1	CH	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	4/127 (3%)	4 (100%)	0	100	100
1	CJ	4/127 (3%)	4 (100%)	0	100	100
1	CK	4/127 (3%)	4 (100%)	0	100	100
1	CL	4/127 (3%)	4 (100%)	0	100	100
1	CM	4/127 (3%)	4 (100%)	0	100	100
1	CN	4/127 (3%)	4 (100%)	0	100	100
1	CO	4/127 (3%)	4 (100%)	0	100	100
1	DA	4/127 (3%)	4 (100%)	0	100	100
1	DB	4/127 (3%)	4 (100%)	0	100	100
1	DC	4/127 (3%)	4 (100%)	0	100	100
1	DD	4/127 (3%)	4 (100%)	0	100	100
1	DE	4/127 (3%)	4 (100%)	0	100	100
1	DF	4/127 (3%)	4 (100%)	0	100	100
1	DG	4/127 (3%)	4 (100%)	0	100	100
1	DH	4/127 (3%)	4 (100%)	0	100	100
1	DI	4/127 (3%)	4 (100%)	0	100	100
1	DJ	4/127 (3%)	4 (100%)	0	100	100
1	DK	4/127 (3%)	4 (100%)	0	100	100
1	DL	4/127 (3%)	4 (100%)	0	100	100
1	DM	4/127 (3%)	4 (100%)	0	100	100
1	DN	4/127 (3%)	4 (100%)	0	100	100
1	DO	4/127 (3%)	4 (100%)	0	100	100
1	EA	4/127 (3%)	4 (100%)	0	100	100
1	EB	4/127 (3%)	4 (100%)	0	100	100
1	EC	4/127 (3%)	4 (100%)	0	100	100
1	ED	4/127 (3%)	4 (100%)	0	100	100
1	EE	4/127 (3%)	4 (100%)	0	100	100
1	EF	4/127 (3%)	4 (100%)	0	100	100
1	EG	4/127 (3%)	4 (100%)	0	100	100
1	EH	4/127 (3%)	4 (100%)	0	100	100
1	EI	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EJ	4/127 (3%)	4 (100%)	0	100	100
1	EK	4/127 (3%)	4 (100%)	0	100	100
1	EL	4/127 (3%)	4 (100%)	0	100	100
1	EM	4/127 (3%)	4 (100%)	0	100	100
1	EN	4/127 (3%)	4 (100%)	0	100	100
1	EO	4/127 (3%)	4 (100%)	0	100	100
1	FA	4/127 (3%)	4 (100%)	0	100	100
1	FB	4/127 (3%)	4 (100%)	0	100	100
1	FC	4/127 (3%)	4 (100%)	0	100	100
1	FD	4/127 (3%)	4 (100%)	0	100	100
1	FE	4/127 (3%)	4 (100%)	0	100	100
1	FF	4/127 (3%)	4 (100%)	0	100	100
1	FG	4/127 (3%)	4 (100%)	0	100	100
1	FH	4/127 (3%)	4 (100%)	0	100	100
1	FI	4/127 (3%)	4 (100%)	0	100	100
1	FJ	4/127 (3%)	4 (100%)	0	100	100
1	FK	4/127 (3%)	4 (100%)	0	100	100
1	FL	4/127 (3%)	4 (100%)	0	100	100
1	FM	4/127 (3%)	4 (100%)	0	100	100
1	FN	4/127 (3%)	4 (100%)	0	100	100
1	FO	4/127 (3%)	4 (100%)	0	100	100
1	GA	4/127 (3%)	4 (100%)	0	100	100
1	GB	4/127 (3%)	4 (100%)	0	100	100
1	GC	4/127 (3%)	4 (100%)	0	100	100
1	GD	4/127 (3%)	4 (100%)	0	100	100
1	GE	4/127 (3%)	4 (100%)	0	100	100
1	GF	4/127 (3%)	4 (100%)	0	100	100
1	GG	4/127 (3%)	4 (100%)	0	100	100
1	GH	4/127 (3%)	4 (100%)	0	100	100
1	GI	4/127 (3%)	4 (100%)	0	100	100
1	GJ	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GK	4/127 (3%)	4 (100%)	0	100	100
1	GL	4/127 (3%)	4 (100%)	0	100	100
1	GM	4/127 (3%)	4 (100%)	0	100	100
1	GN	4/127 (3%)	4 (100%)	0	100	100
1	GO	4/127 (3%)	4 (100%)	0	100	100
1	HA	4/127 (3%)	4 (100%)	0	100	100
1	HB	4/127 (3%)	4 (100%)	0	100	100
1	HC	4/127 (3%)	4 (100%)	0	100	100
1	HD	4/127 (3%)	4 (100%)	0	100	100
1	HE	4/127 (3%)	4 (100%)	0	100	100
1	HF	4/127 (3%)	4 (100%)	0	100	100
1	HG	4/127 (3%)	4 (100%)	0	100	100
1	HH	4/127 (3%)	4 (100%)	0	100	100
1	HI	4/127 (3%)	4 (100%)	0	100	100
1	HJ	4/127 (3%)	4 (100%)	0	100	100
1	HK	4/127 (3%)	4 (100%)	0	100	100
1	HL	4/127 (3%)	4 (100%)	0	100	100
1	HM	4/127 (3%)	4 (100%)	0	100	100
1	HN	4/127 (3%)	4 (100%)	0	100	100
1	HO	4/127 (3%)	4 (100%)	0	100	100
1	IA	4/127 (3%)	4 (100%)	0	100	100
1	IB	4/127 (3%)	4 (100%)	0	100	100
1	IC	4/127 (3%)	4 (100%)	0	100	100
1	ID	4/127 (3%)	4 (100%)	0	100	100
1	IE	4/127 (3%)	4 (100%)	0	100	100
1	IF	4/127 (3%)	4 (100%)	0	100	100
1	IG	4/127 (3%)	4 (100%)	0	100	100
1	IH	4/127 (3%)	4 (100%)	0	100	100
1	II	4/127 (3%)	4 (100%)	0	100	100
1	IJ	4/127 (3%)	4 (100%)	0	100	100
1	IK	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IL	4/127 (3%)	4 (100%)	0	100	100
1	IM	4/127 (3%)	4 (100%)	0	100	100
1	IN	4/127 (3%)	4 (100%)	0	100	100
1	IO	4/127 (3%)	4 (100%)	0	100	100
1	JA	4/127 (3%)	4 (100%)	0	100	100
1	JB	4/127 (3%)	4 (100%)	0	100	100
1	JC	4/127 (3%)	4 (100%)	0	100	100
1	JD	4/127 (3%)	4 (100%)	0	100	100
1	JE	4/127 (3%)	4 (100%)	0	100	100
1	JF	4/127 (3%)	4 (100%)	0	100	100
1	JG	4/127 (3%)	4 (100%)	0	100	100
1	JH	4/127 (3%)	4 (100%)	0	100	100
1	JI	4/127 (3%)	4 (100%)	0	100	100
1	JJ	4/127 (3%)	4 (100%)	0	100	100
1	JK	4/127 (3%)	4 (100%)	0	100	100
1	JL	4/127 (3%)	4 (100%)	0	100	100
1	JM	4/127 (3%)	4 (100%)	0	100	100
1	JN	4/127 (3%)	4 (100%)	0	100	100
1	JO	4/127 (3%)	4 (100%)	0	100	100
1	KA	4/127 (3%)	4 (100%)	0	100	100
1	KB	4/127 (3%)	4 (100%)	0	100	100
1	KC	4/127 (3%)	4 (100%)	0	100	100
1	KD	4/127 (3%)	4 (100%)	0	100	100
1	KE	4/127 (3%)	4 (100%)	0	100	100
1	KF	4/127 (3%)	4 (100%)	0	100	100
1	KG	4/127 (3%)	4 (100%)	0	100	100
1	KH	4/127 (3%)	4 (100%)	0	100	100
1	KI	4/127 (3%)	4 (100%)	0	100	100
1	KJ	4/127 (3%)	4 (100%)	0	100	100
1	KK	4/127 (3%)	4 (100%)	0	100	100
1	KL	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KM	4/127 (3%)	4 (100%)	0	100	100
1	KN	4/127 (3%)	4 (100%)	0	100	100
1	KO	4/127 (3%)	4 (100%)	0	100	100
1	LA	4/127 (3%)	4 (100%)	0	100	100
1	LB	4/127 (3%)	4 (100%)	0	100	100
1	LC	4/127 (3%)	4 (100%)	0	100	100
1	LD	4/127 (3%)	4 (100%)	0	100	100
1	LE	4/127 (3%)	4 (100%)	0	100	100
1	LF	4/127 (3%)	4 (100%)	0	100	100
1	LG	4/127 (3%)	4 (100%)	0	100	100
1	LH	4/127 (3%)	4 (100%)	0	100	100
1	LI	4/127 (3%)	4 (100%)	0	100	100
1	LJ	4/127 (3%)	4 (100%)	0	100	100
1	LK	4/127 (3%)	4 (100%)	0	100	100
1	LL	4/127 (3%)	4 (100%)	0	100	100
1	LM	4/127 (3%)	4 (100%)	0	100	100
1	LN	4/127 (3%)	4 (100%)	0	100	100
1	LO	4/127 (3%)	4 (100%)	0	100	100
All	All	720/22860 (3%)	720 (100%)	0	100	100

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

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

5.3.3 RNA (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)

There are no chain breaks in this entry.

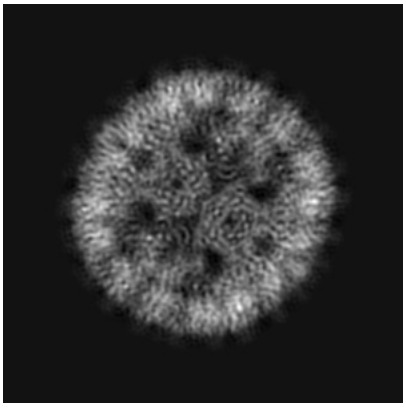
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3543. These allow visual inspection of the internal detail of the map and identification of artifacts.

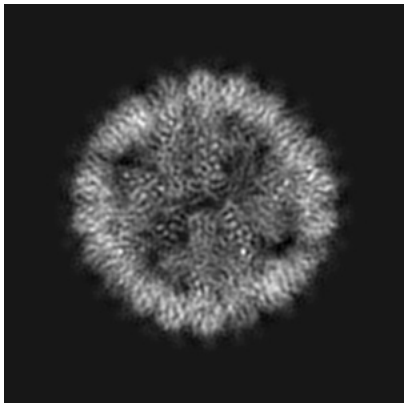
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

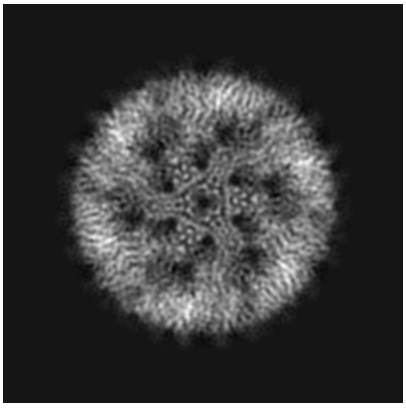
6.1.1 Primary map



X



Y



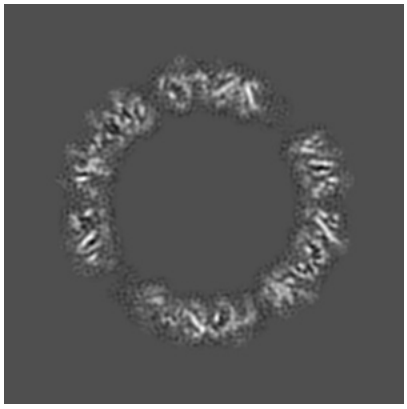
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 150



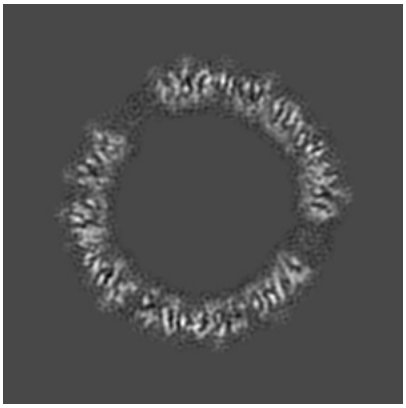
Y Index: 150

Z Index: 150

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 139

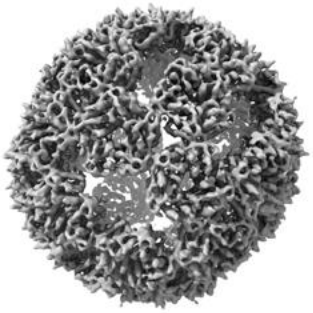
Y Index: 181

Z Index: 151

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

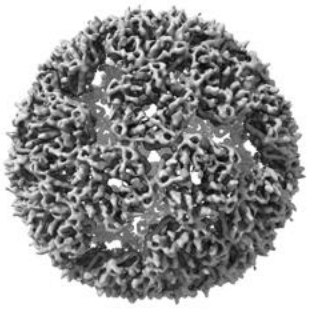
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

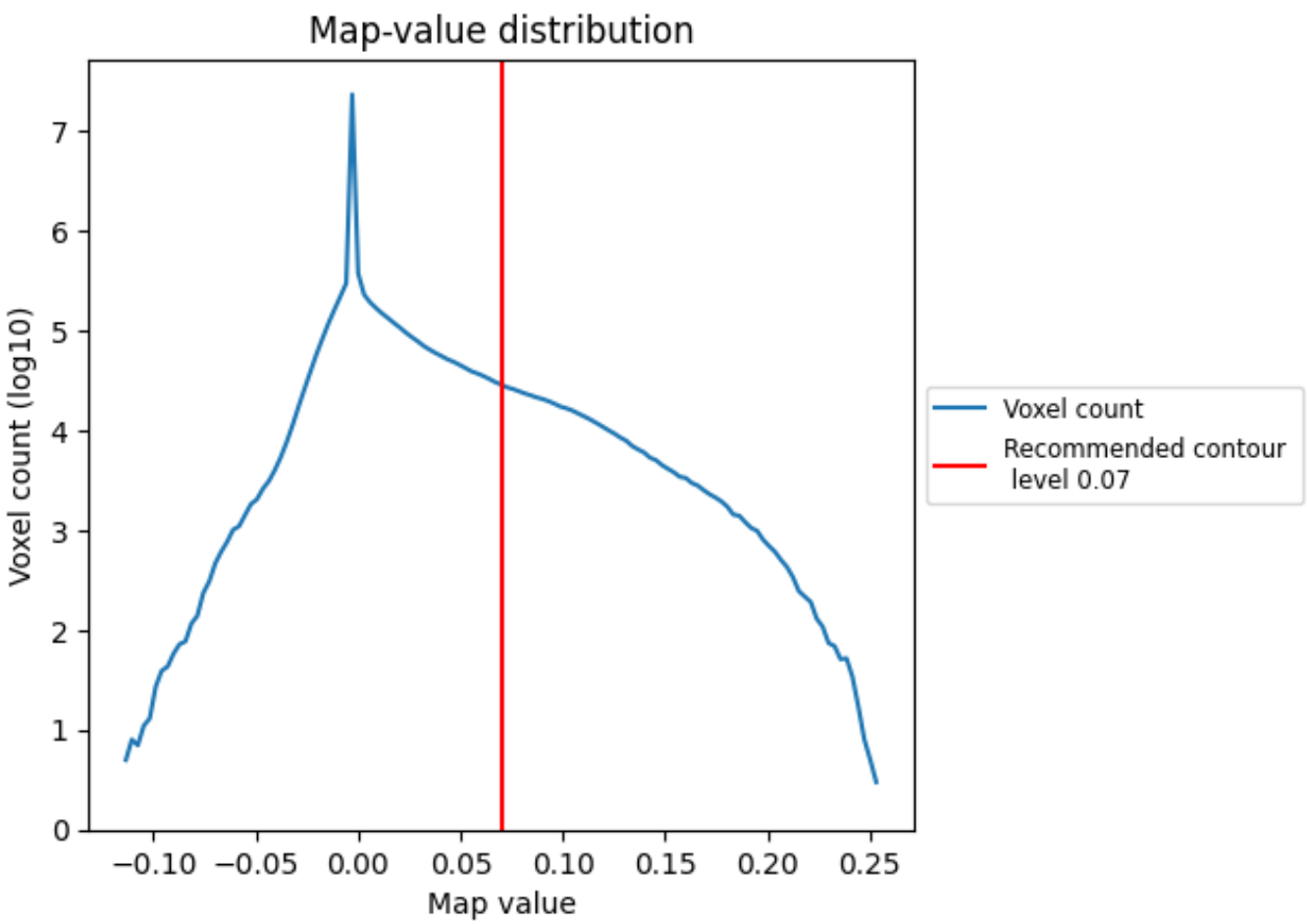
6.5 Mask visualisation (i)

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

7 Map analysis (i)

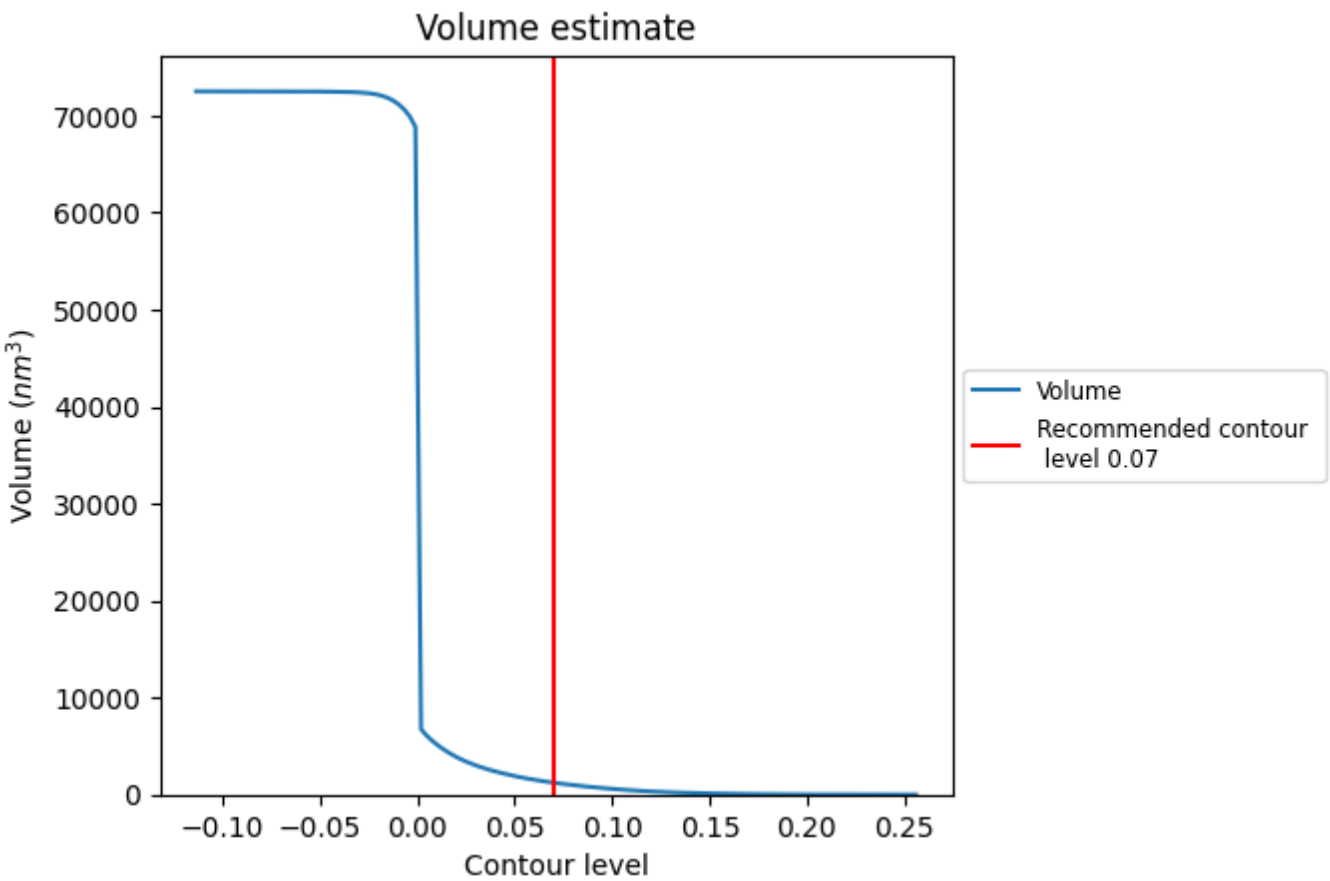
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

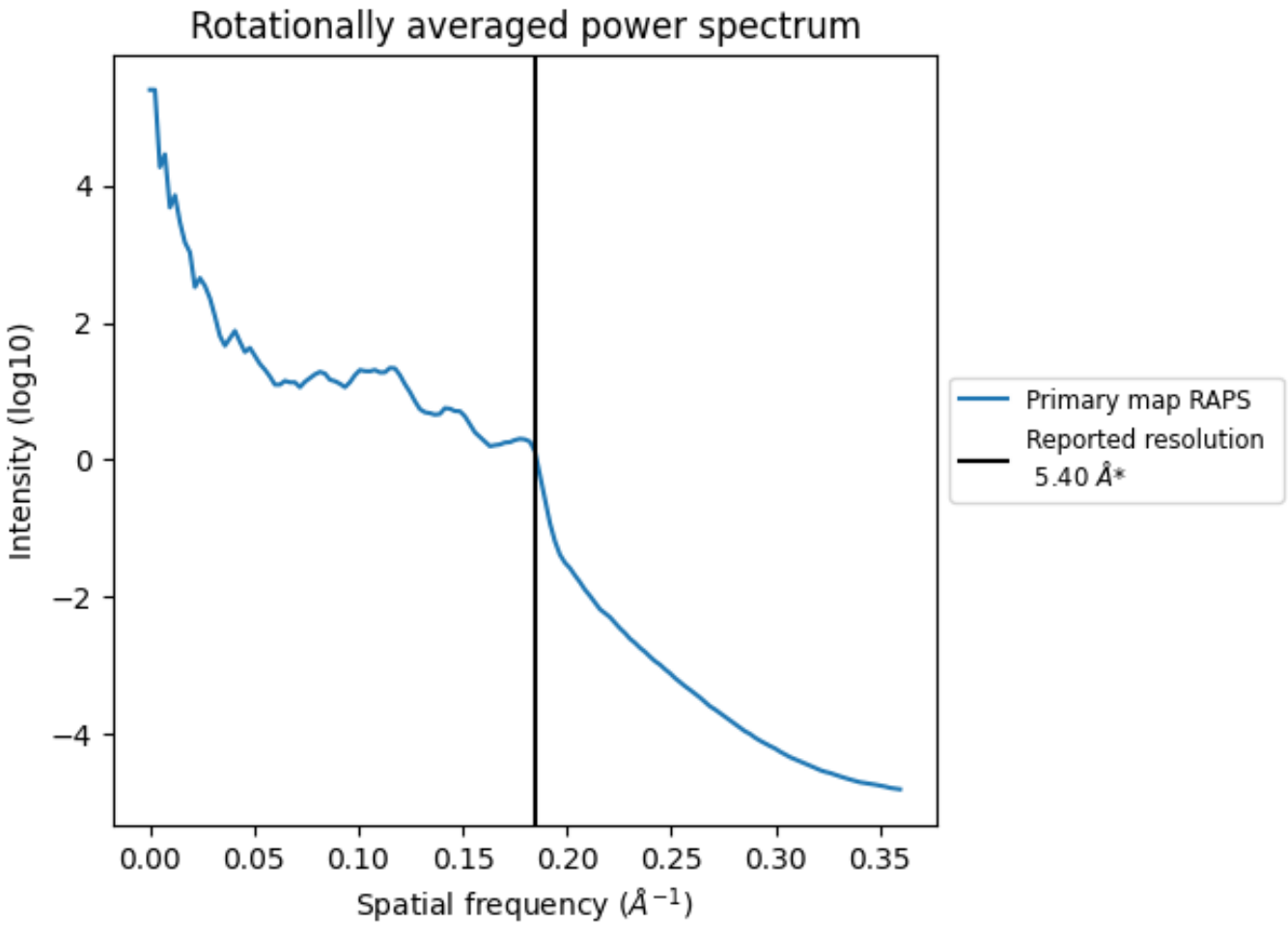
7.2 Volume estimate (i)



The volume at the recommended contour level is 1224 nm^3; this corresponds to an approximate mass of 1106 kDa.

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

7.3 Rotationally averaged power spectrum (i)

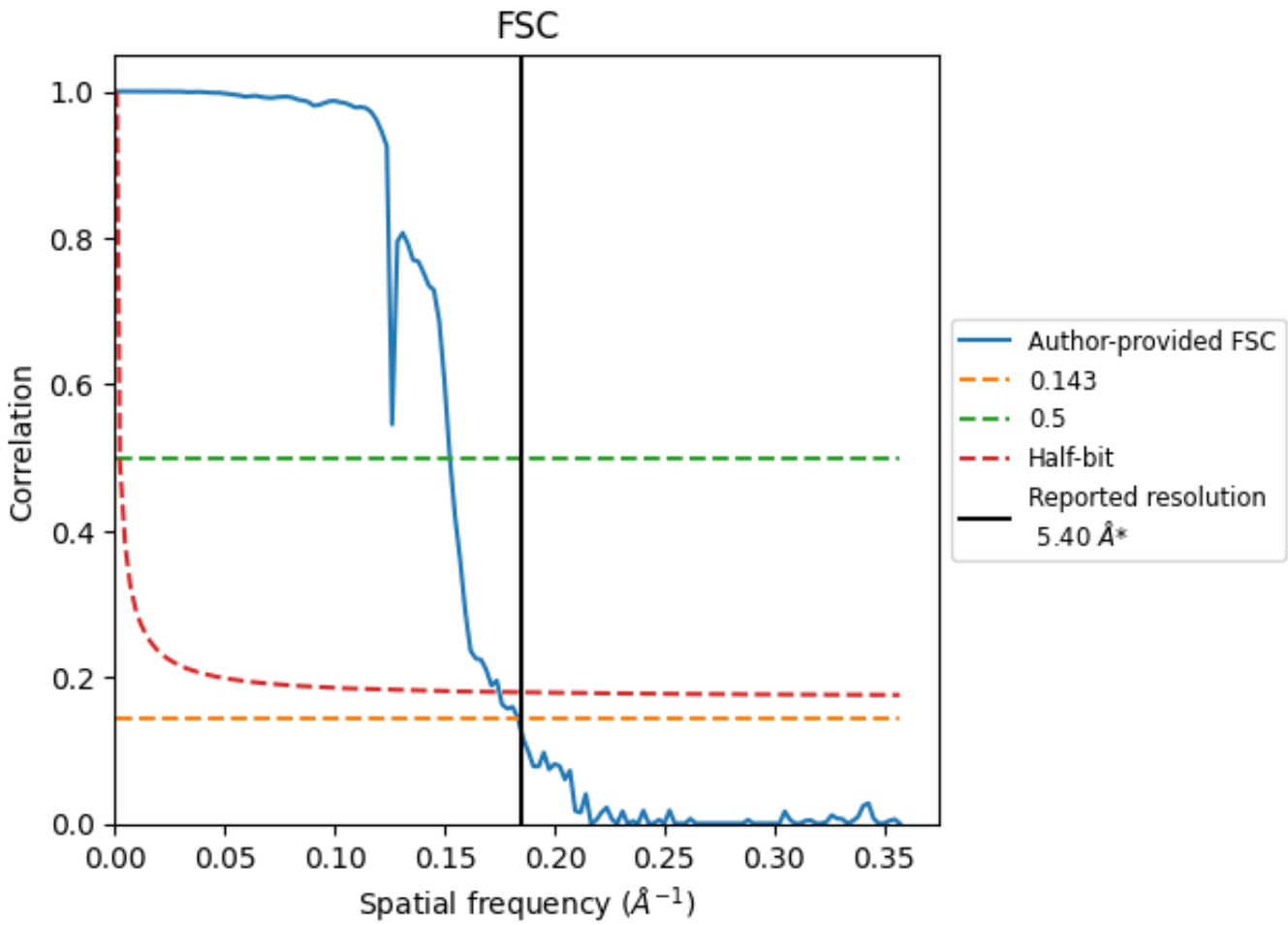


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

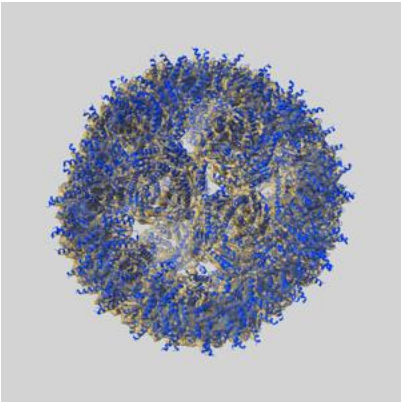
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.45	6.56	5.71
Unmasked-calculated*	-	-	-

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

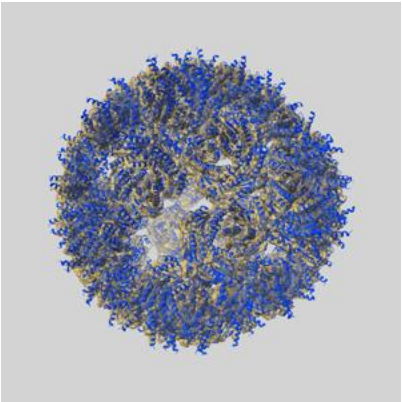
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3543 and PDB model 5MQ3. Per-residue inclusion information can be found in section 3 on page 71.

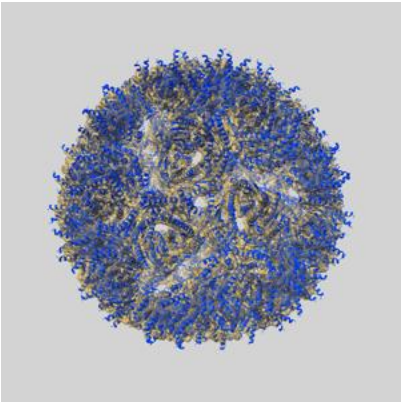
9.1 Map-model overlay (i)



X



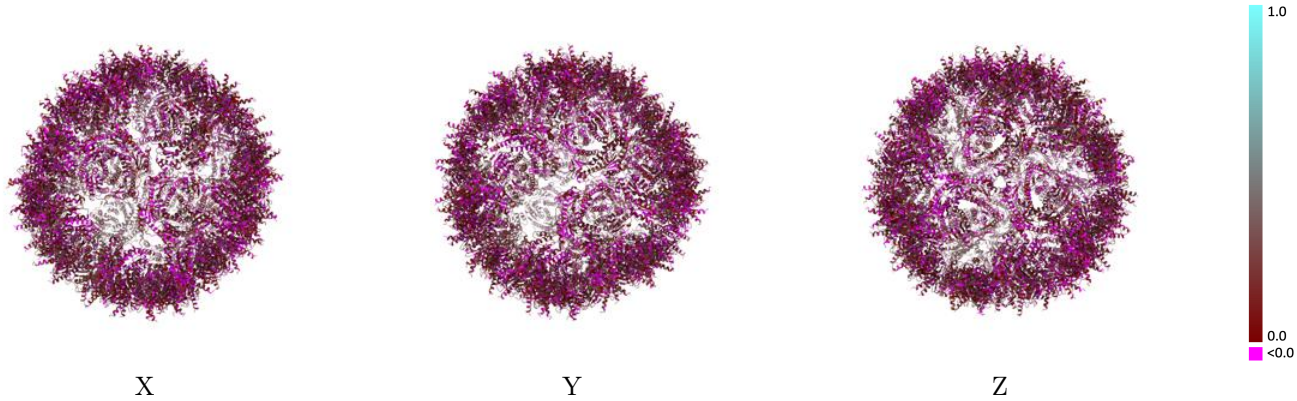
Y



Z

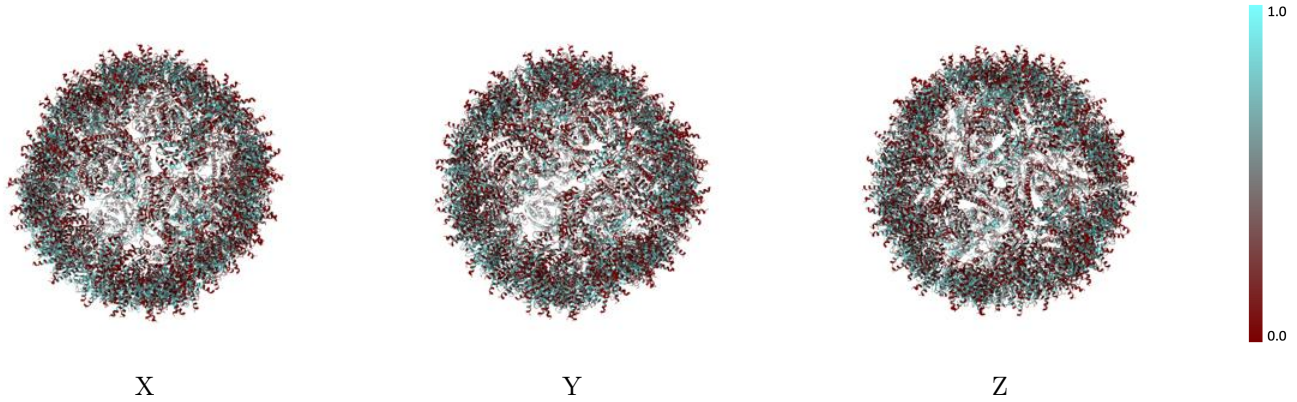
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



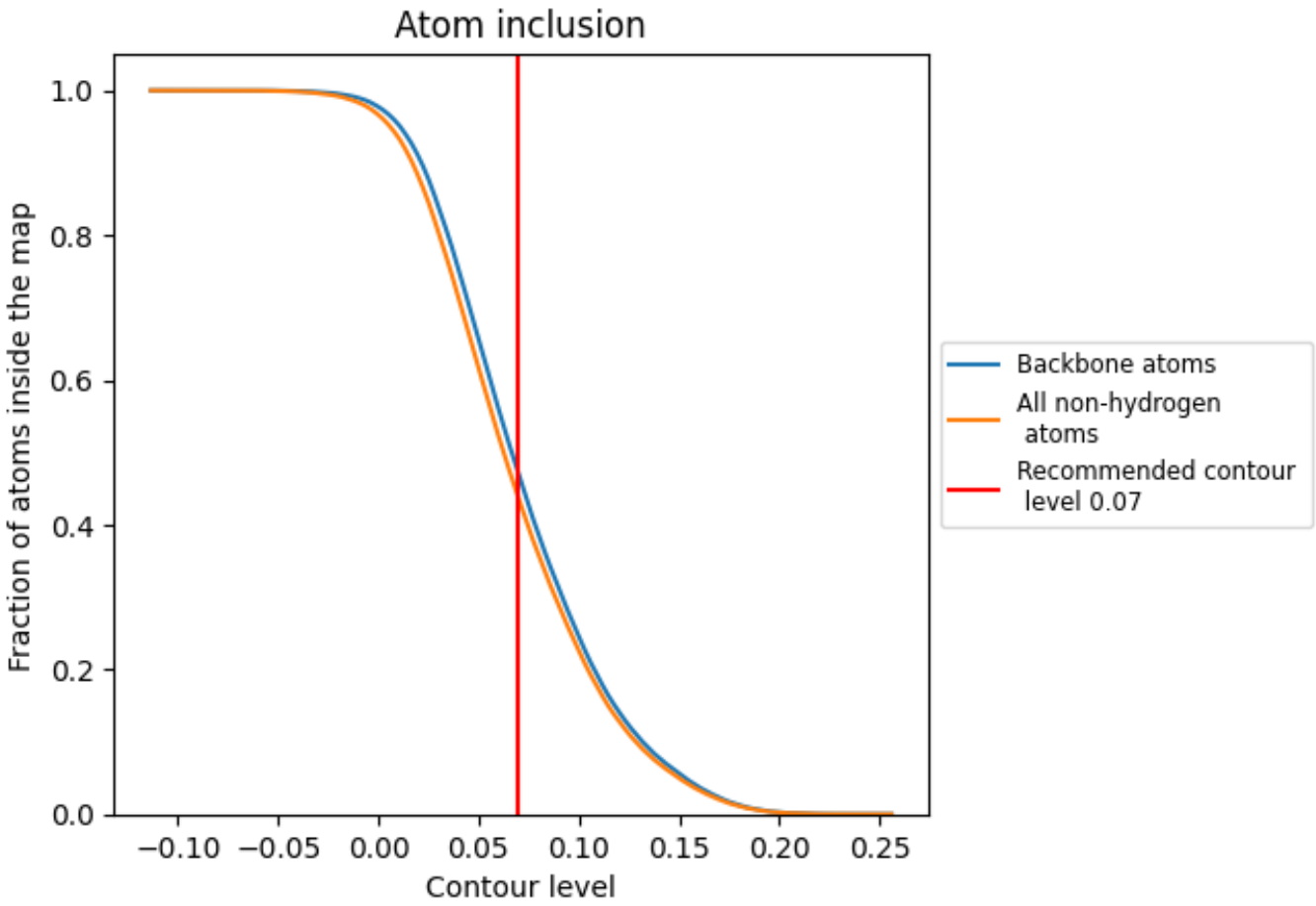
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4361	0.1350
AA	0.4436	0.1520
AB	0.4774	0.1770
AC	0.3922	0.1380
AD	0.3885	0.1120
AE	0.3897	0.1250
AF	0.3584	0.0770
AG	0.3634	0.0860
AH	0.4386	0.1360
AI	0.5150	0.1710
AJ	0.3872	0.1080
AK	0.4085	0.1140
AL	0.3596	0.0920
AM	0.3509	0.0510
AN	0.3910	0.1160
AO	0.4825	0.1800
BA	0.3659	0.0980
BB	0.3622	0.0940
BC	0.4198	0.1330
BD	0.3997	0.1340
BE	0.3546	0.0790
BF	0.3772	0.0820
BG	0.3897	0.1130
BH	0.3860	0.1030
BI	0.4398	0.1300
BJ	0.4599	0.1340
BK	0.4599	0.1440
BL	0.4499	0.1450
BM	0.3496	0.0770
BN	0.3496	0.0720
BO	0.3371	0.0890
CA	0.4449	0.1530
CB	0.4449	0.1450
CC	0.3534	0.0950
CD	0.4073	0.1340

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CE	0.4398	0.1400
CF	0.5802	0.2130
CG	0.5865	0.2150
CH	0.5351	0.2080
CI	0.5025	0.1690
CJ	0.5138	0.1800
CK	0.5075	0.1570
CL	0.4574	0.1550
CM	0.5451	0.2050
CN	0.5576	0.2110
CO	0.5138	0.1910
DA	0.5163	0.1860
DB	0.5827	0.2250
DC	0.5915	0.2270
DD	0.5714	0.2270
DE	0.5188	0.2020
DF	0.4937	0.1730
DG	0.4085	0.1330
DH	0.4323	0.1360
DI	0.5113	0.1690
DJ	0.5338	0.1850
DK	0.5652	0.1920
DL	0.4912	0.1740
DM	0.4524	0.1330
DN	0.4160	0.1440
DO	0.4887	0.1760
EA	0.4085	0.1210
EB	0.3546	0.0940
EC	0.3972	0.1320
ED	0.3885	0.1100
EE	0.4248	0.1300
EF	0.3684	0.0940
EG	0.4298	0.1360
EH	0.4035	0.1250
EI	0.3684	0.0830
EJ	0.3784	0.0680
EK	0.4336	0.1280
EL	0.4273	0.1340
EM	0.4461	0.1390
EN	0.4273	0.1310
EO	0.3885	0.0970
FA	0.3484	0.0640

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FB	0.3521	0.0850
FC	0.3246	0.0760
FD	0.4073	0.1350
FE	0.3897	0.1150
FF	0.5088	0.1540
FG	0.4135	0.1280
FH	0.3571	0.0800
FI	0.3772	0.0550
FJ	0.4085	0.1120
FK	0.3559	0.0590
FL	0.3985	0.1210
FM	0.4912	0.1590
FN	0.4098	0.1320
FO	0.3647	0.0800
GA	0.3421	0.0750
GB	0.3296	0.0530
GC	0.3058	0.0820
GD	0.4499	0.1520
GE	0.4048	0.1310
GF	0.4749	0.1540
GG	0.3897	0.1260
GH	0.3571	0.0700
GI	0.3672	0.0680
GJ	0.4687	0.1370
GK	0.3684	0.0760
GL	0.4198	0.1410
GM	0.4937	0.1650
GN	0.4023	0.1390
GO	0.3571	0.0950
HA	0.4110	0.1210
HB	0.4110	0.1260
HC	0.3997	0.1220
HD	0.3584	0.1140
HE	0.4035	0.1050
HF	0.4073	0.1000
HG	0.4386	0.1470
HH	0.4812	0.1650
HI	0.4912	0.1680
HJ	0.4624	0.1410
HK	0.4436	0.1370
HL	0.4311	0.1250
HM	0.3571	0.0680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HN	0.3759	0.0900
HO	0.3521	0.0870
IA	0.4449	0.1450
IB	0.3584	0.0990
IC	0.3647	0.1140
ID	0.3546	0.0870
IE	0.4023	0.1160
IF	0.3534	0.0790
IG	0.4185	0.1170
IH	0.4298	0.1370
II	0.3672	0.0790
IJ	0.3596	0.0770
IK	0.4098	0.1060
IL	0.4223	0.1310
IM	0.4311	0.1400
IN	0.4261	0.1380
IO	0.3885	0.1090
JA	0.6078	0.2340
JB	0.6140	0.2420
JC	0.5777	0.2220
JD	0.5727	0.2170
JE	0.6153	0.2320
JF	0.5313	0.2000
JG	0.4536	0.1640
JH	0.5326	0.1980
JI	0.6153	0.2210
JJ	0.6040	0.2350
JK	0.5952	0.2110
JL	0.4925	0.1700
JM	0.4499	0.1420
JN	0.4699	0.1730
JO	0.5564	0.2020
KA	0.4361	0.1410
KB	0.4286	0.1380
KC	0.3371	0.0740
KD	0.3885	0.1110
KE	0.3947	0.1090
KF	0.5038	0.1660
KG	0.4812	0.1630
KH	0.4612	0.1580
KI	0.4261	0.1270
KJ	0.4599	0.1370

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
KK	0.4561	0.1290
KL	0.4799	0.1550
KM	0.5489	0.1840
KN	0.5213	0.1890
KO	0.4774	0.1570
LA	0.3960	0.1190
LB	0.4273	0.1600
LC	0.4336	0.1630
LD	0.4474	0.1520
LE	0.4185	0.1400
LF	0.3797	0.0950
LG	0.3659	0.0860
LH	0.4123	0.1080
LI	0.5376	0.1780
LJ	0.4561	0.1350
LK	0.4712	0.1490
LL	0.3734	0.1120
LM	0.3546	0.0670
LN	0.3997	0.1190
LO	0.4925	0.1850